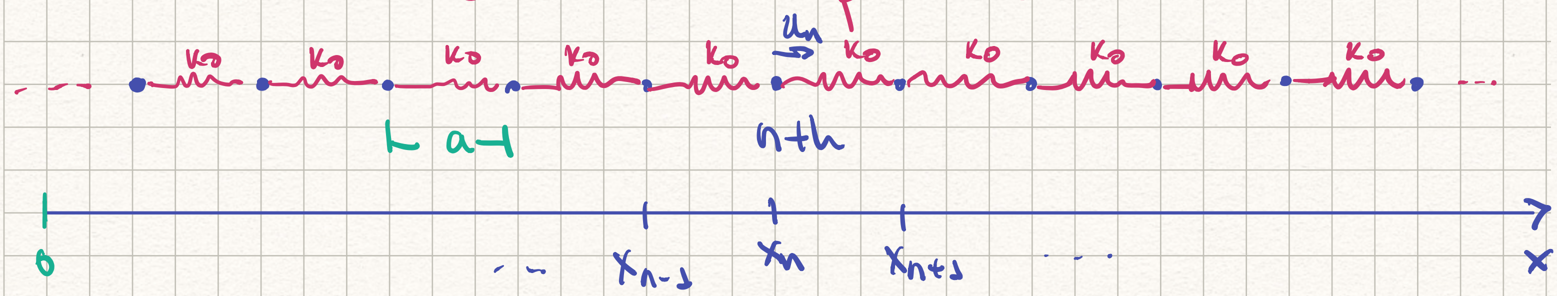
Introduction to phonons



$$m\frac{d^2u_n}{dt^2} = k_0\left(u_{n+1} + u_{n-1} - 2u_n\right)$$ General eq. motion

Assuming that $u_n = A\,e^{i(kx_n - \omega t)}$

x_n: position of equilibrium $\quad x_n = na$

k: wavevector of the wave

$$u_n = A\,e^{i(kna - \omega t)}$$

$$\frac{du_n^2}{dt^2} = -\omega^2 A\,e^{i(kna - \omega t)} = -\omega^2 u_n$$

$$u_{n+1} = A\,e^{i[k(n+1)a - \omega t]} = A\,e^{i[kna - \omega t]}\,e^{ika} = u_n e^{ika}$$

$$u_{n-1} = A\,e^{i[k(n-1)a - \omega t]} = A\,e^{i[kna - \omega t]}\,e^{-ika} = u_n e^{-ika}$$

$$-m\omega^2 u_n = k_0\left[u_n e^{ika} + u_n e^{-ika} - 2u_n\right]$$

$$-m\omega^2 = k_0\left[e^{ika} + e^{-ika} - 2\right]$$

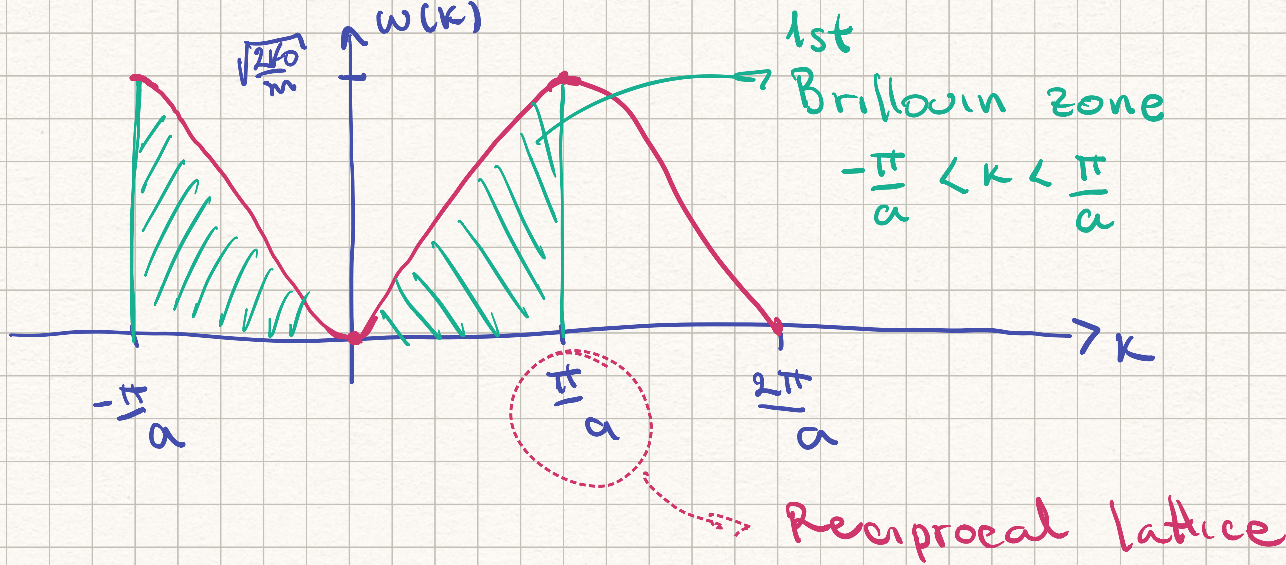
$$= k_0\left[2\cos(ka) - 2\right]$$

$$-m\omega^2 = 2k_0\left[\cos(ka) - 1\right]$$

$$\omega^2 = \frac{2k_0}{m}\left[1 - \cos(ka)\right]$$ using Trig. Id.

$$= \frac{2k_0}{m}\sin^2\left(\frac{ka}{2}\right)$$

$$\boxed{\omega(k) = \sqrt{\frac{2k_0}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$ Dispersion relation



At the edge of the Brillouin zone

$$\frac{d\omega}{dk} = \sqrt{\frac{4K_0}{m}}\,\frac{a}{2}\cos\left(\frac{ka}{2}\right)$$

$$\left.\frac{d\omega}{dk}\right|_{k=\pm\frac{\pi}{a}} = \sqrt{\frac{4K_0}{m}}\,\frac{\pi}{2a}\cos\left(\pm\frac{\pi}{a}\frac{a}{2}\right) = 0$$

At $k = \pm\pi/a$, our solution becomes

$$u_n = Ae^{ikna}e^{-i\omega t} = Ae^{i\pi na/a}e^{-i\omega t} = Ae^{i\pi n}e^{-i\omega t}$$

$$e^{i\pi n} = (e^{i\pi})^n = (-1)^n$$

$$\boxed{u_n = (-1)^n A e^{-i\omega t}}$$

Standing wave of atoms oscillating in opposite phases

The condition $k = \pi/a$ $\qquad k = \frac{2\pi}{\lambda}$

$$\frac{2\pi}{\lambda} = \frac{\pi}{a}$$

λ: wavelenght

$$2a = \lambda$$

Remember Bragg's law: $2d\sin\theta = n\lambda$

$k = \pm\frac{\pi}{a}$ is Bragg's law with $\sin\theta = 1$ and $n = 1$

Group velocity

The velocity of transmission of the wave packet defined

$$v_g = \frac{d\omega}{dk} \qquad \vec{v}_g = \vec{\nabla}_k \, \omega(\vec{k}) \qquad (k_x, k_y, k_z)$$

For our dispersion relation

$$v_g = \sqrt{\frac{\cancel{4K_0}}{m}} \, \frac{a}{2} \cos\left(\frac{ka}{2}\right)$$

$$= \sqrt{\frac{a^2 K_0}{m}} \cos\left(\frac{ka}{2}\right)$$

In the limit of long wavelenghts (small k-vectors)

$$k = \frac{2\pi}{\lambda} << 1$$

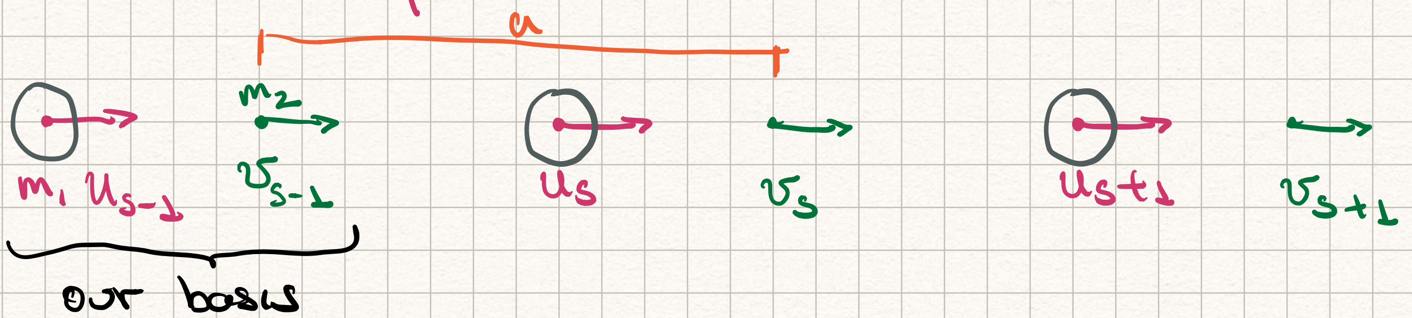
$$\sin\left(\frac{ka}{2}\right) \approx \frac{ka}{2} \qquad \cos\left(\frac{ka}{2}\right) \approx 1$$

The dispersion relation becomes $\omega(k) \approx \sqrt{\frac{a^2 K_0}{m}} \, k$

and the group velocity $v_g = \sqrt{\frac{a^2 K_0}{m}} = \frac{\omega(k)}{k}$

is independent of k

Two atoms per basis



$$m_1 \frac{d^2 u_s}{dt^2} = C\left(v_s + v_{s-1} - 2u_s\right)$$

$$m_2 \frac{d^2 v_s}{dt^2} = C\left(u_{s+1} + u_s - 2v_s\right)$$

we want solution of the type

$$u_s = u\, e^{iska}\, e^{-i\omega t}$$
$$v_s = v\, e^{iska}\, e^{-i\omega t}$$

a: distance between identical planes/atoms

$$-m_1 \omega^2 u = cv(1+e^{-ika}) - 2cu$$
$$-m_2 \omega^2 v = cu(e^{ika}+1) - 2cv$$

Reorganize the eq.

Rewrite in matrix way

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m_1\omega^2 - 2c & c(1+e^{-ika}) \\ c(e^{ika}+1) & m_2\omega^2 - 2c \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\det \begin{pmatrix} m_1\omega^2 - 2c & c(1+e^{-ika}) \\ c(e^{ika}+1) & m_2\omega^2 - 2c \end{pmatrix} = 0$$

$$0 = (m_1\omega^2 - 2c)(m_2\omega^2 - 2c) - c^2(1+e^{-iko})(1+e^{ika})$$
$$= m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 4c^2 - c^2(2+e^{ika}+e^{-ika})$$
$$= m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 4c^2 - c^2[2+2\cos(ka)]$$
$$= m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 4c^2 - 2c^2 - 2c^2\cos(ka)$$
$$= m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 2c^2 - 2c^2\cos(ka)$$
$$0 = m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 2c^2[1-\cos(ka)]$$

$$\omega^2 = \frac{2c(m_1+m_2) \pm \sqrt{4c^2(m_1+m_2)^2 - 8c^2 m_1 m_2[1-\cos(ka)]}}{2m_1m_2}$$

$$4c^2(m_1+m_2)^2 - 8c^2 m_1 m_2[1-\cos(ka)]$$
$$= 4c^2(m_1^2+m_2^2+2m_1m_2) - 8c^2 m_1 m_2 + 8c^2 m_1 m_2 \cos(ka)$$
$$= 4c^2(m_1^2+m_2^2) + 8c^2 m_1 m_2 \cos(ka)$$
$$= 4c^2[m_1^2+m_2^2+2m_1m_2\cos(ka)]$$

$$\omega^2 = \frac{2c\,(m_1+m_2) \pm 2c\sqrt{m_1^2+m_2^2+2m_1m_2\cos(ka)}}{2m_1m_2}$$

$$\omega^2 = \frac{c\,(m_1+m_2) \pm c\sqrt{m_1^2+m_2^2+2m_1m_2\cos(ka)}}{m_1m_2}$$

$$m_1^2+m_2^2+2m_1m_2\cos(ka)+2m_1m_2-2m_1m_2 =$$

$$=(m_1^2+m_2^2+2m_1m_2)+2m_1m_2\left[\cos(ka)-1\right]$$

$$=(m_1+m_2)^2+2m_1m_2\left[\cos(ka)-1\right]$$

$$=(m_1+m_2)^2\left\{1+\frac{2m_1m_2}{(m_1+m_2)^2}\left[\cos(ka)-1\right]\right\}$$