a) The most general solution for a standing wave in a string is

$$Y(x,t) = A\cos(kx + \phi_x)\cos(\omega t + \phi_t)$$

~~Fbw~~ Imposing the boundary conditions

$$Y(0,t) = 0 \quad \Rightarrow \quad A\cos\phi_x = 0 \quad \Rightarrow \quad \phi_x = \pi/2$$

$$Y(L,t) = 0 \quad \Rightarrow \quad A\sin \cancel{\phi} kL = 0 \quad \Rightarrow \quad kL = n\pi$$

Thus, the n-th normal mode of the string is

$$Y_n(x,t) = A_n \sin\left(\frac{n\pi}{L}x\right)\cos(\omega_n t + \phi_t)$$

where

$$\omega_n = n\,\omega_1 = n\,\frac{\pi}{L}\sqrt{\frac{F_T}{\mu}} = n\pi\sqrt{\frac{F_T}{ML}}$$

b) The general formula for the frequency of the n-th mode is

$$\frac{\omega_n}{2\pi} = \frac{n}{2}\sqrt{\frac{F_T}{ML}}$$

The five lowest normal modes are

$$\omega_1 = 2\pi\,\frac{1}{2}\sqrt{\frac{F_T}{ML}} \qquad \omega_3 = 3\omega_1 \qquad \omega_5 = 5\omega_1$$

$$\omega_2 = 2\omega_1 \qquad \omega_4 = 4\omega_1$$

c) Boundary conditions require that the ends of the beads string is held fixed. This gives

$$\omega = 2\omega_0 \sin\left[\frac{m\pi}{2(N+1)}\right] \qquad \omega_0 \equiv \sqrt{\frac{F_T}{\frac{M}{5}\,\frac{L}{6}}} = \sqrt{\frac{30F_T}{ML}}$$

The first five ~~normal modes~~ frequencies are $(N=5)$

$$\omega_1 = 2\pi\frac{\sqrt{120}}{\pi}\sin\left(\frac{\pi}{12}\;\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right) = 0.9\left[2\pi\,\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right]$$

$$\omega_2 = 2\pi\sqrt{\frac{120}{\pi}}\sin\left(\frac{\pi}{6}\;\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right)$$

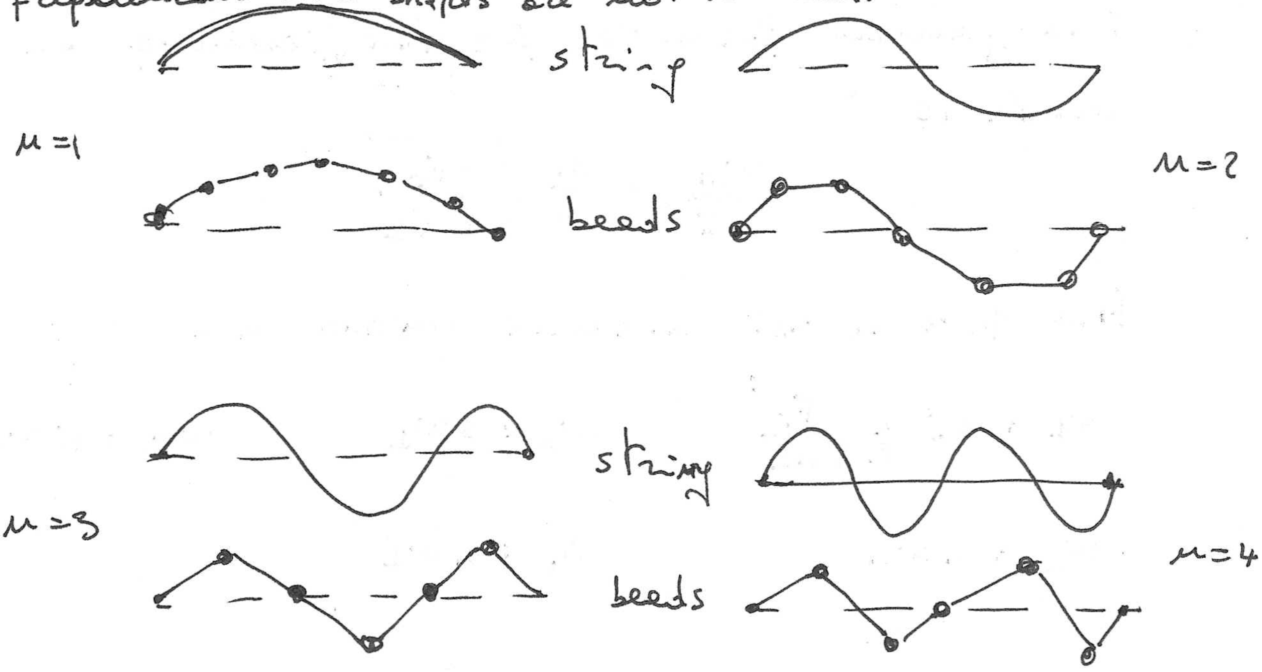
$$\omega_3 = 2\pi\sqrt{\frac{120}{\pi}}\sin\left(\frac{\pi}{4}\;\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right)$$

$$\omega_4 = 2\pi\sqrt{\frac{120}{\pi}}\sin\left(\frac{\pi}{3}\;\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right)$$

$$\omega_5 = 2\pi\sqrt{\frac{120}{\pi}}\sin\left(\frac{5\pi}{12}\;\frac{1}{2}\sqrt{\frac{F_T}{ML}}\right)$$

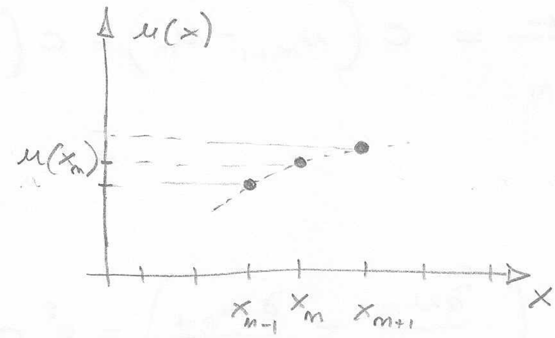
d) e)

Since $N=5$ is still not $N \gg 1$, the normal modes frequencies and shapes are not identical.



# CONNECTION WITH THE THEORY OF ELASTICITY

a) For $ka \ll 1$ ($a \ll \lambda$) the displacements of each ion is small and the chain of N atoms can be approximated with a continuous function $u(x)$




$x_{m+1} = x_m + a$

The relation between $u_m$ and $u_{m+1}$

$$u_{m+1} = u_m e^{ika} \Rightarrow u_{m+1} - u_m = (e^{ika} - 1)\, u_m$$

can be approximate as

$$u_{m+1} - u_m \cong ika\, u_m.$$

$$u_m(x_m,t) = A e^{i(kx_m - \omega t)} \quad ; \quad \frac{\partial}{\partial x} u_m = ik\, u_m$$

$$\Rightarrow u_{m+1} - u_m \cong a \left.\frac{\partial u}{\partial x}\right|_{x=x_m}$$

This is equivalent of expanding $u(x)$ in Taylor series around a generic point $x_m$.

Given the harmonic potential

$$V_{harm} = \frac{1}{2} c \sum_{m=0}^{N} (u_m - u_{m+1})^2$$

the discrete equations of motion

$$F_m = -\frac{\partial V_{harm}}{\partial x_m} = c\left(u_{m+1} - u_m\right) + c\left(u_{m-1} - u_m\right)$$

can be approximated

$$m \frac{\partial^2 u_m}{\partial t^2} \cong a c \left( \frac{\partial u_m}{\partial x} - \frac{\partial u_{m-1}}{\partial x} \right) = a^2 c \; \frac{\frac{\partial u_m}{\partial x} - \frac{\partial u_{m-1}}{\partial x}}{a}$$

$$\simeq a^2 c \frac{\partial^2 u_m}{\partial x^2}$$

$$v^2 \equiv \frac{a^2 C}{m} \qquad \left( \text{for } ka \ll 1 \text{ we found } v_g = \frac{\partial \omega}{\partial k} = \frac{c}{m} a \right)$$

The relation for the speed of sound is equivalent to the usual definition $v^2 = F_T/\mu$, with $\mu = \frac{m}{a}$ and $F_T = Ca$

b) As also shown in Ch. 4 of Kittel, 8th ed., the generalization of the dispersion relation to p nearest ions is

$$\omega_p^2 = \frac{2}{m} \sum_{p>0} C_p \left(1 - \cos pka\right)$$

Writing the harmonic potential with p interacting sites

$$V_{harm} = \sum_{m} \sum_{p>0} \frac{1}{2} C_p \left[ u_m - u_{m+p} \right]^2$$

the equation of motion is

$$m \frac{\partial^2 u_m}{\partial t^2} = - \frac{\partial V_{harm}}{\partial x_m}$$

$$m \frac{\partial^2 u_m}{\partial t^2} = \sum_{p>0} - c_p \left[ 2 u_m - u_{m-p} - u_{m+p} \right].$$

We seek for solutions of the itinerant form

$$u_m(x,t) = e^{i(k x_m - \omega t)}$$

where $k = \frac{2\pi}{a} \frac{n}{N}$ $n$ is an integer and $a$ equilibrium length.

By substitution we have for values lying between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$

$$\omega_p^2 = \frac{2}{m} \sum_{p>0} c_p (1 - \cos pka)$$

For $ka \ll 1$

$$v^2 = \frac{1}{m} \sum_{p>0} p^2 a^2 c_p$$

# ION VIBRATIONS IN METAL

a) The Coulomb force on an ion displaced by a distance $r$ from the center of a sphere of a static electron sea can be calculated using the Gauss law and is

$$F = -e\vec{E}(\vec{r}) = \begin{cases} -\alpha \dfrac{e^2}{R^3}\vec{r} & r \leq R \\ -\alpha \dfrac{e^2}{r^2}\hat{r} & r \geq R \end{cases} \qquad \text{where} \quad \alpha = \begin{cases} 1 & \text{Gauss units} \\ \dfrac{1}{4\pi\epsilon_0} & \text{S.I.} \end{cases}$$

Using the Gauss unit system, for $r \leq R$ the force constant is

$$c = \frac{e^2}{R^3}$$

The oscillation angular frequency (which is similar to the plasma frequency)

$$\omega^2 = \frac{e^2}{MR^3}$$

[See also Ashcroft and Mermin p. 512]

b) For Na

$$M \simeq 4\times10^{-23}\ g \qquad R \cong 2\times10^{-8}\ cm \quad \Rightarrow \quad \omega_0 \cong 3\times10^{13}\ s^{-1}$$

c) The maximum phonon wavevector is of the order of $10^8\ cm^{-1}$. If we suppose that $\omega_0$ is associated with $k_{MAX}$, the speed can be estimated

$$v = \frac{\omega_0}{k_{MAX}} \approx 3\times10^5\ cm/s$$

, which is of the same order of magnitude of the speed of sound in metals.

# WAVE PULSE PROPAGATION

a) By the Fourier theorem, any wave can be viewed as a sum of plane waves. We can solve this problem by taking

$$f(\vec{k}') = \int_{-\infty}^{+\infty} d^3r \left( e^{-i\vec{k}\cdot\vec{r}} e^{-\alpha r^2} \right) e^{i\vec{k}'\cdot\vec{r}}$$

$$= \int_{-\infty}^{+\infty} d^3r \, e^{-\alpha r^2} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}$$

$$= \left(\frac{\pi}{\alpha}\right)^{3/2} e^{-|\vec{k}-\vec{k}'|^2/4\alpha}$$

We have used the result that the Fourier transform of a Gaussian is another Gaussian.

The Fourier transform gives the relative weight of each plane-wave component in the pulse. To find the wave form at ~~t~~ time $t>0$, we can multiply each component plane wave at $t=0$ with the phase factor $e^{i\omega t}$

$$y(\vec{r},t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d^3k' \, f(\vec{k}') \, e^{-i\vec{k}'\cdot\vec{r}} \, e^{i\omega(\vec{k}')t}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} d^3k' \left(\frac{\pi}{\alpha}\right)^{3/2} e^{-|\vec{k}-\vec{k}'|^2/4\alpha} \, e^{-i(\vec{k}'\cdot\vec{r}-\omega(\vec{k}')t)}$$

Expanding $\omega(k)$

$$\omega(\vec{k}') \simeq \omega + \vec{v}_g \cdot \vec{K} ,$$

where we have defined

$$\vec{k}' = \vec{k} + \vec{K} .$$

Then we have

$$\psi(\vec{r},t) = \frac{1}{2\pi}\left(\frac{\pi}{\alpha}\right)^{3/2} \int_{-\infty}^{+\infty} d^3K \, e^{-K^2/4\alpha} \exp\left[-i\left(\vec{K}\cdot\vec{r} - \vec{K}\cdot\vec{v}_g t\right)\right] \exp\left[-i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right]$$

$$= \exp\left[-i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right] e^{-\alpha|\vec{r} - \vec{v}_g t|^2}$$

This expression is the original plane wave modulated by an evelope function centered at a point $\vec{r}$ that moves with velocity $\vec{v}_g$. From this we see that the wave fronts move with the phase velocity $v_\phi = \frac{\omega}{k}$ in the directions of $\vec{k}$, while the evelope of the pulse moves with velocity $v_g = \nabla_{\vec{k}}\,\omega$, which is not necessarily in the same direction as the vector $\vec{k}$.

b) If we expand $\omega(k)$ to the second order,

$$\omega(\vec{k}') \simeq \omega + v_g\,(k' - k) + \frac{1}{2} B\,(k' - k)^2 \qquad B \equiv \frac{\partial^2}{\partial k^2}\omega$$

Let ~~us~~ define

$$h = k' - k$$

and insert the expansion into the equation for $\psi(\vec{r},t)$ above mentioned. (Since we are in 1D we use the variable $x_p$)

$$\psi(x,t) = \frac{1}{2\sqrt{\pi\alpha}} \int_{-\infty}^{+\infty} dh \; e^{-h^2/4\alpha} \exp\left[-i(hx - h v_g t)\right] \exp\left[-i(kx-\omega t)\right] e^{iBh^2t/2}$$

$$= \exp\left[-i(kx-\omega t)\right] \frac{1}{2\sqrt{\pi\alpha}} \int_{-\infty}^{+\infty} dh \; \exp\left[-h^2\left(\frac{1}{4\alpha} - i\frac{Bt}{2}\right)\right] \exp\left[-ih(x-v_g t)\right]$$

$$= \exp\left[-i(kx-\omega t)\right] \frac{1}{\sqrt{1-2i\alpha Bt}} \exp\left[-\frac{i\alpha(x-v_g t)^2}{i+2\alpha Bt}\right]$$

The square of the width of the wave packet will be determined by the real part of the exponential factor in the numerator of the fraction, which takes the form

$$\exp\left[\frac{-i\alpha(x-v_g t)^2}{i+2\alpha Bt}\right] = \exp\left[\frac{\alpha(x-v_g t)^2 - 2i\alpha Bt\alpha(x-v_g t)^2}{(2\alpha Bt)^2+1}\right] =$$

$$= \exp\left[\frac{\alpha(x-v_g t)^2}{(2\alpha Bt)^2+1}\right] \exp\left[\frac{-2i\alpha Bt\alpha(x-v_g t)^2}{(2\alpha Bt)^2+1}\right]$$

The second term is the exponential of a purely imaginary number. The width is given by

$$\left[\frac{(2\alpha Bt)^2+1}{\alpha}\right]^{1/2}.$$

We can see that the wavepacket broadens as a function of time only if ~~the~~ $B \neq 0$.

# SINGULARITY IN DENSITY OF STATES

a) The dispersion relation for a monoatomic linear lattice of N atoms with nearest-neighbor interactions is

$$\omega = \omega_m \left| \sin \frac{1}{2} ka \right| \qquad \omega_m \equiv \sqrt{\frac{4C}{M}}$$

then

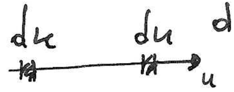
$$k = \frac{2}{a} \sin^{-1} \frac{\omega}{\omega_m}$$

and

$$\frac{dk}{d\omega} = \frac{2}{a} \frac{1}{\sqrt{\omega_m^2 - \omega^2}} .$$

dimension

$$D(\omega)\, d\omega = \left(\frac{L}{2\pi}\right)^d \int_{\text{shell}} d^d k$$




for $d = 1$

$$D(\omega) = \frac{L/\pi}{d\omega/dk} = \frac{2L}{\pi a} \frac{1}{\sqrt{\omega_m^2 - \omega^2}}$$

using eq. (15) in Kittel.

b) The volume of a sphere of radius k in the k-space is

$$\Omega = \frac{4}{3} \pi k^3 = \frac{4}{3} \pi \left[ \frac{\omega_0 - \omega}{A} \right]^{3/2}$$

with

$$k = \left( \frac{\omega_0 - \omega}{A} \right)^{1/2}$$ from the optical phonon branch

and the density of states near $\omega_0$ is

$$D(\omega) = \left(\frac{L}{2\pi}\right)^3 \left| \frac{d\Omega}{dk} \right| = \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A^{3/2}} \sqrt{\omega_0 - \omega} \qquad \text{for } \omega < \omega_0$$