

Assignment 5

Solution

Question 1:-

a)

$$\begin{aligned}\vec{a} &= a \hat{i} \\ \vec{b} &= a \left[\cos 60^\circ \hat{i} + \sin 60^\circ \hat{j} \right] \\ &= \frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j}\end{aligned}$$

b)

$$\vec{a}^* = \frac{2\pi}{a} \frac{\vec{b} \times \hat{z}}{\vec{a} \cdot (\vec{b} \times \hat{z})}; \quad \vec{b}^* = \frac{2\pi}{a} \frac{\hat{z} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \hat{z})}$$

$$\vec{b} \times \hat{z} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{z} \\ a/2 & \sqrt{3}a/2 & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{\sqrt{3}}{2} a \hat{i} - \frac{a}{2} \hat{j}$$

$$\vec{a} \cdot (\vec{b} \times \hat{z}) = \frac{\sqrt{3}}{2} a^2$$

$$\hat{z} \times \vec{a} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{z} \\ 0 & 0 & 1 \\ a & 0 & 0 \end{vmatrix} = a \hat{j}$$

$$\Rightarrow \vec{a}^* = 2\pi \left(\frac{2}{\sqrt{3}a^2} \right) \left[\frac{\sqrt{3}}{2} a \hat{i} - \frac{a}{2} \hat{j} \right] = \frac{2\pi}{\sqrt{3}a} (\sqrt{3} \hat{i} - \hat{j})$$

$$\vec{b}^* = 2\pi \left(\frac{2}{\sqrt{3}a^2} \right) (a\hat{j}) = \frac{4\pi}{\sqrt{3}a} \hat{j}$$

To find that the Wigner-Seitz Cell is hexagonal:-

$$\vec{a}^* \cdot \vec{b}^* = \left(\frac{-2\pi}{\sqrt{3}a} \right) \left(\frac{4\pi}{\sqrt{3}a} \right) = -\frac{8\pi^2}{3a^2}$$

$$|\vec{a}^*| = \sqrt{\frac{4\pi^2}{a^2} + \frac{4\pi^2}{3a^2}} = \frac{2\pi}{a} \sqrt{\frac{4}{3}}$$

$$= \frac{4\pi}{\sqrt{3}a}$$

$$|\vec{b}^*| = \frac{4\pi}{\sqrt{3}a}$$

$$\cos\theta = \frac{\vec{a}^* \cdot \vec{b}^*}{|\vec{a}^*| |\vec{b}^*|} = \left(\frac{-8\pi^2}{3a^2} \right) / \left(\frac{16\pi^2}{3a^2} \right)$$

$$= -\frac{1}{2}$$

$$\Rightarrow \theta = 120^\circ$$

$$\text{or } \theta = 180^\circ - 120^\circ = 60^\circ$$

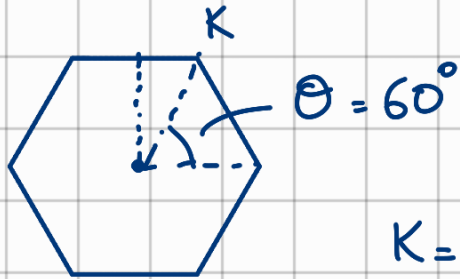
This makes Wigner-Seitz cell around $\Gamma = (0, 0)$ a regular hexagon.

Coordinates of :-

- M : midpoint of upper horizontal edge of hexagon

$$\Rightarrow M = \left(0, \frac{4\pi}{\sqrt{3}a} \left(\frac{1}{2} \right) \right) = \left(0, \frac{2\pi}{\sqrt{3}a} \right)$$

• K :



$$K = \frac{4\pi}{\sqrt{3}a} \left(\cos 60^\circ, \sin 60^\circ \right)$$

$$= \left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{a} \right)$$

c)

$$\Phi'_{0,x} = -\alpha (\hat{\omega}_1 \cdot \hat{x}) (\hat{\omega}_1 \cdot \hat{x}) = -\alpha (1)(1)$$

$$= -\alpha \quad \text{where } \hat{\omega}_1 = (1, 0)$$

Similarly,

$$\Phi'_{0,y} = \Phi'_{0,x} = \Phi'_{0,y} = 0$$

With $\hat{\omega}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right) :-$

$$\Phi'_{0,x} = -\alpha (\hat{\omega}_2 \cdot \hat{x}) (\hat{\omega}_2 \cdot \hat{x})$$

$$= \frac{-\alpha}{4}$$

$$\Phi'_{0,y} = \Phi'_{0,x} = -\alpha (\hat{\omega}_2 \cdot \hat{x}) (\hat{\omega}_2 \cdot \hat{y})$$

$$= -\frac{\sqrt{3}}{4} \alpha$$

$$\Phi'_{0,y} = -\alpha \left(\frac{\sqrt{3}}{2} \right)^2 = -\frac{3}{4} \alpha$$

With $\hat{\omega}_3 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) :-$

$$\begin{aligned}\bar{\Phi}_{0,x}^{3,x} &= -\alpha (\hat{\omega}_3 \cdot \hat{x}) (\hat{\omega}_3 \cdot \hat{x}) \\ &= \frac{-\alpha}{4}\end{aligned}$$

$$\begin{aligned}\bar{\Phi}_{0,y}^{3,x} &= \bar{\Phi}_{0,x}^{3,y} = -\alpha (\hat{\omega}_3 \cdot \hat{x}) (\hat{\omega}_3 \cdot \hat{y}) \\ &= + \frac{\sqrt{3}}{4} \alpha\end{aligned}$$

$$\bar{\Phi}_{0,y}^{3,y} = -\alpha \left(\frac{\sqrt{3}}{2}\right)^2 = -\frac{3}{4} \alpha$$

With $\hat{\omega}_4 = (-1, 0) :-$

$$\begin{aligned}\bar{\Phi}_{0,x}^{4,x} &= -\alpha (\hat{\omega}_4 \cdot \hat{x}) (\hat{\omega}_4 \cdot \hat{x}) \\ &= -\alpha\end{aligned}$$

$$\bar{\Phi}_{0,y}^{4,x} = \bar{\Phi}_{0,x}^{4,y} = \bar{\Phi}_{0,y}^{4,y} = 0$$

With $\hat{\omega}_5 = \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right) :-$

$$\begin{aligned}\bar{\Phi}_{0,x}^{5,x} &= -\alpha (\hat{\omega}_5 \cdot \hat{x}) (\hat{\omega}_5 \cdot \hat{x}) \\ &= \frac{-\alpha}{4}\end{aligned}$$

$$\begin{aligned}\bar{\Phi}_{0,y}^{5,x} &= \bar{\Phi}_{0,x}^{5,y} = -\alpha (\hat{\omega}_5 \cdot \hat{x}) (\hat{\omega}_5 \cdot \hat{y}) \\ &= -\frac{\sqrt{3}}{4} \alpha\end{aligned}$$

$$\bar{\Phi}_{0,y}^{5,y} = -\alpha \left(-\frac{\sqrt{3}}{2}\right)^2 = -\frac{3}{4} \alpha$$

With $\hat{\omega}_6 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) :-$

$$\begin{aligned}\Phi_{0,x}^{6,x} &= -\alpha (\hat{\omega}_6 \cdot \hat{x}) (\hat{\omega}_6 \cdot \hat{x}) \\ &= \frac{-\alpha}{4}\end{aligned}$$

$$\begin{aligned}\Phi_{0,y}^{6,x} &= \Phi_{0,x}^{6,y} = -\alpha (\hat{\omega}_6 \cdot \hat{x}) (\hat{\omega}_6 \cdot \hat{y}) \\ &= + \frac{\sqrt{3}}{4} \alpha\end{aligned}$$

$$\Phi_{0,y}^{6,y} = -\alpha \left(\frac{\sqrt{3}}{2}\right)^2 = -\frac{3}{4} \alpha$$

d)
$$D_{n,i}^{m,j} = \frac{1}{M} \sum_m \Phi_{n,i}^{m,j} e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_n)}$$

$$\begin{aligned}D_{0,x}^{m,x} &= \frac{1}{M} \sum_m \Phi_{0,x}^{m,x} e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_0)} \\ &= \frac{1}{M} \left[-\alpha e^{ik_x a} - \alpha e^{-ik_x a} - \frac{\alpha}{4} e^{ik_x a/2} e^{iky\sqrt{3}a/2} + \right. \\ &\quad \left. - \frac{\alpha}{4} e^{-ik_x a/2} e^{iky\sqrt{3}a/2} - \frac{\alpha}{4} e^{-ik_x a/2} e^{-iky\sqrt{3}a/2} + \right. \\ &\quad \left. - \frac{\alpha}{4} e^{ik_x a/2} e^{-iky\sqrt{3}a/2} \right] \\ &= \frac{-\alpha}{4M} \left[8 \cos(k_x a) + 2 e^{ik_x a/2} \cos\left(\frac{\sqrt{3} k_y a}{2}\right) + \right. \\ &\quad \left. + 2 e^{-ik_x a/2} \cos\left(\frac{\sqrt{3} k_y a}{2}\right) \right] \\ &= \frac{-\alpha}{M} \left[2 \cos(k_x a) + \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{\sqrt{3} k_y a}{2}\right) \right]\end{aligned}$$

$$D_{0,y}^{m,x} = \frac{1}{M} \sum_m \Phi_{0,y}^{m,x} e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_0)}$$

$$= \frac{1}{M} \left[-\frac{\sqrt{3}\alpha}{4} e^{ik_x a/2} e^{iky\sqrt{3}a/2} + \frac{\sqrt{3}\alpha}{4} e^{-ik_x a/2} e^{iky\sqrt{3}a/2} \right. \\ \left. - \frac{\sqrt{3}\alpha}{4} e^{-ik_x a/2} e^{-iky\sqrt{3}a/2} + \frac{\sqrt{3}\alpha}{4} e^{ik_x a/2} e^{-iky\sqrt{3}a/2} \right]$$

$$= \frac{\sqrt{3}\alpha}{M} \sin\left(\frac{k_x a}{2}\right) \sin\left(\frac{\sqrt{3}k_y a}{2}\right)$$

$$\therefore D_{0,x}^{m,y} = D_{0,y}^{m,x} = \frac{\sqrt{3}\alpha}{M} \sin\left(\frac{k_x a}{2}\right) \sin\left(\frac{\sqrt{3}k_y a}{2}\right)$$

$$D_{0,y}^{m,y} = \frac{-3\alpha}{4M} \left[e^{ik_x a/2} e^{iky\sqrt{3}a/2} + e^{-ik_x a/2} e^{iky\sqrt{3}a/2} + \right. \\ \left. e^{-ik_x a/2} e^{-iky\sqrt{3}a/2} + e^{ik_x a/2} e^{-iky\sqrt{3}a/2} \right]$$

$$= \frac{-3\alpha}{M} \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{\sqrt{3}k_y a}{2}\right)$$

$$|D - \omega^2 \mathbb{1}| = 0$$

$$\Rightarrow \left[\frac{-\alpha}{M} \left[2 \cos(k_x a) + \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \right] - \omega^2 \right] \times \\ \left[\frac{-3\alpha}{M} \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{\sqrt{3}k_y a}{2}\right) - \omega^2 \right] +$$

$$- \frac{3\alpha^2}{M^2} \sin^2\left(\frac{k_x a}{2}\right) \sin^2\left(\frac{\sqrt{3}k_y a}{2}\right) = 0$$

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In[ ]:= Q = DiagonalMatrix[{-ω^2 + (2 + Cos[ky + Sqrt[3]/2] - 3), -ω^2 + 3 + (Cos[ky + Sqrt[3]/2] - 1)}]
Out[ ]:= {{-1 - ω^2 + Cos[ $\frac{\sqrt{3} ky}{2}$ ], 0}, {0, -ω^2 + 3 - (1 + Cos[ $\frac{\sqrt{3} ky}{2}$ ])}}
In[ ]:= Solve[Simplify[Det[Q]] == 0, ω]
Out[ ]:= {{ω -> -√{-1 + Cos[ $\frac{\sqrt{3} ky}{2}$ ]}, {ω -> √{-1 + Cos[ $\frac{\sqrt{3} ky}{2}$ ]}, {ω -> -√3 √{-1 + Cos[ $\frac{\sqrt{3} ky}{2}$ ]}, {ω -> √3 √{-1 + Cos[ $\frac{\sqrt{3} ky}{2}$ ]}}
Q = DiagonalMatrix[{-ω^2 + (2 + Cos[ky + Sqrt[3]/2] - 3), -ω^2 + 3 + (Cos[ky + Sqrt[3]/2] - 1)}]
In[ ]:= A = {{(-ω^2 + α/M * (3 - 2 + Cos[kx + a] - Cos[kx + a/2]) + Cos[ky + Sqrt[3] * a/2]), Sqrt[3] * α/M * Sin[kx + a/2] + Sin[ky + Sqrt[3] * a/2]),
(Sqrt[3] * α/M * Sin[kx + a/2] + Sin[ky + Sqrt[3] * a/2]), -ω^2 + 3 + α/M * (1 - Cos[kx + a/2] + Cos[ky + Sqrt[3] * a/2])}}
Out[ ]:= {{-ω^2 +  $\frac{\alpha (3 - 2 \cos[ax] - \cos[\frac{akx}{2}]) \cos[\frac{1}{2} \sqrt{3} aky]}{M}$ ,  $\frac{\sqrt{3} \alpha \sin[\frac{akx}{2}] \sin[\frac{1}{2} \sqrt{3} aky]}{M}$ }, { $\frac{\sqrt{3} \alpha \sin[\frac{akx}{2}] \sin[\frac{1}{2} \sqrt{3} aky]}{M}$ ,  $-\omega^2 + \frac{3 \alpha (1 - \cos[\frac{akx}{2}] - \cos[\frac{1}{2} \sqrt{3} aky])}{M}$ }}

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e)

From Γ to M

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In[ ]:= FullSimplify[Solve[FullSimplify[Det[A /. kx -> 0]] == 0, ω]]

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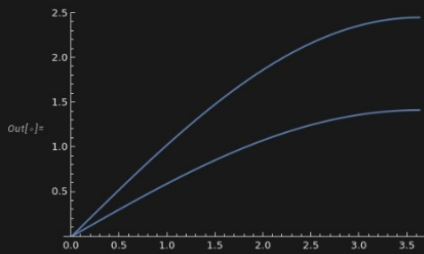
Out[ ]:= {{ω -> -√ $\frac{4 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 - 2 \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}$ }, {ω -> √ $\frac{4 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 - 2 \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}$ },
{ω -> -√2 √ $\frac{2 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 + \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}$ }, {ω -> √2 √ $\frac{2 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 + \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}$ }}

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In[ ]:= q1 = Plot[FullSimplify[ $\left\{ \sqrt{\frac{4 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 - 2 \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}}, \sqrt{2} \sqrt{\frac{2 M \alpha \sin[\frac{1}{4} \sqrt{3} aky]^2 + \sqrt{M^2 \alpha^2 \sin[\frac{1}{4} \sqrt{3} aky]^4}}{M^2}} \right\} /. (\alpha \rightarrow 1, a \rightarrow 1, M \rightarrow 1)$ ,
{ky, 0, 2 * Pi / Sqrt[3]}, PlotRange -> {0, 2.5}]

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From M to K

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In[ ]:= FullSimplify[Solve[FullSimplify[Det[A /. ky -> 2 * Pi / (a + Sqrt[3])]] == 0, ω]]

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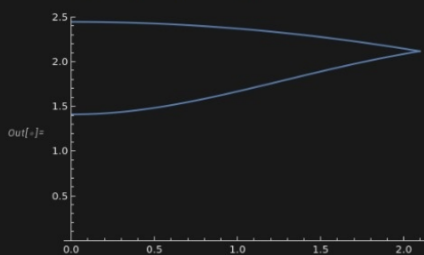
Out[ ]:= {{ω -> -√ $\frac{-2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}$ }, {ω -> √ $\frac{-2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}$ },
{ω -> -√ $\frac{2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}$ }, {ω -> √ $\frac{2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}$ }}

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In[ ]:= q2 = Plot[FullSimplify[ $\left\{ \sqrt{\frac{2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}}, \sqrt{\frac{-2 \sqrt{M^2 \alpha^2 \cos[\frac{akx}{4}]^4 (1 - 2 \cos[\frac{akx}{2}])^2 + M \alpha (3 + 2 \cos[\frac{akx}{2}] - \cos[akx])}{M^2}} \right\} /. (\alpha \rightarrow 1, a \rightarrow 1, M \rightarrow 1)$ ,
{kx, 0, 2 * Pi / 3}, PlotRange -> {0, 2.5}]

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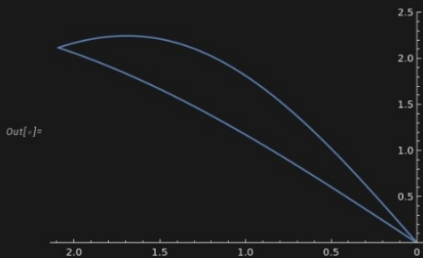


From K to Γ

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In[ ]:= Solve[Det[A /. ky -> Sqrt[3] * kx] == 0,  $\omega$ ]
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Out[ ]:= {{ $\omega \rightarrow -\frac{\sqrt{3} \sqrt{\alpha - \alpha \cos[a kx]}}{\sqrt{M}}$ }, { $\omega \rightarrow \frac{\sqrt{3} \sqrt{\alpha - \alpha \cos[a kx]}}{\sqrt{M}}$ }, { $\omega \rightarrow -\frac{\sqrt{3 \alpha - \alpha \cos[a kx] - 2 \alpha \cos[2 a kx]}}{\sqrt{M}}$ }, { $\omega \rightarrow \frac{\sqrt{3 \alpha - \alpha \cos[a kx] - 2 \alpha \cos[2 a kx]}}{\sqrt{M}}$ }}}
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In[ ]:= q3 = Plot[FullSimplify[{ $\frac{\sqrt{3} \sqrt{\alpha - \alpha \cos[a kx]}}{\sqrt{M}}$ ,  $\frac{\sqrt{3 \alpha - \alpha \cos[a kx] - 2 \alpha \cos[2 a kx]}}{\sqrt{M}}$ }] /. { $\alpha \rightarrow 1$ ,  $a \rightarrow 1$ ,  $M \rightarrow 1$ }, {kx, 2 * Pi / 3, 0}, ScalingFunctions -> {"Reverse", Identity}, PlotRange -> {0, 2.5}]
```



Question 2:-

$$a) \quad s_n = u_n e^{i(kna - \omega t)} = u_n e^{i(kna - \omega t)} e^{-\eta na}$$

For a monoatomic 1D lattice,

$$\ddot{s}_n = \frac{\alpha}{M} (s_{n+1} + s_{n-1} - 2s_n)$$

$$-\omega^2 s_n = \frac{\alpha}{M} (s_n e^{i(k+n)a} + s_n e^{-i(k+n)a} - 2s_n)$$

For arbitrary s_n :

$$-M\omega^2 = \alpha (e^{i(k+n)a} + e^{-i(k+n)a} - 2)$$

$$\cosh \beta = \frac{e^\beta + e^{-\beta}}{2}$$

$$\begin{aligned} \rightarrow \cosh [i(k+n)] &= \cos(k+n) = \cos(k)\cos(n) - \sin(k)\sin(n) \\ &= \cos(k)\cosh(n) - i\sin(k)\sinh(n) \end{aligned}$$

$$\cos \cosh(i\theta) = \frac{e^{i\theta} + e^{-i\theta}}{2} = \cos \theta$$

$$\cos(in) = \frac{e^{+i(in)} + e^{-i(in)}}{2} = \frac{e^{-n} + e^n}{2} = \cosh(n)$$

$$\sin(in) = \frac{e^{i(in)} - e^{-i(in)}}{2} = \frac{e^{-n} - e^n}{2i} = i \sinh(n)$$

$$\Rightarrow D = \frac{2\alpha}{M} [1 - \cos(k)\cosh(n) + i\sin(k)\sinh(n)]$$

$$\omega = \sqrt{\frac{2\alpha}{M}} \sqrt{1 - \cos(k) \cosh(\eta) + i \sin(k) \sinh(\eta)}$$

is complex

If $\eta \ll k$ (η is small),

$$\cosh(\eta) = \frac{e^\eta + e^{-\eta}}{2} \approx \frac{1}{2} (1 + \eta + 1 - \eta) \approx 1$$

$$\sinh(\eta) \approx \frac{1}{2} (1 + \eta - 1 + \eta) \approx \eta$$

$$\therefore \omega = \sqrt{\frac{2\alpha}{M}} \sqrt{1 - \cos(k) + i\eta \sin(k)}$$

$\Rightarrow k$ small \rightarrow acoustic, near $k=0$

$$\omega = \sqrt{\frac{2\alpha}{M}} \sqrt{1 - \left(1 - \frac{k^2}{2}\right) + ik\eta}$$

$$\omega = \sqrt{\frac{2\alpha}{M}} \left(\frac{k^2}{2} + ik\eta\right)^{1/2} = \sqrt{\frac{\alpha k}{M}} \left[1 + ik\eta \frac{2}{k^2}\right]^{1/2}$$

b)

as $k \gg \eta$,

$$\omega = \sqrt{\frac{\alpha k}{M}} \left(1 + \frac{i\eta}{k}\right)$$

$$\operatorname{Re}(\omega) = \sqrt{\frac{\alpha k}{M}} \quad ; \quad \operatorname{Im}(\omega) = \sqrt{\frac{\alpha k}{M}} \frac{\eta}{k}$$