Transport III → Dielectrics and Conductors (a.)

→ Have been exploring matter, using transport as probe.

→ Lesson: Scales and Scale Orderings determine transport properties

→ So far: Dilute gas, weakly ionized gas, Plasma.

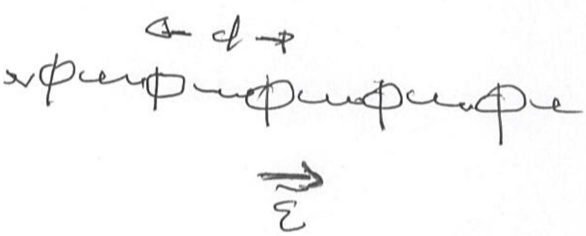
→ Now: Dielectric (crystal), Conductor.

4.) Dielectric / Insulator

→ no free charge, i.e. insulator

→ crystalline solid. Other possibilities are amorphous solid, glass, liquid.

What is it? – Essential Ideas



– Lattice of $\left\{\begin{array}{l}\text{atoms} \\ \text{ions,}\end{array}\right.$ harmonically bound

– small oscillations

– very non-dilute, i.e. $T \ll \bar{U}$

– basic element – lattice wave, phonon (akin chain pblm)

– transport by phonons ...

→ Key issues:

i.) – rms displacement

ii.) – T vs e^2/d ? → vs. gas.

iii.) – mean displacement ?

⇒ anharmonicity

⇒ thermal expansion ↔ $\boxed{\text{asymmetry}}$

iv.) – dispersion characteristics ↔ wave properties ⇒ what sets speed ?

v.) – transport → λ, what is l_{mfp} ?

→ RMS Displacement

– For crystal-as-lattice-of-oscillators, can expect thermal vibrations at

$$T \sim \tfrac{1}{2} M \omega_0^2 \underbrace{\mathcal{E}_T^2}_{\text{displacement}} \qquad M \to \text{mass ion}$$

$$\Rightarrow \mathcal{E}_T \sim \left(T/M\omega_0^2\right)^{1/2} \quad \to \text{vibration amplitude}$$

What is ω_0 ?

$d \equiv$ spacing

$$F \simeq -\nabla U, \quad U = e^2/d + \mathcal{E}$$

What about quantum effects?

$\Rightarrow$ will require $T >$ something

Now $\rightarrow$ vibration frequency ω_0 $\Rightarrow$
so quanta energy $E \sim \hbar\omega_0$

For classical analysis, need:
temp. must exceed energy quantum.

$T > E \sim \hbar\omega_0$ $\qquad \omega_0 = (e^2/Md^3)^{1/2}$

but $1/d^3 \sim n$

$$\Rightarrow \boxed{T > \hbar\,(n_0 e^2/M)^{1/2}} \qquad \omega_0 = (n_0 e^2/M)^{1/2}$$

$$\hbar\,(n_0 e^2/M)^{1/2} \equiv T_{Debye} \leftrightarrow \Theta$$

Defines Debye temperature

$$\Theta = 100 - 500\ K.$$

classical mechanics ok at room temperature!

ii) Now $\boxed{\text{anharmonicity}}$, non-equilibrium etc

- Many important characteristics of crystal depend on anharmonic nature of restoring force (non-linearity)
- ultimately, especially important for

$c(\omega_0)$)

→ Now, consider thermal expansion an equilibrium process.

→ how does $\langle \xi \rangle$ scale with temperature

mean displacement

(i.e. expect crystal to expand).

↳ heat ⟺ expand

Now, if $U = \frac{1}{2} M \omega_0^2 \xi^2$

$$\langle \xi \rangle = 0$$

so require anharmonic correction, i.e. i.e. some asymmetry must enter.. odd term

$$U \cong \frac{1}{2} M \omega_0^2 \xi^2 + g \xi^3$$

$F = -K_{eff} \xi = -K_0 \xi + |\alpha| \xi^2$ for $\xi \ll d$

(for expansion need $g < 0$)

$$U'' \cong M \omega_0^2 + g \xi$$

$> 0 \Rightarrow$ stable.

$U \sim \frac{1}{2} K_{eff} \xi^2$

$K_{eff} = K_0 - |\alpha| \xi$ (weaker spring)

Now, to estimate $|g|$, exploit $\xi < d$ requirement, i.e.

$$U = \underset{①}{\frac{1}{2} M \omega_0^2 \xi^2} + \underset{②}{g \xi^3}$$

should ... for $\xi \sim d$ → "feel"

so

$$g d^3 \sim M\omega_0^2 d^2$$

→ estimated by ordering ΔT
→ effectively scale for d.

$$g \sim M\omega_0^2/d \sim e^2/d^4$$

$$\Rightarrow \quad U \cong M\omega_0^2\left[\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{d}\right]$$

$$\cong M\omega_0^2\varepsilon^2\left[\frac{1}{2} - \frac{\varepsilon}{d}\right]$$

Now, for $\langle \varepsilon \rangle$:

$$\rho(\varepsilon) \cong \exp\left[-\overset{\text{potential}}{U}(\varepsilon)/T\right]$$

~ probability of a certain displacement.
~ must normalize

so

$$\langle \varepsilon \rangle \cong \int d\varepsilon \; \varepsilon \exp\left[-U(\varepsilon)/T\right]$$

Now, for anharmonic contribution small, expand:

$$\exp\left[-\left(\frac{\frac{1}{2}M\omega_0^2\varepsilon^2}{T} - \frac{g\varepsilon^3}{T}\right)\right] \cong \left(1 + \frac{g\varepsilon^3}{T}\right)\exp\left[-\frac{M\omega_0^2\varepsilon^2}{T}\right]$$

so

$$\mathcal{E}_T^3 = T/M\omega_0^2$$

$$\langle \mathcal{E} \rangle = \int \frac{d\mathcal{E}}{\mathcal{E}_T} \frac{|g|\mathcal{E}^4}{T} \exp\left[-\mathcal{E}^2/\mathcal{E}_T^2\right]$$

where:

- normalized ρ
- $\langle \mathcal{E} \rangle > 0 \Rightarrow$ + sign

$\Downarrow$

expansion

$$\langle \mathcal{E} \rangle \sim \frac{|g|}{T}\mathcal{E}_T^4 \sim \frac{g}{T} d^4 \left(\frac{T^2 d^2}{(e^2)^2}\right)$$

$$\mathcal{E}_T \sim d\,(Td/e^2)^{1/2} \ll d$$

$$|g| \sim e^2/d^4$$

$$\langle \mathcal{E} \rangle \sim \frac{\cancel{e^2}}{\cancel{d^4}} \frac{1}{\cancel{T}} \cancel{d^3} \frac{T^{\cancel{2}} \cancel{d}\,\cancel{d}\, d}{(e^2)^{\cancel{2}}}$$

$$\sim \left(\frac{Td}{e^2}\right) d \longrightarrow \text{mean displacement}$$

$$\boxed{\langle \mathcal{E} \rangle \sim d\,\left(Td\right)}$$

$\int$ where

Note:

$$\boxed{\langle \xi \rangle \sim d\,(T d/e^2)}$$ $\Rightarrow$ mean displacement due anharmonicity

so

$$\alpha \sim \frac{1}{d}\frac{d\langle \xi \rangle}{dT} \sim d/e^2 \text{ , indep. } T$$

coefficient of linear expansion

observe:

- $\langle \xi \rangle \ll d$
- $\langle \xi \rangle^2 / \xi_T^2 \sim \dfrac{d^2 (Td/e^2)^2}{(Td/e^2)} \sim d^2\, Td/e^2$

$$\boxed{\langle \xi \rangle \ll \xi_T} \rightarrow \boxed{\xi_{rms} \gg \bar{\xi}}$$

i.e. expansion displacement small relative to thermal displacement amplitude.

Scales:

$$\boxed{\bar{\xi} < \xi_T < \bar{r} \simeq d < l_{mfp} < L}$$

IV.) Dispersion Characteristics

Linear Chains, etc.

→ Here, we explore / study wave/oscillation patterns / properties in crystal in greater depth.

→ point is to understand collective modes of crystal.

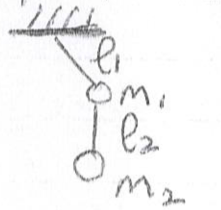
⇒

→ model: linear chain

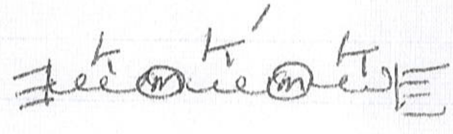
→ acoustic waves
optical mode.

→ Small Oscillations II — { Chains, Strings and the Transition Discrete → Continuous

- previously, considered few-degree-of-freedom systems, i.e.

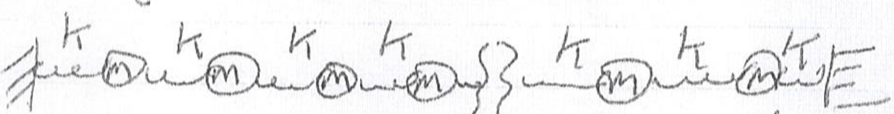


or



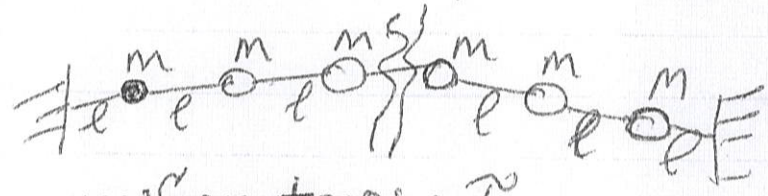
now, consider systems with $N \gg 1$ degrees of freedom, i.e. (separated by ℓ at equilibrium)

i) - linear chain (1-D oscillators)



(application → solid) (identical components) → monatomic

ii) - massless string (loaded)



uniform tension T

uniform { mass m, separation ℓ }

For i)

$$L = \sum_{i=1}^{N} \left(\frac{1}{2} m \dot{x}_i^2 - \left(\frac{1}{2} k (x_i - x_{i-1})^2 + \underbrace{\frac{1}{2} k (x_{i+1} - x_i)^2}_{\frac{1}{2}k(x_{i+1}-x_i)^2} \right) \right)$$

$$\begin{cases} x_0 \equiv 0 \\ x_{N+1} \equiv 0 \end{cases}$$

or simply
$$L = \sum_{i=1}^{N}\left(\frac{1}{2}m\dot{x}_i^2 - \frac{k}{2}(x_{i+1}-x_i)^2\right)$$
{Compressional Modes

For ii.),
$$L = \sum_{i=1}\left(\frac{1}{2}m\dot{y}_i^2 - \frac{\tau}{2\ell}(y_{i+1}-y_i)^2\right)$$
{transverse modes

≈ identical systems.

∴ hereafter, focus on i.)

motivations for i.)
- monatomic chain is simplest example of elastic wave in solid
- step toward continuous system i.e. now discrete → masses separated by ℓ

Proceeding:

$$m\ddot{x}_i - k\left[(x_{i+1}-x_i) + (x_{i-1}-x_i)\right] = 0$$

$$\ddot{x}_i + \frac{k}{m}\left[2x_i - (x_{i+1}+x_{i-1})\right] = 0$$

$$x_i = \hat{x}_i e^{-i\omega t}$$

$$\left(\frac{2k}{m} - \omega^2\right)\hat{X}_i - \frac{k}{m}\left(\hat{X}_{i-1} + \hat{X}_{i+1}\right) = 0$$

For eigenvalues, $\det \underline{A} = 0$

$$\underline{A} = \begin{vmatrix} \frac{2k}{m} - \omega^2 & -k/m & & & \\ -k/m & \frac{2k}{m} - \omega^2 & -k/m & & 0 \\ & -k/m & \frac{2k}{m} - \omega^2 & -k/m & \\ 0 & & -k/m & \frac{2k}{m} - \omega^2 & -k/m \end{vmatrix}$$

i.e. A tri-diagonal.

Now, taking masses separated by ℓ, take

$$\hat{X}_n \sim e^{i(n\ell)\alpha}$$

wave-vector

$\left\{\begin{array}{l} n \equiv \text{bead \#} \\ \alpha \equiv \text{wave \#} \\ \ell \equiv \underline{\text{spacing}} \end{array}\right.$ ℓ ℓ

$$\Rightarrow \left(\frac{2k}{m} - \omega^2\right)e^{i[i\,\ell\alpha]} - \frac{k}{m}\left(e^{i[(i+1)\,\ell\alpha]} + e^{i[(i-1)\,\ell\alpha]}\right) = 0$$

careful i's.

$$\therefore \left(\frac{2k}{m} - \omega^2\right) - \frac{2k}{m}\cos\left[(\alpha\ell)\right] = 0$$

Note: says $\hat{X}_{n+m} = e^{im\ell\alpha}\,\hat{X}_n$

phase displ $\sim m\ell$

Sol/ $$\omega^2 = \frac{2k}{m}(2)\left[\frac{1-\cos(\alpha l)}{2}\right]$$

$$= \frac{4k}{m}\sin^2\left(\frac{\alpha l}{2}\right)$$

$$\Rightarrow \boxed{\omega^2 = \frac{4k}{m}\sin^2(\alpha l/2)}$$

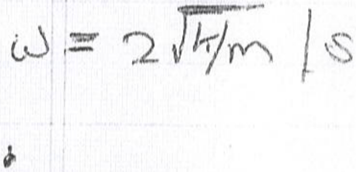
$$\omega = 2\sqrt{k/m}\,|\sin \alpha l/2|$$

Note:

① − $\omega = \omega_{max}\,|\sin l\alpha/2|$; $\omega_{max}^2 = 4k/m$

$$\begin{cases} \omega(\alpha) = \omega(-\alpha) \\ \alpha' = \alpha + 2\pi/l \quad \text{leaves } \omega \text{ invariant} \end{cases}$$

i.e. need only define α on $[-\pi/l, \pi/l]$



& repeats

i.e. { First Brillouin Zone, only needed

② − for $l\alpha/2 \ll 1$

i.e. wavelength $\alpha^{-1} >>$ bead spacing l

→ continuum limit

then $\omega = \sqrt{k/m}\, \ell\, \alpha$

$= \alpha \left[\ell \sqrt{k/m} \right]$

akin to acoustic wave

$$\omega = k\, c_o \qquad \begin{cases} k \leftrightarrow \alpha \\ c_o \leftrightarrow \ell\sqrt{k/m} \\ \dfrac{\chi_p}{\rho} \leftrightarrow \dfrac{\ell^2 k}{m} \end{cases}$$

$\ell^2 k \rightarrow$ stored elastic energy (springiness)

$m \rightarrow$ inertia

③ – observe maximum frequency propagated is:

$\omega^2 = \omega_{max}^2 = 4k/m$ i.e. $\begin{cases} \omega^2 > \omega_{max}^2 & \text{not propagated} \\ \omega^2 < \omega_{max}^2 & \text{propagated} \end{cases}$

$\begin{cases} \text{Chain acts as low-pass filter} \\ \text{Higher frequencies evanescent!} \end{cases}$

④ – for propagation structure;

$\omega = 2\sqrt{k/m}\, \left[\sin(\alpha \ell/2) \right]$

$V_{gr} = d\omega/d\alpha = \ell\sqrt{k/m}\, \cos(\alpha \ell/2)$

i.e. $V_{gr} = \ell\sqrt{k/m} \sim c_{s\,eff}$ for $\alpha \ell \ll 1$
(a la' sound)

but $\lim_{\alpha \to \pi/\ell} v_{gr} = \ell\sqrt{k/m}\cos(\pi/2) \to 0$

i.e. modes at edge of Brillouin zone non - propagating

modes in middle of zone propagate at acoustic speed.

Can also observe that:

$$x_{i+1} + x_{i-1} - 2x_i = e^{i[\alpha\ell i]}\left(e^{i\alpha\ell} + e^{-i\alpha\ell} - 2\right)$$

$$= 2e^{i[i\alpha\ell]}\left(\cos\alpha\ell - 1\right)$$

so $\cos\alpha\ell / 1 \sim$ ratio of $(x_{i+1} + x_{i-1})/2x_i$

$\sim$ mean phase ratio

so $\alpha\ell \ll 1$ (in zone) $\Rightarrow$ neighbors on chain vibrate in phase $\to$ propagation

$\cos = 1$

$\alpha\ell \sim \pi$ (zone boundary) $\Rightarrow$ neighbors on chain vibrate out of phase $\to$ no propagation

$\cos = -1$

What if?:

→ Boundary Conditions

Can distinguish 2 cases — periodic B.C.'s / fixed end B.C.'s.

1) Periodic B.C.'s

Now, $x_i = Ae^{i[i \ell\alpha]}$

notational clarity ⇒ $x_n = Ae^{i[n\ell\alpha]}$

$1 < n < N.$

For periodic B.C.'s,

$x_n = x_{n+N} \Rightarrow e^{iN\ell\alpha} = 1$ → mode indx

$\therefore \quad N\ell\alpha = 2\pi p$

$$\Rightarrow \boxed{\alpha = \frac{2\pi p}{N\ell}} \qquad p = \begin{cases} 0, \pm 1, \ldots \pm \frac{1}{2}(N-1) & N \text{ odd} \\ 0, \pm 1, \ldots \frac{1}{2}N & N \text{ even} \end{cases}$$

Note: guarantees N normal modes.

2, Fixed end B.C.'s : $\left.\begin{array}{l} X_0 = 0 \\ X_{N+1} = 0 \end{array}\right\}$ guarantees ends fixed

$$\Rightarrow \quad X_0 = X_{N+1} = 0$$

$$X_n = Ae^{in\alpha\ell} + Be^{-in\alpha\ell}$$

$$= A\sin(n\ell\alpha) + B\cos(n\ell\alpha)$$

$$B = 0 \rightarrow n = 0 \checkmark$$

$$(N+1)\alpha\ell = p\pi \quad ; \quad p = 1, \ldots N$$

mode index

$$\Rightarrow \quad \boxed{\alpha_p = p\pi/\ell(N+1)}$$

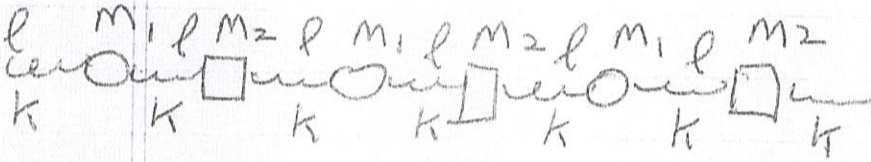
{acts to quantize k

$$\therefore \quad X_n(t) = A_n \sin\left(\frac{n\cancel{\alpha}\ell p\pi}{\cancel{\alpha}\ell(N+1)}\right) e^{-i\omega_p t}$$

$$\text{where} \quad \omega_p^2 = \frac{4k}{m}\sin^2\left(\frac{p\pi\cancel{\ell}}{2\cancel{\ell}(N+1)}\right)$$

– Diatomic Chain

→ consider slightly richer toy model, namely the diatomic chain



{un-equal masses!

then, no loss of generality to associate

$$m_1 \to x_{2n} \quad \text{(evens)}$$
$$m_2 \to x_{2n+1} \quad \text{(odds)}$$

> positions

∴ can immediately write dynamical equations

$$m_1 \ddot{x}_{2n} = -k\left(2x_{2n} - x_{2n-1} - x_{2n+1}\right)$$

$$m_2 \ddot{x}_{2n+1} = -k\left(2x_{2n+1} - x_{2n} - x_{2n+2}\right)$$

solution of form:

$$x_{2n} = A e^{i n \ell \alpha} e^{-i\omega t} \qquad \text{(evens)}$$

$$x_{2n+1} = B e^{i(2n+1)\ell\alpha} e^{-i\omega t} \qquad \text{(odds)}$$

(consider one mass → d, co)

$$-m_1\omega^2 A = -k\left(2A - \left(e^{il\alpha} + e^{-il\alpha}\right)B\right)$$

$$-m_2\omega^2 B = -k\left(2B - \left(e^{il\alpha} + e^{-il\alpha}\right)A\right)$$

$\Rightarrow$

$$(-m_1\omega^2 + 2k)A - k(2\cos l\alpha)\ B = 0$$

$$(-2k\cos l\alpha)A + (-m_2\omega^2 + 2k)B = 0$$

$\therefore$

$$\boxed{(\omega^2 - 2k/m_1)(\omega^2 - 2k/m_2) - \frac{4k^2}{m_1 m_2}\cos^2 l\alpha = 0}$$

$\Rightarrow$ dispersion relation:

$$\omega^2 = k\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm k\left\{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2(\alpha l)}{m_1 m_2}\right\}^{1/2}$$

$1/\mu \equiv 1/m_1 + 1/m_2$ $\Rightarrow$ reduced mass, as usual.

$$\omega^2 = k/\mu \pm k/\mu\left\{1 - \frac{4\mu^2}{m_1 m_2}\sin^2(\alpha l)\right\}^{1/2}$$

$\therefore$ dispersion relation:

$$\boxed{\omega^2 = \frac{k}{\mu}\left\{1 \pm 1\left\{1 - \frac{4\mu^2}{m_1 m_2}\sin^2(\alpha l)\right\}^{1/2}\right\}}$$

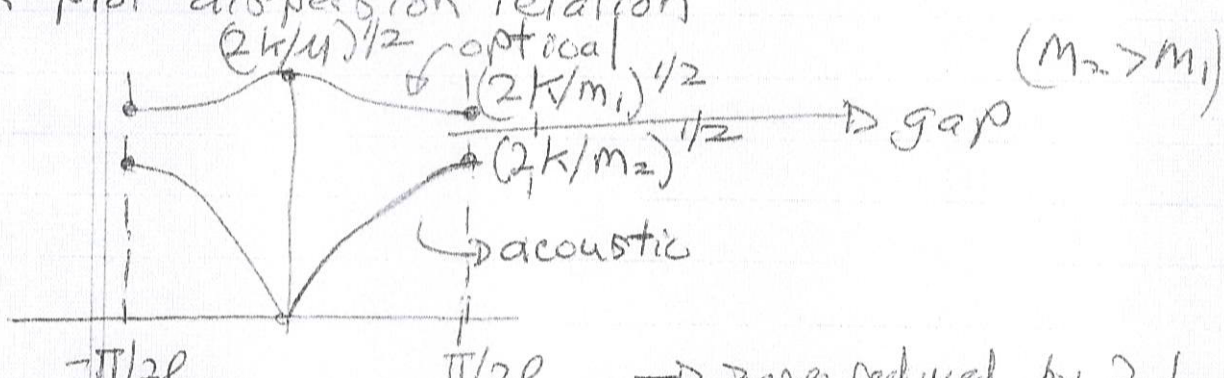
Can immediately observe:

→ system supports 2 modes

- low frequency → "acoustic" mode (a.k.a. sound)
  → analogous to mode of monatomic chain

- high frequency → "optical" mode (a.k.a. plasma) (vibration)
  → new

Can plot dispersion relation



→ zone reduced by 2! (scale)

Note: - acoustic mode $\omega \sim \alpha \left(\frac{k\ell^2}{m_2 + m_1} \right)^{1/2}$

$\sim k c_{s\,eff}$

as $k\ell \to 0$ ⇒ mass neighbors vibrate <u>in phase</u>

$x_n = x_{n+1}$

solid → phonon ($\omega = kc$)

optical mode $\quad \omega \sim (2k/\mu)^{1/2}$

as $kl \to 0$; $m_1 x_n + m_2 x_{n+1} = 0$

i.e. neighboring masses vibrate <u>out</u> of phase, weighted by masses

solid $\to$ analogous collective mode is EM wave

$\omega^2 = \omega_{pe}^2 + c^2 k^2$ or plasmon

$\omega^2 = \omega_{pe}^2 + k^2 v_{Te}^2$

i.e. $k \to 0$, frequency constant!

$\to$ Note <u>gap</u> $\to$ no propagation for

$$(2k/m_2)^{1/2} < \omega < (2k/m_1)^{1/2}$$

$\to$ consequence of fact

phonon $\leftrightarrow$ inertia of heavy mass

optical $\leftrightarrow$ inertia of light mass (in ω_p^2)

→ Transition to Continuum

To recover continuum $\left\{ \underline{\text{i.e.}} \begin{array}{l} \text{elastic medium} \\ \text{massive string} \end{array} \right.$

take $\begin{array}{l} N \to \infty \\ \ell \to 0 \end{array}$ $\underline{\underline{\text{with}}}$ $\underline{\underline{\text{constant}}}$ $\begin{array}{l} L = (N+1)\ell \\ \left\{ \begin{array}{l} \frac{m}{\ell} = \mu = \text{const.} \\ K\ell = \mathcal{K} = \text{const.} \end{array} \right. \end{array}$

Note: "$N \to \infty$" means $N > p$, for all modes p.

Then;

$$\omega_p^2 = \frac{4K}{m} \sin^2\left(\frac{p\pi}{2(N+1)}\right)$$

$$\cong \frac{4K}{m}\left(\frac{p\pi}{2(N+1)}\right)^2$$

$$= \frac{(p\pi)^2}{((N+1)\ell)^2} \frac{K\ell^2}{m}$$

$$= \left(\frac{p\pi}{L}\right)^2 \left(\frac{\mathcal{K}}{\mu}\right) = \left(\frac{p\pi}{L}\right)^2 c_s^2$$

$$c_s^2 = K\ell^2/m = (K\ell)\,\ell/m = \mathcal{K}/\mu$$

$\to \quad \omega^2 = k^2 c_s^2 \quad ; \quad \begin{array}{l} c_s^2 = \mathcal{K}/\mu \\ k = p\pi/L \end{array}$

Short Form – Linear Chain

Have oscillation equation:

$$\boxed{M\ddot{\xi}_i + K\left[2\xi_i - (\xi_{i+1} + \xi_{i-1})\right] = 0}$$

$K = M\omega_0^2 = e^2/d^3$ → spring const.
set by electrostatics
⇒ stiffness.

Now, spacing is d, so:

$$2\xi_i - (\xi_{i+1} + \xi_{i-1}) = \xi_i - \xi_{i+1} + \xi_i - \xi_{i-1}$$

but $\xi_{i+1} = \xi_i(x+d)$, for d small ⇒
displ. at position
i.e. $Kd \ll 1$
considered K.

$$\cong \underbrace{\xi_i + d\frac{d\xi_i}{dx} + \frac{d^2}{2}\frac{d^2\xi_i}{dx^2}}_{\text{expand!}}$$

so

$$M\ddot{\xi}_i - d^2K\, d^2\xi_i/dx^2 = 0$$

or

Clarity $k \to C = e^2/d^3$

$\downarrow$ spring const.

Sound / acoustic wave speed:

$$\boxed{\begin{aligned} c_s^2 &= d^2 k/M = d^2 C/M \\ &= e^2/dM \end{aligned}}$$

$c_s^2 \sim dP/d\rho \sim T/M$ i.e. $\rho \frac{\partial \tilde{v}}{\partial t} = -c_s^2 \nabla \tilde{\rho}$

$\partial \tilde{\rho} = -\rho_0 \nabla \cdot \tilde{v}$

here energy density electrostatic, not thermal, so

$c_s^2 \sim e^2/dM \gg T/M$, as $e^2/d > T$ here.

→ speed sound larger in crystal, as crystal is stiffer i.e. stores more energy

(n.b. at fixed temperature)

→ highest frequency:

$$\omega_{max} \sim \frac{1}{d} c_s \sim \left(e^2/Md^3\right)^{1/2}$$

→ in diatomic chain, optical mode has $v_{gr} \sim 0$. So phonons carry energy of lattice vibration.

→ $c_s \sim \left(e^2/dM\right)^{1/2}$ is key speed for transport in crystal.