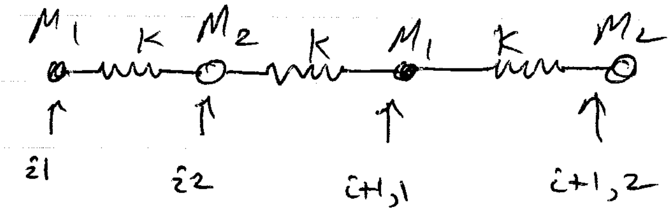
PHY 521 Solutions Problem Set 8

1)



Since atoms are different, we have BL with basis.

BL: $R_n = 2na$ n = integer, a = spacing between ions

basis: $0, a$

RL: $K = \frac{2\pi}{2a} n = \frac{\pi}{a} n$

1st BZ $k \in \left(-\frac{\pi}{2a}, \frac{\pi}{2a}\right)$

label the M_1 atom at site R_i "$i1$". label the M_2 atom at site $R_i + a$ "$i2$".

a) The displacements are u_{i1} and u_{i2}

Equations of motion for atoms $i1$ and $i2$ are

$$M_1 \ddot{u}_{i1} = -K(u_{i1} - u_{i2}) - K(u_{i1} - u_{i-1,2})$$

$$M_2 \ddot{u}_{i2} = -K(u_{i2} - u_{i+1,1}) - K(u_{i2} - u_{i1})$$

Assume solution of the form

$$\begin{pmatrix} u_{i1}(t) \\ u_{i2}(t) \end{pmatrix} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} e^{i(kR_i - \omega t)}$$

Plug in to get

$$\begin{cases} -\omega^2 M_1 \epsilon_1 = -K(\epsilon_1 - \epsilon_2) - K(\epsilon_1 - \epsilon_2 e^{-2ika}) & \text{since } R_{i-1} = R_i - 2a \\ -\omega^2 M_2 \epsilon_2 = -K(\epsilon_2 - \epsilon_1 e^{2ika}) - K(\epsilon_2 - \epsilon_1) & \text{since } R_{i+1} = R_i + 2a \end{cases}$$

Put into matrix form

$$\begin{pmatrix} -\omega^2 M_1 + 2K & -K[1+e^{-2ika}] \\ -K[1+e^{2ika}] & -\omega^2 M_2 + 2K \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = 0$$

there exists a non trivial solution only when the determinant of the matrix vanishes. This gives the dispersion relations $\omega_\pm(k)$.

$$(-\omega^2 M_1 + 2K)(-\omega^2 M_2 + 2K) - K^2(1+e^{-2ika})(1+e^{2ika}) = 0$$

$$\Rightarrow \omega^4 M_1 M_2 - 2K(M_1+M_2)\omega^2 + 4K^2 - K^2(2+2\cos 2ka) = 0$$

$$\Rightarrow \omega^4 - \frac{2K(M_1+M_2)}{M_1 M_2} + \frac{2K^2}{M_1 M_2}(1-\cos 2ka) = 0$$

$$\Rightarrow \omega_\pm^2 = \frac{K(M_1+M_2)}{M_1 M_2} \pm \sqrt{\left[\frac{K(M_1+M_2)}{M_1 M_2}\right]^2 - \frac{2K^2}{M_1 M_2}(1-\cos 2ka)}$$

$$= \frac{K}{M_1 M_2}\left\{M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 - 2M_1 M_2(1-\cos 2ka)}\right\}$$

$$\boxed{\omega_\pm^2 = \frac{K}{M_1 M_2}\left\{M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos 2ka}\right\}}$$

b) For $ka \ll 1$ approx $\cos(2ka) \simeq 1 - \frac{1}{2}(2ka)^2 = 1 - 2k^2a^2$

$$\omega_\pm^2 = \frac{K}{M_1M_2}\left\{M_1+M_2 \pm \sqrt{M_1^2+M_2^2+2M_1M_2-4M_1M_2k^2a^2}\right\}$$

$$= \frac{K}{M_1M_2}\left\{M_1+M_2 \pm \sqrt{(M_1+M_2)^2-4M_1M_2k^2a^2}\right\}$$

$$= \frac{K}{M_1M_2}\left\{M_1+M_2 \pm (M_1+M_2)\sqrt{1-\frac{4M_1M_2}{(M_1+M_2)^2}k^2a^2}\right\}$$

$$\simeq \frac{K}{M_1M_2}\left\{M_1+M_2 \pm (M_1+M_2)\left(1-\frac{2M_1M_2}{(M_1+M_2)^2}k^2a^2\right)\right\}$$

look at + root

$$\omega_+^2 = \frac{K}{M_1M_2}\left\{2(M_1+M_2)\left(1-\frac{M_1M_2}{(M_1+M_2)^2}k^2a^2\right)\right\}$$

$$\omega_+ \simeq \sqrt{\frac{K}{M_1M_2}2(M_1+M_2)}\left(1-\frac{M_1M_2}{2(M_1+M_2)^2}k^2a^2\right)$$

$$\boxed{\omega_+ \simeq \sqrt{\frac{2K(M_1+M_2)}{M_1M_2}}\left(1-\frac{M_1M_2}{2(M_1+M_2)^2}k^2a^2\right) \qquad ka \ll 1}$$

as $k\to 0$ same ω as if block of reduced mass $\frac{1}{\mu}=\frac{1}{M_1}+\frac{1}{M_2}$, spring $2K$

look at − root

$$\omega_-^2 = \frac{K}{M_1M_2}\frac{2M_1M_2}{(M_1+M_2)}k^2a^2$$

$$\boxed{\omega_- \simeq \sqrt{\frac{2K}{(M_1+M_2)}}\,ka \qquad ka \ll 1}$$

Same ω as if monatomic chain with average mass $(M_1+M_2)/2$

so we see that ω_- is an acoustic mode with $\omega_-(k) \sim ck$ at small k

$c = \sqrt{\frac{2K}{(M_1+M_2)}}\,a$ is speed of sound.

ω_+ is an optical mode with $\omega_+(k) \to \omega_0$ constant as $k \to 0$.

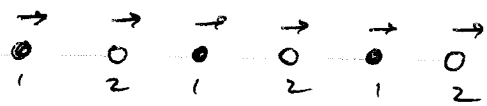
We can get the eigenvectors from the matrix equation

$$\epsilon_2 = \frac{(2K - \omega_\pm^2 M_1)\,\epsilon_1}{K(1+e^{-2ika})} \simeq \frac{2K - \omega_\pm^2 M_1}{2K} \quad \text{as } k \to 0$$

for the acoustic mode ω_- as $k \to 0$

$$\epsilon_2 = \frac{\left(2K - \frac{2K}{(M_1+M_2)} k^2 a^2\right)}{2K}\,\epsilon_1 = \epsilon_1 \quad \text{as } k \to 0$$

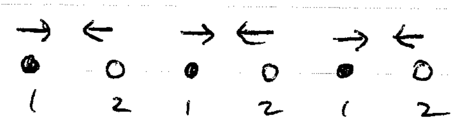
So M_1 and M_2 oscillate in phase $\boxed{\epsilon_2 = \epsilon_1}$



for the optical mode ω_+ as $k \to 0$

$$\epsilon_2 = \frac{\left(2K - \frac{2K(M_1+M_2)M_1}{M_1 M_2}\right)}{2K}\,\epsilon_1 = -\frac{M_1}{M_2}\,\epsilon_1$$

So M_1 and M_2 oscillate π out of phase $\boxed{\epsilon_2 = -\frac{M_1}{M_2}\epsilon_1}$



for $k = \frac{\pi}{2a} + \delta k$

$$\cos(2ka) \simeq \cos(\pi + 2\delta ka) = -\cos(2\delta ka)$$
$$\simeq -\left(1 - \tfrac{1}{2}(2\delta ka)^2\right) = -1 + 2(\delta ka)^2$$

$$\omega_\pm^2 = \frac{K}{M_1M_2}\left\{M_1+M_2 \pm \sqrt{M_1^2+M_2^2 - 2M_1M_2 + 4M_1M_2(\delta ka)^2}\right\}$$

$$= \frac{K}{M_1M_2}\left\{M_1+M_2 \pm \sqrt{(M_1-M_2)^2 + 4M_1M_2(\delta ka)^2}\right\}$$

$$= \frac{K}{M_1M_2}\left\{M_1+M_2 \pm |M_1-M_2|\sqrt{1 + \frac{4M_1M_2}{(M_1-M_2)^2}(\delta ka)^2}\right\}$$

$$\simeq \frac{K}{M_1M_2}\left\{M_1+M_2 \pm |M_1-M_2|\left(1 + \frac{2M_1M_2}{(M_1-M_2)^2}(\delta ka)^2\right)\right\}$$

let us take M_1 to be the larger mass, $M_1 > M_2$

+ root:

$$\omega_+^2 = \frac{K}{M_1M_2}\left\{M_1+M_2 + M_1 - M_2 + \frac{2M_1M_2}{M_1-M_2}(\delta ka)^2\right\}$$

$$= \frac{K}{M_1M_2}\, 2M_1\left(1 + \frac{M_2}{M_1-M_2}(\delta ka)^2\right)$$

$$\boxed{\omega_+ = \sqrt{\frac{2K}{M_2}}\left(1 + \frac{M_2\,(\delta ka)^2}{2(M_1-M_2)}\right)}$$

− root:

$$\omega_-^2 = \frac{K}{M_1M_2}\left\{M_1+M_2 - M_1 + M_2 - \frac{2M_1M_2}{M_1-M_2}(\delta ka)^2\right\}$$

$$= \frac{K}{M_1M_2}\, 2M_2\left(1 - \frac{M_1}{M_1-M_2}(\delta ka)^2\right)$$

Note both ω_+ and ω_- $\sim$ const $+ (\delta ka)^2$

$\Rightarrow$ dispersion curves hit BZ edge with zero slope!

$$\boxed{\omega_- = \sqrt{\frac{2K}{M_1}}\left(1 - \frac{M_1}{2(M_1-M_2)}(\delta ka)^2\right)}$$

<u>eigenvectors</u>

$$\epsilon_2 = \frac{(2K - \omega_\pm^2 M_1)\,\epsilon_1}{K(1+e^{-2ika})}$$

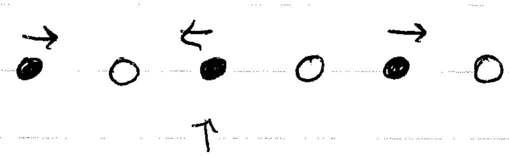
$$e^{-2ika} = e^{-i\pi}e^{-2i\delta ka} = -e^{-2i\delta ka}$$

<u>acoustic mode</u> ω_- as $k \to \frac{\pi}{2a}$

$$\epsilon_2 = \frac{2K - (2K)\left(1 - \frac{M_1}{2(M_1-M_2)}(\delta ka)^2\right)}{K\left(1-(1-2i\delta ka)\right)}$$

$$= \frac{\frac{2M_1}{2(M_1-M_2)}(\delta ka)^2}{2i\delta ka} = \frac{-iM_1\,\delta ka}{(M_1-M_2)\,2} \to 0 \quad \text{as } \delta k \to 0$$

so $\boxed{\epsilon_2 = 0}$



plane wave factor gives relative phase e^{ik2a} between adjacent M_1 atoms $= e^{i\pi} = -1$ for $k = \frac{\pi}{2a}$

optical mode ω_+ as $k \to \frac{\pi}{2a}$

$$\epsilon_2 = \frac{\left(2K - 2K\frac{M_1}{M_2}\right)}{K(2i\delta ka)}\epsilon_1$$ blows up as $\delta k \to 0$

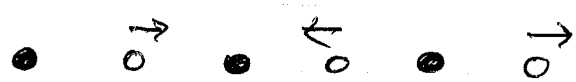
instead we use (also from matrix equation)

$$\epsilon_1 = \frac{(-\omega_+^2 M_2 + 2K)\,\epsilon_2}{K[1+e^{2ika}]}$$ $e^{2ika} = -e^{2i\delta ka} = -(1+2i\delta ka)$

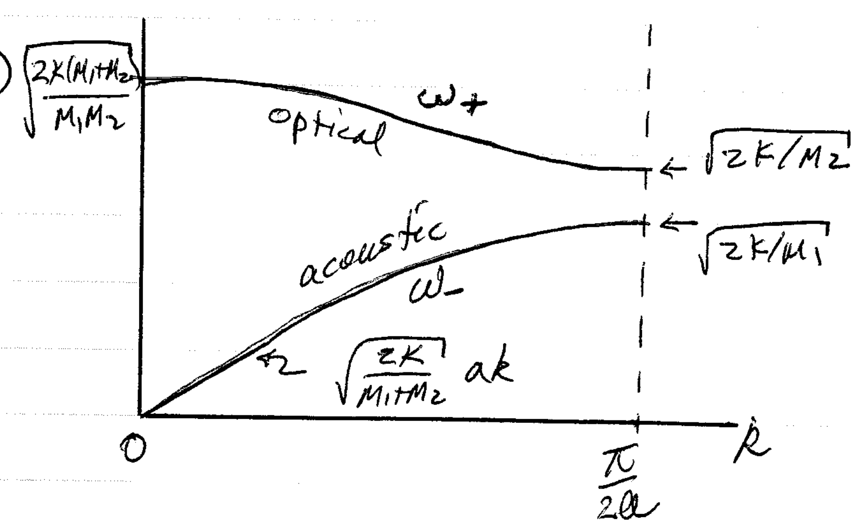
$$= \frac{2K - 2K\left(1 + \frac{M_2(\delta ka)^2}{2(M_1-M_2)}\right)}{-K\,2i\delta ka}\,\epsilon_2$$

$$= \frac{M_2(\delta ka)^2}{2(M_1-M_2)\,i\delta ka}\,\epsilon_2 = \frac{-iM_2\delta ka}{2(M_1-M_2)} \to 0 \text{ as } \delta k \to 0$$

$$\boxed{\epsilon_1 = 0}$$



c)



d) $M_1 \gg M_2$

$$\omega_\pm^2 = \frac{K}{M_1 M_2}\left\{ M_1 + M_2 \pm M_1\sqrt{1 + \frac{2M_2}{M_1}\cos 2ka + \frac{M_2^2}{M_1^2}} \right\}$$

to $O(M_2/M_1)$

$$\omega_\pm^2 = \frac{K}{M_1 M_2}\left\{ M_1 + M_2 \pm M_1\left(1 + \frac{M_2}{M_1}\cos 2ka\right)\right\}$$

optical mode

$$\omega_+^2 = \frac{K}{M_1 M_2}\left\{ 2M_1 + M_2(1+\cos 2ka)\right\}$$

$$= \frac{2K}{M_2}\left\{ 1 + \frac{M_2}{2M_1}(1+\cos 2ka)\right\}$$

$$\omega_+ = \sqrt{\frac{2K}{M_2}}\left(1 + \frac{M_2}{4M_1}(1+\cos 2ka)\right)$$

$$\frac{1+\cos 2ka}{2} = \cos^2 ka$$

$$\boxed{\omega_+ = \sqrt{\frac{2K}{M_2}}\left(1 + \frac{M_2}{2M_1}\cos^2 ka\right)}$$

acoustic mode

$$\omega_-^2 = \frac{K}{M_1 M_2}\left\{ M_2 - M_2\cos 2ka\right\}$$

$$\frac{1-\cos 2ka}{2} = \sin^2 ka$$

$$= \frac{K}{M_1}\left\{1 - \cos 2ka\right\} = \frac{K}{M_1}2\sin^2 ka$$

$$\boxed{\omega_- = \sqrt{\frac{2K}{M_1}}\sin ka}$$

speed of sound is $C = \sqrt{\frac{2K}{M_1}}\, a$

eigenvectors

optical mode

use

$$\epsilon_1 = \frac{-\omega_+^2 M_2 + 2K}{K(1+e^{2ika})}\,\epsilon_2$$

$$= \frac{2K - 2K\left(1 + \frac{M_2}{2M_1} 2\cos^2 ka\right)}{K(1+e^{2ika})}\,\epsilon_2$$

$$\boxed{\epsilon_1 = -\frac{2M_2\cos^2 ka}{M_1\,(1+e^{2ika})}\,\epsilon_2}$$

$\epsilon_1 = -\frac{2M_2}{M_1}\epsilon_2 \ll \epsilon_2$ for $k=0$

optical mode M_1 moves only a little compared to M_2

M_1 π out of phase with M_2

$\epsilon_1 \simeq 0$ when $k = \frac{\pi}{2a}$

acoustic mode

use $\epsilon_2 = \frac{-\omega_-^2 M_1 + 2K}{K(1+e^{-2ika})}\,\epsilon_1$

$$= \frac{2K - 2K\sin^2 ka}{K(1+e^{-2ika})}\,\epsilon_1$$

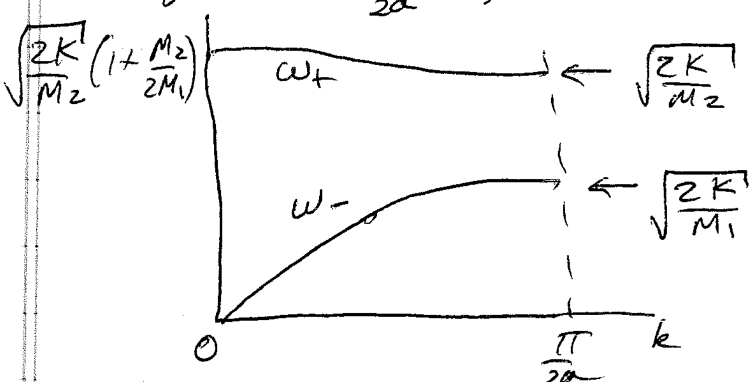
$$\boxed{\epsilon_2 = \frac{2\cos^2 ka}{1+e^{-2ika}}\,\epsilon_1}$$

use $2\cos^2 ka = 1+\cos 2ka = \frac{1}{2}(1+e^{2ika})(1+e^{-2ika})$

$$\boxed{\epsilon_2 = \frac{1}{2}(1+e^{2ika})\,\epsilon_1}$$

for small ka, $\epsilon_2 \simeq \epsilon_1$ — M_1 and M_2 are in phase

for $k = \frac{\pi}{2a}$, $\epsilon_2 = 0$



optical mode has <u>very flat</u> dispersion

e) $M_1 = M_2 + \delta M$, $\delta M \to 0$

$$\omega_\pm^2 = \frac{K}{(M_2+\delta M)M_2}\left\{M_2+\delta M+M_2 \pm \sqrt{(M_2+\delta M)^2+M_2^2+2(M_2+\delta M)M_2 \times \cos 2ka}\right\}$$

to $O\left(\frac{\delta M}{M_2}\right)$

$$\omega_\pm^2 = \frac{K}{M_2^2\left(1+\frac{\delta M}{M_2}\right)}\left\{M_2+\delta M+M_2 \pm M_2\sqrt{1+\frac{2\delta M}{M_2}+\underbrace{\frac{\delta M^2}{M_2^2}}_{\text{ignore}}+1+2\left(1+\frac{\delta M}{M_2}\right)\cos 2ka}\right\}$$

$$= \frac{K}{M_2^2\left(1+\frac{\delta M}{M_2}\right)}\left\{2M_2+\delta M \pm M_2\left[2\left(1+\frac{\delta M}{M_2}\right)(1+\cos 2ka)\right]^{1/2}\right\}$$

$$= \frac{K}{M_2^2\left(1+\frac{\delta M}{M_2}\right)}\left\{2M_2+\delta M \pm M_2\left[4\left(1+\frac{\delta M}{M_2}\right)\cos^2 ka\right]^{1/2}\right\}$$

$$\omega_\pm^2 = \frac{K}{M_2^2\left(1+\frac{\delta M}{M_2}\right)}\left\{2M_2+\delta M \pm 2M_2\cos ka\left(1+\frac{\delta M}{2M_2}\right)\right\}$$

$$\omega_\pm^2 = \frac{2K\left(1+\frac{\delta M}{2M_2}\right)(1 \pm \cos ka)}{M_2\left(1+\frac{\delta M}{M_2}\right)}$$

expand denominator

$$\omega_\pm^2 \simeq \frac{2K}{M_2}(1 \pm \cos ka)\left(1 - \frac{\delta M}{2M_2}\right)$$

In limit $\delta M \to 0$

$$\boxed{\omega_\pm^2 = \frac{2K}{M_2}(1 \pm \cos ka)}$$

acoustic mode

$$\omega_-^2 = \frac{2K}{M_2}(1 - \cos ka) = \frac{4K}{M_2}\sin^2\frac{ka}{2}$$

$$\boxed{\omega_- = 2\sqrt{\frac{K}{M_2}}\sin\frac{ka}{2}}$$

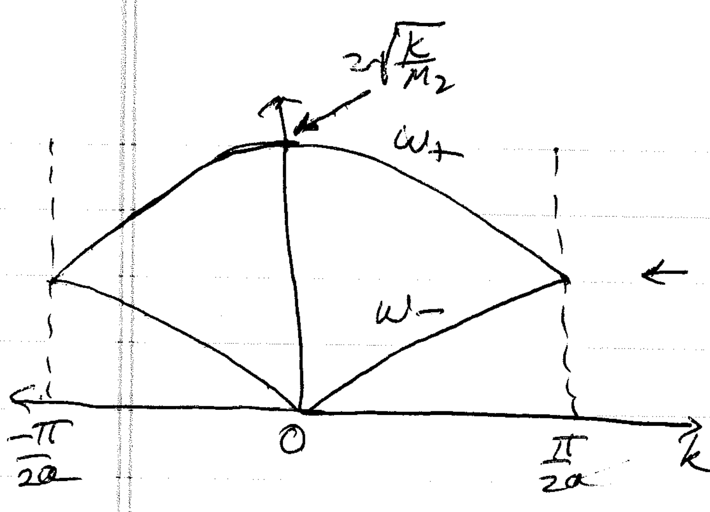
identical to a monatomic chain of atoms of mass M_2

optical mode

$$\omega_+^2 = \frac{2K}{M_2}(1 + \cos ka) = \frac{4K}{M_2}\cos^2\frac{ka}{2}$$

$$\boxed{\omega_+ = 2\sqrt{\frac{K}{M_2}}\cos\left(\frac{ka}{2}\right)}$$

At $k = \frac{\pi}{2a}$, note $\omega_+\left(\frac{\pi}{2a}\right) = \omega_-\left(\frac{\pi}{2a}\right) = \sqrt{\frac{2K}{M_2}}$



$$\omega_+\left(\frac{\pi}{2a}\right) = \omega_-\left(\frac{\pi}{2a}\right) = \sqrt{\frac{2K}{M_2}}$$

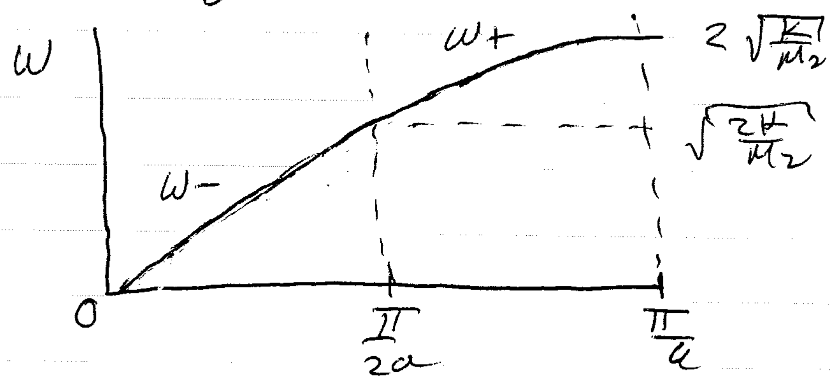
← note, slopes of $\omega_\pm(k)$ do not vanish at $k = \frac{\pi}{2a}$ as they did when δM was finite (see part b)

Note: we can write $\cos\left(\frac{ka}{2}\right) = \sin\left(\frac{\pi}{2} - \frac{ka}{2}\right)$

If $K \equiv \frac{\pi}{a}$ is the smallest non zero RL vector

then $\cos\left(\frac{ka}{2}\right) = \sin\left(\frac{Ka}{2} - \frac{ka}{2}\right) = \sin\left(\frac{(K-k)a}{2}\right)$

In this way we see that the optical branch can be translated from $\left(-\frac{\pi}{2a}, 0\right)$ to $\left(\frac{\pi}{2a}, \frac{\pi}{a}\right)$ to smoothly continue the acoustic branch



This is just the dispersion relation for a monatomic chain of atoms of mass M_2 and separation a, with a 1^{st} BZ that goes from $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$. But that is just how it should be when $\delta M \to 0$!

2) From lecture we know that the frequencies are given by

$$\omega_s(\vec{k}) = \sqrt{\frac{\lambda_s(\vec{k})}{M}}$$

where $\lambda_s(\vec{k})$ is an eigenvalue of the Dynamical matrix $\mathbb{D}(\vec{k})$. $\mathbb{D}(\vec{k})$ is the Fourier trans of $\mathbb{D}(\vec{R})$

$$\mathbb{D}(\vec{k}) = \sum_i e^{-i\vec{k}\cdot\vec{R}_i}\, \mathbb{D}(\vec{R}_i) \qquad \text{BL vectors } \{\vec{R}_i\}$$

From lecture we had $\sum_i \mathbb{D}(R_i) = 0$ and if crystal has inversion symmetry (monatomic BL does) then $\mathbb{D}(\vec{R}) = \mathbb{D}(-\vec{R})$. So we can write

$$\mathbb{D}(\vec{R}=0) = -\sum_{R_i \neq 0} \mathbb{D}(\vec{R}_i)$$

and so

$$\mathbb{D}(\vec{k}) = \mathbb{D}(\vec{R}=0) + \sum_{R_i\neq 0} e^{-i\vec{k}\cdot\vec{R}_i}\, \mathbb{D}(\vec{R}_i)$$

$$= \sum_{R_i \neq 0} \left(e^{-i\vec{k}\cdot\vec{R}_i} - 1\right) \mathbb{D}(\vec{R}_i)$$

$$= \frac{1}{2}\sum_{R_i\neq 0} \Big\{\left[e^{-i\vec{k}\cdot\vec{R}_i} - 1\right]\mathbb{D}(\vec{R}_i) + \left[e^{i\vec{k}\cdot\vec{R}_i} - 1\right]\mathbb{D}(-\vec{R}_i)\Big\}$$

$$= \frac{1}{2}\sum_{R_i\neq 0}\left[e^{i\vec{k}\cdot\vec{R}_i} + e^{-i\vec{k}\cdot\vec{R}_i} - 2\right]\mathbb{D}(\vec{R}_i)$$

$$\mathbb{D}(\vec{k}) = \frac{1}{2}\sum_{\vec{R}_i \neq 0} 2(\cos \vec{k}\cdot\vec{R}_i - 1)\, \mathbb{D}(\vec{R}_i)$$

$$= -2\sum_{\vec{R}_i \neq 0} \sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right) \mathbb{D}(\vec{R}_i)$$

Now take a model with pairwise nearest neighbor interactions only, given by a general interaction potential $\phi(|\vec{r}|)$ that depends only on the separation between the ions $|\vec{r}|$. If $\vec{R}_i$ are the BL sites, then ions are at positions $\vec{R}_i + \vec{u}(R_i)$ where $\vec{u}$ is the displacement with respect to $\vec{R}_i$.

The ion interaction potential is then

$$U^{ion} = \sum_{\langle ij \rangle} \phi(|\vec{R}_i + \vec{u}(\vec{R}_i) - R_j - \vec{u}(\vec{R}_j)|)$$

sum over nearest neighbor bonds

By translational invariance, the real space dynamical matrix is given by

$$\mathbb{D}_{\alpha\beta}(\vec{R}_i) = \left.\frac{\partial^2 U^{ion}}{\partial u_\alpha(0)\, \partial u_\beta(\vec{R}_i)}\right|_{\{\vec{u}(R_i)=0\}}$$

evaluated at zero displacements

For pairwise nearest neighbor interactions, above $\mathbb{D}(\vec{R}_i) = 0$ unless $\vec{R}_i$ is one of the smallest non zero BL vectors, ie the nearest neighbors of the origin. Let $d \equiv |\vec{R}_i|$ be length of these nearest neighbor $\vec{R}_i$, ie d is distance between nearest neighbor ions.

$$\frac{\partial U^{ion}}{\partial u_\alpha(0)} = \sum_{nn} \phi'(|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|)\ \frac{\partial|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|}{\partial u_\alpha(0)}$$

only sum over nearest neighbors $\vec{R}_i$ of origin

in above $\phi'(|\vec{r}|) \equiv \frac{d\phi}{dr}$

now use $\frac{\partial|\vec{r}|}{\partial r_\alpha} = \frac{\partial}{\partial r_\alpha}\sqrt{r_x^2+r_y^2+r_z^2} = \frac{1}{2}\frac{1}{|\vec{r}|}2r_\alpha = \frac{r_\alpha}{|\vec{r}|}$

$$\frac{\partial U^{ion}}{\partial u_\alpha(0)} = \sum_{nn} \phi'(|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|)\ \frac{u_\alpha(0)-R_{i\alpha}-u_\alpha(\vec{R}_i)}{|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|}$$

For $\vec{R}_i$ a nn of origin

$$\frac{\partial^2 U^{ion}}{\partial u_\alpha(0)\partial u_\beta(\vec{R}_i)} = -\phi''(|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|)\ \frac{[u_\alpha(0)-R_{i\alpha}-u_\alpha(\vec{R}_i)]}{|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|}\ \frac{[u_\beta(0)-R_{i\beta}-u_\beta(\vec{R}_i)]}{|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|}$$

$$+\ \phi'(|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|)\left\{\frac{-\delta_{\alpha\beta}}{|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|} + \frac{[u_\alpha(0)-R_{i\alpha}-u_\alpha(\vec{R}_i)][u_\beta(0)-R_{i\beta}-u_\beta(\vec{R}_i)]}{|\vec{u}(0)-\vec{R}_i-\vec{u}(\vec{R}_i)|^3}\right\}$$

now evaluate above at $\vec{u}(0)=\vec{u}(\vec{R}_i)=0$, use $|\vec{R}_i|=d$

$$D_{\alpha\beta}(\vec{R}_i) = -\phi''(d)\ \frac{R_{i\alpha}R_{i\beta}}{|\vec{R}_i|^2} - \frac{\phi'(d)}{d}\delta_{\alpha\beta} + \frac{\phi'(d)}{d}\frac{R_{i\alpha}R_{i\beta}}{|\vec{R}_i|^2}$$

$$= -\frac{\phi'(d)}{d}\delta_{\alpha\beta} - \left[\phi''(d) - \frac{\phi'(d)}{d}\right]\hat{R}_{i\alpha}\hat{R}_{i\beta}$$

Now for $\phi(|\vec{r}|) = \frac{1}{2}K(|\vec{r}|-d)^2$

$$\phi'(d) = K(d-d) = 0$$
$$\phi''(d) = K$$

$$\Rightarrow \; D_{\alpha\beta}(\vec{R}_i) = -K \, \hat{R}_{i\alpha} \hat{R}_{i\beta}$$

So $$\boxed{\mathbb{D}(\vec{k}) = 2K \sum_{nn} \sin^2\left(\frac{\vec{k}\cdot\vec{R}_i}{2}\right) \hat{R}_{i\alpha} \hat{R}_{i\beta}}$$

sum is over only nearest neighbor $\vec{R}_i$ to origin
ie the smallest non-zero BL vectors.

If $\lambda_s(\vec{k})$, $s=1,2,3$ are the three eigenvalues of $\mathbb{D}(\vec{k})$, then normal mode frequencies are

$$\omega_s(\vec{k}) = \sqrt{\frac{\lambda_s(\vec{k})}{M}}$$

3) <u>fcc lattice</u>

12 nearest neighbor $\{\vec{R}_i\} = \frac{a}{2}(\pm\hat{x} \pm \hat{y})$

$$\frac{a}{2}(\pm\hat{y} \pm \hat{z})$$
$$\frac{a}{2}(\pm\hat{z} \pm \hat{x})$$

$$D(\vec{k}) = 2K \sum_{nn} \sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right) \hat{R}_\alpha \hat{R}_\beta \qquad d = |\vec{R}_i| = \frac{a}{2}\sqrt{2} = \frac{a}{\sqrt{2}}$$

$$= \frac{4K}{a^2} \sum_{nn} \sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right) \vec{R}_\alpha \vec{R}_\beta$$

since the terms in the sum are symmetric under $\vec{R} \to -\vec{R}$, we can sum over only the 6 vectors

$$\frac{a}{2}(\hat{x} \pm \hat{y}), \quad \frac{a}{2}(\hat{y} \pm \hat{z}), \quad \frac{a}{2}(\hat{z} \pm \hat{x})$$

and multiply the sum by a factor 2

$$D(\vec{k}) = \frac{8K}{a^2} \sum_{\substack{\frac{a}{2}(\hat{x}\pm\hat{y}) \\ \frac{a}{2}(\hat{y}\pm\hat{z}) \\ \frac{a}{2}(\hat{z}\pm\hat{x})}} \sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right) \vec{R}_\alpha \vec{R}_\beta$$

a) For $\vec{k} = (k, 0, 0)$ the only terms for which $\sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right)$ do not vanish are $\vec{R} = \frac{a}{2}(\hat{x} \pm \hat{y})$, $\frac{a}{2}(\hat{z} \pm \hat{x})$

$$D(\vec{k}) = \frac{8K}{a^2} \frac{a^2}{4} \sin^2\left(\frac{ka}{4}\right) \Big\{ (\hat{x}+\hat{y})(\hat{x}+\hat{y}) + (\hat{x}-\hat{y})(\hat{x}-\hat{y}) + (\hat{z}+\hat{x})(\hat{z}+\hat{x}) + (\hat{z}-\hat{x})(\hat{z}-\hat{x}) \Big\}$$

$$= 2K \sin^2\left(\frac{ka}{4}\right) \Big\{ 2\hat{x}\hat{x} + 2\hat{y}\hat{y} + 2\hat{z}\hat{z} + 2\hat{x}\hat{x} \Big\}$$

$$= 4K \sin^2\left(\frac{ka}{4}\right) \Big\{ 2\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z} \Big\}$$

In matrix form,

$$\mathbb{D}(\vec{k}) = 4K \sin^2\left(\frac{ka}{4}\right) \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

eigenvalues are
$$\lambda_1(\vec{k}) = 8K \sin^2\left(\frac{ka}{4}\right)$$
$$\lambda_2(\vec{k}) = 4K \sin^2\left(\frac{ka}{4}\right)$$
$$\lambda_3(\vec{k}) = 4K \sin^2\left(\frac{ka}{4}\right)$$

eigenvectors are

$$\vec{\epsilon}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \parallel \vec{k} \quad \text{so longitudinal}$$

$$\vec{\epsilon}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \perp \vec{k} \quad \text{so transverse}$$

$$\vec{\epsilon}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \perp \vec{k} \quad \text{so transverse}$$

The two transverse modes are <u>degenerate</u>.
So we have

$$\boxed{\begin{aligned} \omega_L(\vec{k}) &= 2\sqrt{\frac{2K}{M}} \sin\left(\frac{ka}{4}\right) \\ \omega_T(\vec{k}) &= 2\sqrt{\frac{K}{M}} \sin\left(\frac{ka}{4}\right) \end{aligned}}$$

b) For $\vec{k} = (\kappa, \kappa, \kappa)$ $\qquad k = \sqrt{3}\,\kappa$

The only terms for which $\sin^2\left(\frac{\vec{k}\cdot\vec{R}}{2}\right)$ do not vanish are $\vec{R} = \frac{a}{2}(\hat{x}+\hat{y}), \frac{a}{2}(\hat{y}+\hat{z}), \frac{a}{2}(\hat{z}+\hat{x})$

$$\mathbb{D}(\vec{k}) = \frac{8K}{a^2}\frac{a^2}{4}\sin^2\left(\frac{2\kappa a}{4}\right)\Big\{(\hat{x}+\hat{y})(\hat{x}+\hat{y}) + (\hat{y}+\hat{z})(\hat{y}+\hat{z}) + (\hat{z}+\hat{x})(\hat{z}+\hat{x})\Big\}$$

$$= 2K\sin^2\left(\frac{\kappa a}{2}\right)\Big\{2\hat{x}\hat{x} + 2\hat{y}\hat{y} + 2\hat{z}\hat{z} + \hat{x}\hat{y} + \hat{y}\hat{x} + \hat{y}\hat{z} + \hat{z}\hat{y} + \hat{z}\hat{x} + \hat{x}\hat{z}\Big\}$$

in matrix form

$$\mathbb{D}(\vec{k}) = 2K \sin^2\left(\frac{\kappa a}{2}\right) \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

eigenvectors ad eigenvalues are

$$\vec{\epsilon}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \lambda_1 = 8K\sin^2\left(\frac{\kappa a}{2}\right) \quad \vec{\epsilon}_1 \parallel \vec{k} \text{ longitudinal}$$

$$\vec{\epsilon}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad \lambda_2 = 2K\sin^2\left(\frac{\kappa a}{2}\right) \quad \vec{\epsilon}_2 \perp \vec{k} \text{ transverse}$$

$$\vec{\epsilon}_3 = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \quad \lambda_3 = 2K\sin^2\left(\frac{\kappa a}{2}\right) \quad \vec{\epsilon}_3 \perp \vec{k} \text{ transverse}$$

so

$$\boxed{\begin{aligned} \omega_L(\vec{k}) &= 2\sqrt{\frac{2K}{M}}\sin\left(\frac{\kappa a}{2}\right) \\ \omega_L(\vec{k}) &= \sqrt{\frac{2K}{M}}\sin\left(\frac{\kappa a}{2}\right) \end{aligned}} \qquad \kappa = \frac{k}{\sqrt{3}}$$

c) $\vec{k} = (\kappa, \kappa, 0) \qquad k = \sqrt{2}\,\kappa$

$$\vec{k}\cdot\vec{R} = \begin{cases} \frac{2\kappa a}{2} & \text{for } \frac{a}{2}(\hat{x}+\hat{y}) \\ 0 & \text{for } \frac{a}{2}(\hat{x}-\hat{y}) \\ \frac{\kappa a}{2} & \text{for } \frac{a}{2}(\hat{y}\pm\hat{z}) \\ \pm\frac{\kappa a}{2} & \text{for } \frac{a}{2}(\hat{z}\pm\hat{x}) \end{cases}$$

$$\mathbb{D}(\vec{k}) = \frac{8K}{a^2}\frac{a^2}{4}\Big[\sin^2\left(\frac{2ka}{4}\right)(\hat{x}+\hat{y})(\hat{x}+\hat{y})$$

$$+\sin^2\left(\frac{ka}{4}\right)\Big\{(\hat{y}+\hat{z})(\hat{y}+\hat{z}) + (\hat{y}-\hat{z})(\hat{y}-\hat{z}) + (\hat{z}+\hat{x})(\hat{z}+\hat{x}) + (\hat{z}-\hat{x})(\hat{z}-\hat{x})\Big\}\Big]$$

$$= 2K\Big[\sin^2\left(\frac{2ka}{4}\right)\Big\{\hat{x}\hat{x}+\hat{y}\hat{y}+\hat{x}\hat{y}+\hat{y}\hat{x}\Big\}$$

$$+\sin^2\left(\frac{ka}{4}\right)\Big\{2\hat{y}\hat{y}+2\hat{x}\hat{x}+4\hat{z}\hat{z}\Big\}\Big]$$

$$= 2K\begin{pmatrix} \sin^2\left(\frac{ka}{2}\right)+2\sin^2\left(\frac{ka}{4}\right) & \sin^2\left(\frac{ka}{2}\right) & 0 \\ \sin^2\left(\frac{ka}{2}\right) & \sin^2\left(\frac{ka}{2}\right)+2\sin^2\left(\frac{ka}{4}\right) & 0 \\ 0 & 0 & 4\sin^2\left(\frac{ka}{4}\right) \end{pmatrix}$$

eigenvectors and eigenvalues are

$\vec{\epsilon}_1 = \begin{pmatrix}1\\1\\0\end{pmatrix}$ $\lambda_1 = 2K\left[2\sin^2\left(\frac{ka}{2}\right)+2\sin^2\left(\frac{ka}{4}\right)\right]$ $\vec{\epsilon}_1 \parallel \vec{k}$ long

$\vec{\epsilon}_2 = \begin{pmatrix}0\\0\\1\end{pmatrix}$ $\lambda_2 = 8K\sin^2\left(\frac{ka}{4}\right)$ $\vec{\epsilon}_2 \perp \vec{k}$ transverse

$\vec{\epsilon}_3 = \begin{pmatrix}1\\-1\\0\end{pmatrix}$ $\lambda_3 = 4K\sin^2\left(\frac{ka}{4}\right)$ $\vec{\epsilon}_3 \perp \vec{k}$ transverse

$$\boxed{\begin{aligned} \omega_L(\vec{k}) &= 2\sqrt{\frac{K}{M}\left[\sin^2\left(\frac{\kappa a}{2}\right) + \sin^2\left(\frac{\kappa a}{4}\right)\right]} \\ \omega_{T1}(\vec{k}) &= 2\sqrt{\frac{2K}{M}}\sin\left(\frac{\kappa a}{4}\right) \qquad \kappa = \frac{k}{\sqrt{2}} \\ \omega_{T2}(\vec{k}) &= 2\sqrt{\frac{K}{M}}\sin\left(\frac{\kappa a}{4}\right) \end{aligned}}$$

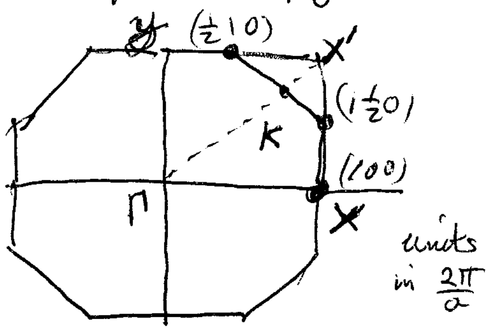
Here we have ω_{T1} and ω_{T2} are <u>NOT</u> degenerate

d) fcc has bcc RL with unit cell of side $\frac{4\pi}{a}$

In the 100 direction the edge of the 1st BZ is the Bragg plane that bisects $\vec{K} = \frac{4\pi}{a}\hat{x}$ so the edge is at $k_x = \frac{2\pi}{a}\hat{x}$.
In the 111 direction the edge of the 1st BZ is the Bragg plane that bisects the $\vec{K} = \frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ to the body centered site so $\vec{k}_o = \frac{\pi}{a}(1,1,1)$

So for $\vec{k}$ in (100) direction $k_{max} = \frac{2\pi}{a}$
for $\vec{k}$ in (111) direction $K_{max} = \frac{\pi}{a}$ $\qquad k = \sqrt{3}\,K$

For $\vec{k}$ in (110) direction we can use info in AM prob 9.3 pg 171 to draw the BZ in the xy plane



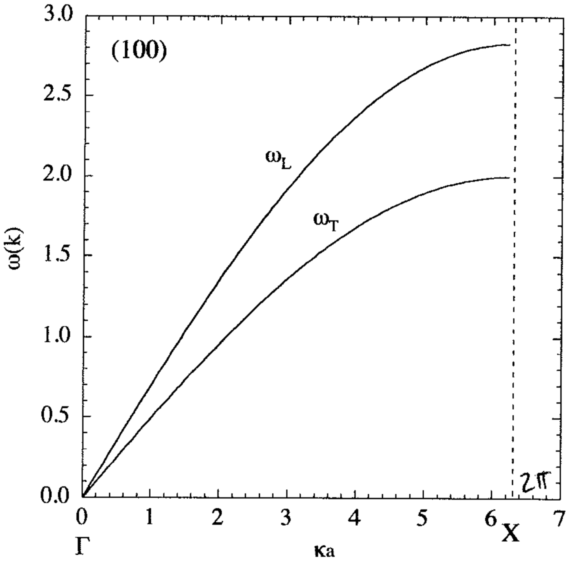
pt K is at $\frac{2\pi}{a}\left(\frac{3}{4}, \frac{3}{4}, 0\right)$
pt X' is at $\frac{2\pi}{a}(1,1,0)$

Γ is origin, X is edge in (100), K is edge in (110)

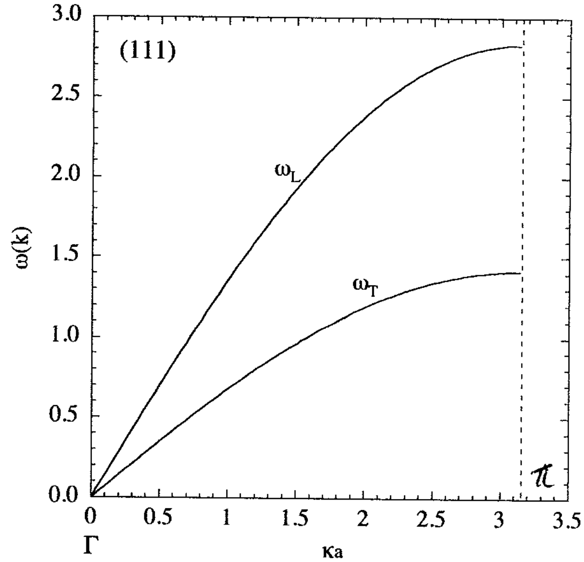
from AM fig 22.13 we see that pt X' is equivalent to pt X when viewed in the repeated zone scheme.

So for $\vec{k}$ in (110) direction $K_{max} = \frac{2\pi}{a}\frac{3}{4}$ to pt K

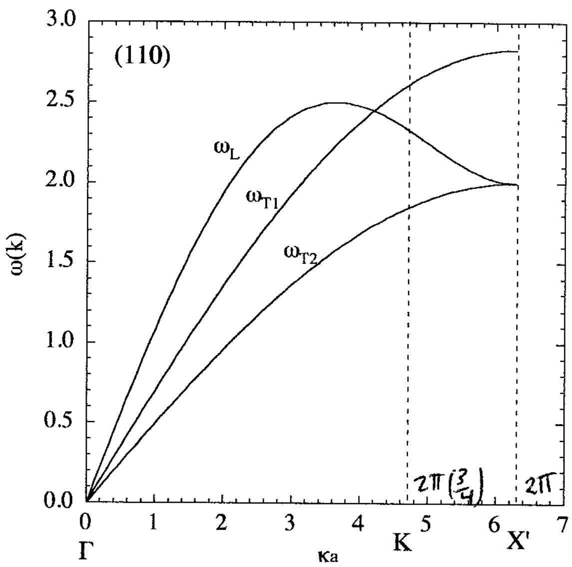
$\frac{2\pi}{a}$ to pt X'



$\kappa = |\vec{k}|$



$\kappa = \frac{|\vec{k}|}{\sqrt{3}}$



$\kappa = \frac{|\vec{k}|}{\sqrt{2}}$

Note that the "L" mode in (100) becomes "T" mode in (110) at ~~point~~ X, and that "L" mode in (110) becomes "T" mode in (100) at point X'.

This can happen because

$$\vec{k}_{X'} = \frac{2\pi}{a}(1,1,0) = \vec{k}_X + \vec{K}$$

where $\vec{k}_X = \frac{2\pi}{a}(0,0,1)$

$\vec{K} = \frac{2\pi}{a}(1,1,-1)$ a RL vector

so $\vec{k}_{X'}$ and $\vec{k}_X$ are equivalent wavevectors — they differ only by a RL. vector.

yet $\vec{k}_{X'} \cdot \vec{k}_X = 0$ ie $\vec{k}_{X'} \perp \vec{k}_X$ so the orientation of the mode, whether transverse or longitudinal, is ambiguous at high symmetry point X.