Jo

Q1

(a) Acoustic (with $-$ sign)

$$\frac{d\omega_-}{dk} = \frac{a\gamma \sin(ka)}{2 m_a m_b \sqrt{\frac{1}{M_a^2}+\frac{1}{M_b^2}+\frac{2\cos(ak)}{M_a M_b}}\sqrt{\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}-\sqrt{\frac{1}{M_a^2}+\frac{1}{M_b^2}+\frac{2\cos(ak)}{M_a M_b}}\right)}}$$

(1)

Optical branch (with + sign)

$$\frac{d\omega_+}{dk} = -\frac{a\gamma \sin(ka)}{2 M_a M_b \sqrt{\frac{1}{M_a^2}+\frac{1}{M_b^2}+\frac{2\cos(ak)}{M_a M_b}}\sqrt{\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}+\sqrt{\frac{1}{M_a^2}+\frac{1}{M_b^2}+\frac{2\cos(ak)}{M_a M_b}}\right)}}$$

(2)

(b) For the optical branch

$$\omega^2 = \gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right) + \gamma\sqrt{\left(\frac{1}{M_a}+\frac{1}{M_b}\right)^2 - \left(\frac{4}{M_a M_b}\right)\sin^2\left(\frac{ka}{2}\right)}$$

$$\omega^2\Big|_{k=0} = 2\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right).$$

Putting this into Eq. 3, with $k=0$

$$\left(-2\gamma\left(\frac{1}{m_a}+\frac{1}{M_b}\right)+\frac{2\gamma}{m_a}\right)u_1 - \frac{\gamma}{\sqrt{m_a M_b}}(1+1)\,u_2 = 0.$$

$$\left(\cancel{\frac{1}{M_a}} - \cancel{\frac{1}{M_a}} - \frac{1}{M_b}\right)u_1 - \frac{1}{\sqrt{m_a M_b}}\,u_2 = 0$$

$$\frac{1}{M_b}\frac{u_1}{u_2} = -\frac{1}{\sqrt{m_a M_b}}$$

$$\frac{u_1}{u_2} = -\sqrt{\frac{M_b}{m_a}}$$

$$\cancel{\frac{S_1}{S_2} = \frac{u_1}{\sqrt{m_a}}\frac{\sqrt{M_b}}{u_2} = -\sqrt{\frac{M_b}{m_a}}}$$

$$\frac{u_1}{u_2} = \frac{\sqrt{m_a}\,S_1}{\sqrt{m_b}\,S_2} \Rightarrow \frac{S_1}{S_2} = \frac{S_{n,a}}{S_{n,b}} = \frac{u_1}{u_2}\sqrt{\frac{m_b}{m_a}}$$

$$\frac{S_1}{S_2} = -\frac{m_b}{m_a}$$ (out of phase as required).

(b) $g(\omega) = \frac{L}{2\pi} \frac{1}{d\omega/dk}$

Acoustic branch first

$\frac{d\omega_-}{dk} = 0$ when $\sin(ka) = 0 \Rightarrow k = 0, \pm\frac{\pi}{a}$

Insert these values of k in the dispersion relat.

$$\omega_-\Big|_{k=0} = \sqrt{\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right) - \gamma\sqrt{\left(\frac{1}{M_a}+\frac{1}{M_b}\right)^2}}$$

$$= \sqrt{\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right) - \gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right)} = 0$$

and

$$\omega_-\Big|_{k=\pm\pi/a} = \sqrt{\gamma\left(\frac{1}{M_a}+\frac{1}{M_b}\right) - \gamma\sqrt{\left(\frac{1}{M_a}+\frac{1}{M_b}\right)^2 - \frac{4}{M_aM_b}}}$$

Let's put in some representative values, Say $M_b = M_a/2 = \frac{M}{2}$

$$\omega_-^2\Big|_{k=\pm\pi/a} = \gamma\left(\frac{1}{M}+\frac{2}{M}\right) - \gamma\sqrt{\left(\frac{1}{M}+\frac{2}{M}\right)^2 - \frac{4\times 2}{M^2}}$$

$$= \frac{\gamma 3}{M} - \gamma\sqrt{\frac{9}{M^2} - \frac{8}{M^2}}$$

$$= \frac{\gamma 3}{M} - \frac{\gamma}{M}\sqrt{1} = \frac{3\gamma}{M} - \frac{\gamma}{M} = \frac{2\gamma}{M}$$

$$\omega_-\Big|_{k=\pm\pi/2} = \sqrt{\frac{2\gamma}{M}}$$

$\boxed{\text{So we have singularities in } g(\omega) \text{ at } \omega = 0 \text{ and } \omega = \sqrt{\frac{2\gamma}{M}} \text{ when } M_b = M_a/2.}$

Optical branch

From Eq. ②, $\frac{d\omega_+}{dk} = 0$ also when

$ka = 0$ or $ka = \pi$.

Putting these values into ω_+:

$$\omega_+\Big|_{k=0} = \sqrt{2\gamma\left(\frac{1}{M_a} + \frac{1}{M_b}\right)}$$

and

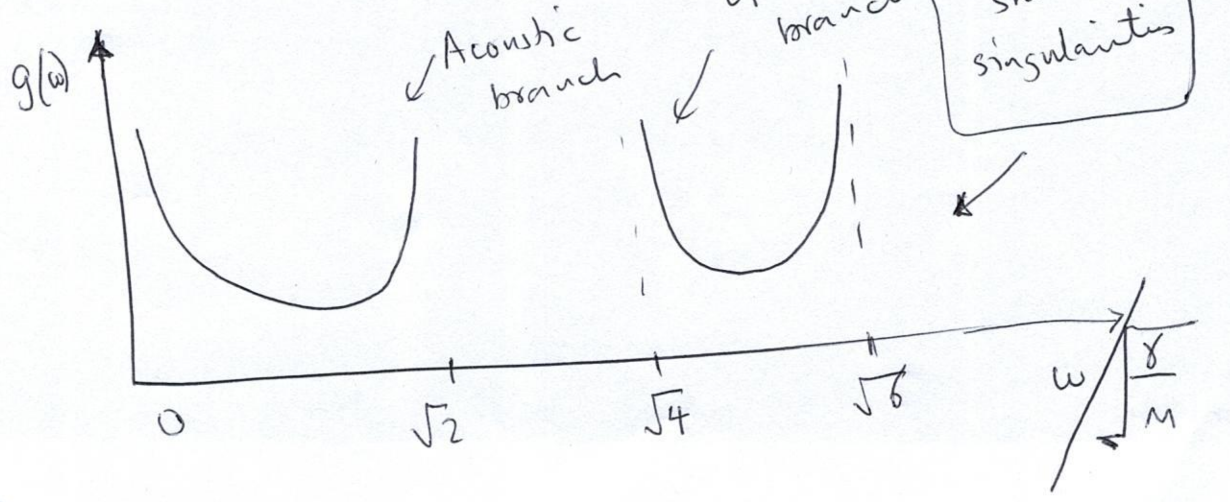
$$\omega_+\Big|_{k=\frac{\pi}{a}} = \sqrt{\gamma\left(\frac{1}{M_a} + \frac{1}{M_b}\right) + \gamma\sqrt{\left(\frac{1}{M_a} + \frac{1}{M_b}\right)^2 - \left(\frac{4}{M_a M_b}\right)}}$$

Let's use our representative masses, $M_b = M_a/2$.

$$\omega_+\Big|_{k=0} = \sqrt{\frac{6\gamma}{m}}$$

$$\omega_+\Big|_{k=\pi/a} = \sqrt{\frac{4\gamma}{m}}$$

Possible form of the density of states showing singularities



Question 2:-

$$U = \frac{3V k_B^4 T^4}{2\pi^2 \hbar^3 v^3} \int_0^{x_D} dx \, \frac{x^3}{e^x - 1}$$

where $x_{(D)} = \frac{\hbar \omega_{(D)}}{k_B T}$; in low T limit: $x_D \to \infty$

In low T limit:

$$U = \frac{3V k_B^4 T^4}{2\pi^2 \hbar^3 v^3} \underbrace{\int_0^{\infty} dx \, \frac{x^3}{e^x - 1}}_{= \pi^4/15}$$

$$\approx \frac{3V k_B^4 T^4}{2\pi^2 \hbar^3 v^3} \frac{\pi^4}{15}$$

$$\Rightarrow C_v = \left.\frac{\partial U}{\partial T}\right|_v = \frac{2V k_B^4 \pi^2}{5 \hbar^3 v^3} T^3$$

$C_v \propto T^3$ at ultra-low temperatures

Question 3 :-

$$\begin{pmatrix} -\omega^2 + \frac{2\gamma}{m_a} & -\frac{\gamma}{\sqrt{m_a m_b}}\left(1 + e^{-ika}\right) \\ -\frac{\gamma}{\sqrt{m_a m_b}}\left(1 + e^{ika}\right) & -\omega^2 + \frac{2\gamma}{m_b} \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = 0$$

$$S_{n,a} = \frac{U_a}{\sqrt{m_a}} e^{ikna} \quad , \quad S_{n,b} = \frac{U_b}{\sqrt{m_b}} e^{ikna}$$

a) For acoustic branch at $k = 0$,

$$\omega = 0$$

$$\Rightarrow \begin{pmatrix} \frac{2\gamma}{m_a} & \frac{-2\gamma}{\sqrt{m_a m_b}} \\ \frac{-2\gamma}{\sqrt{m_a m_b}} & \frac{2\gamma}{m_b} \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = 0$$

$$\Rightarrow \frac{\cancel{2\gamma}}{m_a} U_1 - \frac{\cancel{2\gamma}}{\sqrt{m_a m_b}} U_2 = 0$$

$$U_1 = \sqrt{\frac{m_a}{m_b}}\, U_2$$

$$\Rightarrow \frac{S_{n,a}}{S_{n,b}} = \frac{U_a/\sqrt{m_a}}{U_b/\sqrt{m_b}} = \frac{U_a}{U_b}\sqrt{\frac{m_b}{m_a}} = \sqrt{\frac{m_a}{m_b}}\sqrt{\frac{m_b}{m_a}} = +1$$

$$\therefore \frac{S_{n,a}}{S_{n,b}} = 1 \longrightarrow$$ acoustic, both atoms move with same displacement amplitude and are in phase

Question 4:-

a) For the harmonic oscillator :-

$$U = \frac{1}{2} \sum_{\substack{m,n,\\a,b}} \Phi^{m,b}_{n,a} \, s_{n,a} s_{m,b} \quad \text{———} \quad (1)$$

There are two atoms in a unit cell n : a_n, b_n
with displacements $u_{n,a}$ and $u_{n,b}$
The spring constants are related as:
↳ α : $a_n - b_n$
β : $b_n - a_{n+1}$

One can construct the potential energy as:

$$U = \frac{1}{2} \sum_n \left[\alpha \left(s_{n,b} - s_{n,a} \right)^2 + \beta \left(s_{n+1,a} - s_{n,b} \right) \right]$$

$$= \frac{1}{2} \sum_n \left[\alpha \left(s_{n,b}^2 + s_{n,a}^2 - 2 s_{n,b} s_{n,a} \right) + - \beta \left(s_{n+1,a}^2 + s_{n,b}^2 - 2 s_{n+1,a} s_{n,b} \right) \right] \quad \text{—} \quad (2)$$

Comparing (1) and (2) together:-

1) $\Phi^{n,a}_{n,a} = \Phi^{n,b}_{n,b} = \alpha + \beta$

2) $\Phi^{n,b}_{n,a} = \Phi^{n,a}_{n,b} = -\alpha$

3) $\Phi^{n+1,a}_{n,b} = \Phi^{n-1,b}_{n,a} = -\beta$

All other Φs are 0.

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b) $$D^b_a = \sum_m \Phi^{m,b}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$D^a_a = \sum_m \Phi^{m,a}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$= \Phi^{n,a}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_n-\vec{r}_n)} = \alpha+\beta$$

$$D^b_b = \sum_m \Phi^{m,b}_{n,b}\, e^{i\vec{k}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$= \Phi^{n,b}_{n,b}\, e^{i\vec{k}\cdot(\vec{r}_n-\vec{r}_n)} = \alpha+\beta$$

$$D^a_b = \sum_m \Phi^{m,a}_{n,b}\, e^{i\vec{k}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$= \Phi^{n,a}_{n,b}\, e^{i\vec{k}\cdot(\vec{r}_n-\vec{r}_n)} + \Phi^{n+1,a}_{n,b}\, e^{i\vec{k}\cdot(\vec{r}_{n+1}-\vec{r}_n)}$$

$$= -\alpha - \beta e^{-ika}$$

$$D^b_a = \sum_m \Phi^{m,b}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$= \Phi^{n,b}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_n-\vec{r}_n)} + \Phi^{n-1,b}_{n,a}\, e^{i\vec{k}\cdot(\vec{r}_{n-1}-\vec{r}_n)}$$

$$= -\alpha - \beta e^{-ika}$$

c) $$D(k) = \begin{pmatrix} \alpha+\beta & -\alpha-\beta e^{-ika} \\ -\alpha-\beta e^{+ika} & \alpha+\beta \end{pmatrix}$$

$$|D - \omega^2 I| = 0$$

$$\begin{vmatrix} \alpha+\beta-\omega^2 & -\alpha-\beta e^{ika} \\ -\alpha-\beta e^{-ika} & \alpha+\beta-\omega^2 \end{vmatrix} = 0$$

$$\Rightarrow \left(\alpha+\beta-\omega^2\right)^2 - \left(\alpha+\beta e^{-ika}\right)\left(\alpha+\beta e^{ika}\right) = 0$$

$$\left(\alpha+\beta-\omega^2\right)^2 - \left[\alpha^2+\beta^2+2\alpha\beta\frac{\left(e^{ika}+e^{-ika}\right)}{2}\right] = 0$$

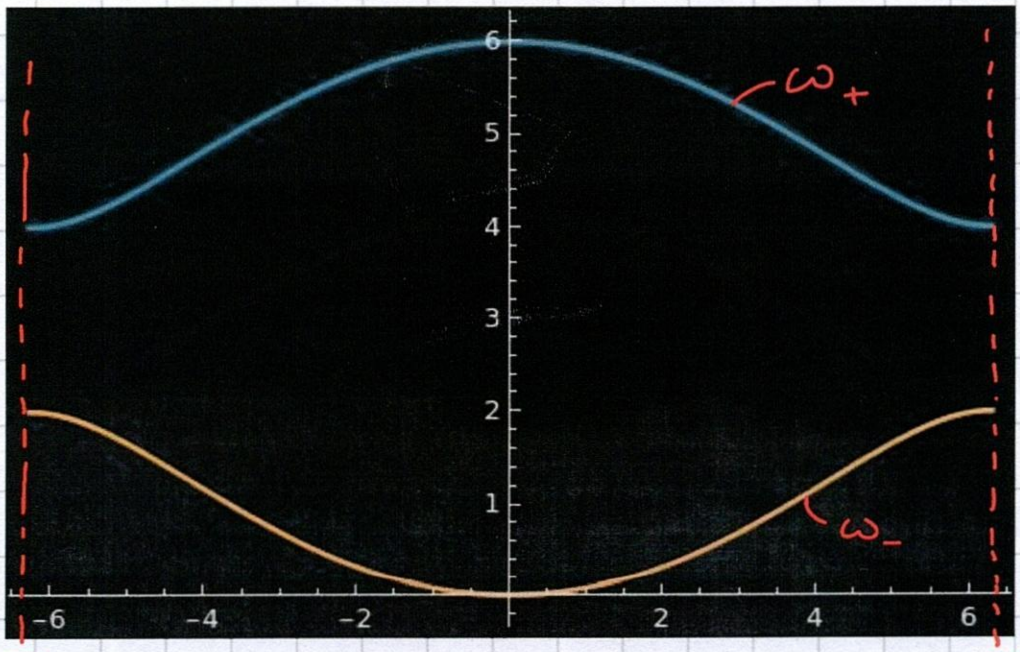
$$\left(\alpha+\beta-\omega^2\right)^2 - \left[\alpha^2+\beta^2+2\alpha\beta\cos(ka)\right] = 0$$

$$\left(\alpha+\beta-\omega^2\right)^2 = \left[\alpha^2+\beta^2+2\alpha\beta\cos(ka)\right]$$

$$\alpha+\beta-\omega^2 = \pm\sqrt{\alpha^2+\beta^2+2\alpha\beta\cos(ka)}$$

$$\Rightarrow \omega_\pm^2 = \frac{\alpha+\beta \pm\sqrt{\alpha^2+\beta^2+2\alpha\beta\cos(ka)}}{M}$$

don't forget the M



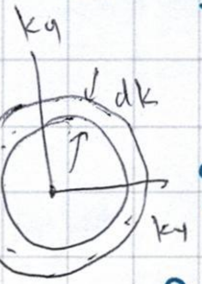
$-\pi/2$ $+\pi/2$

Question 5:-

a) Assuming $\omega = vk$ and working in 2D space,

$$dN = g(\omega)\,d\omega = g(k)\,dk$$

$$= \frac{A}{(2\pi)^2}(2\pi k)\,dk$$



$$g(\omega)\,d\omega = \frac{A}{2\pi}\,k\,dk$$

Since, $\omega = vk \Rightarrow d\omega = v\,dk$

$$\Rightarrow g(\omega)\,d\omega = \frac{A}{2\pi}\frac{\omega}{v}\frac{d\omega}{v}$$

$$g(\omega)\,d\omega = \frac{A}{2\pi}\frac{\omega}{v^2}\,d\omega \quad \text{for one branch}$$

For both branches in 2D,

$$g(\omega)\,d\omega = \frac{A}{\pi v^2}\,\omega\,d\omega$$

$$\therefore \; g(\omega) = \frac{A}{\pi v^2}\,\omega$$

b) Total number of modes in a crystal with N atoms = 2N

$$\Rightarrow \int_0^{\omega_D} g(\omega)\,d\omega = 2N$$

$$\int_0^{\omega_D} \frac{A}{\pi v^2}\,\omega\,d\omega = 2N$$

$$\frac{A\omega_D^2}{2\pi v^2} = 2N$$

Better way ↓

$$dN = \frac{2\pi k\,dk}{(2\pi)^2/L^2}$$

L^2 = area of the solid

$$dN = g(\omega)\,d\omega$$

$$\therefore g(\omega)\,d\omega = \frac{2\pi k L^2}{4\pi^2}\,dk$$

$$\boxed{g(\omega) = \frac{k}{2\pi}L^2\frac{1}{\frac{d\omega}{dk}}}$$

✓

$\omega = vk$ (v = speed of sound)

$d\omega/dk = v$

$$g(\omega) = \frac{kL^2}{2\pi}\cdot\frac{1}{v}$$

$$\boxed{g(\omega) = \frac{L^2}{2\pi}\frac{\omega}{v^2}}$$

(We assume oscillations ⊥ plane not possible).

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$$\omega_D^2 = \frac{4\pi N v^2}{A}$$

as $n = N/A$;

$$\therefore \quad \omega_D = v\sqrt{4\pi n}$$

c) $$E = \int_0^{\omega_D} \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}\, g(\omega)\, d\omega$$

$$= \frac{A\hbar}{\pi v^2}\int_0^{\omega_D} \frac{\omega^2}{e^{\beta\hbar\omega}-1}\, d\omega$$

$x = \beta\hbar\omega$; $d\omega = (1/\beta\hbar)dx$ where $\beta = 1/k_BT$

$$= \frac{k_BT}{\hbar}\, dx$$

and $\theta_D = \dfrac{\hbar\omega_D}{k_B}$

$$\Rightarrow E = \frac{A\hbar}{\pi v^2}\left(\frac{k_BT}{\hbar}\right)^3 \int_0^{\theta_D/T} \frac{x^2}{e^x-1}\, dx$$

$$= \frac{A(k_BT)^2}{\pi v^2\hbar^2}\int_0^{\theta_D/T} \frac{x^2}{e^x-1}\, dx$$

d) In low temperature limit,

$$\frac{\theta_D}{T} \longrightarrow \infty$$

$$E = \frac{A(k_BT)^3}{\pi v^2\hbar^2}\int_0^{\infty} \frac{x^2}{e^x-1}\, dx$$

$2\zeta(3) = 2.404$

$$U = \frac{2.404\, A(k_BT)^3}{\pi v^2\hbar^2}$$

$$\Rightarrow C_v = \left.\frac{\partial U}{\partial T}\right|_V = \frac{3(2.404)\,A\,k_B^3}{\pi v^2 \hbar^2}\, T^2 \propto T^2$$

at low temperatures

✓