# Phonons

P715

# Phonons

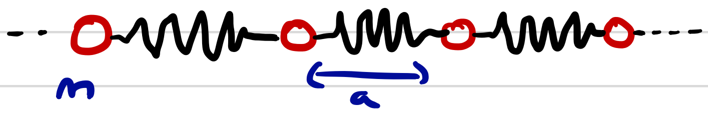
- Atoms form crystal but aren't fully fixed in place.

collective vibrations = phonons.

- A lot of the physics at play here can be understood in 1d, using classical physics.

## (I) Classical phonons in 1d

### (a) Monoatomic chain




$u_n = x_n - na$, small

atom: $x_n(t)$, equilibrium location: $x_n^{eq} = n a$

Potential: $V(x_{n+1} - x_n) \longrightarrow V(u_{n+1} - u_n) = Cst + \frac{V''(a)}{2}(u_{n+1} - u_n)^2 + \ldots$

$$V'\big|_{x_{eq}} = 0$$

$\lambda = V''\big|_{eq}$ spring constant

$$\Rightarrow \mathcal{H} = \sum_n \frac{p_n^2}{2m} + \frac{\lambda}{2}\sum_n (u_{n+1} - u_n)^2$$

Equations of motion: $m\ddot{u}_n = -\lambda(u_n - u_{n-1}) - \lambda(u_n - u_{n+1})$

Look for solutions: $u_n(t) = A\, e^{-i\omega_k t + ikna}$

$k \to k + \frac{2\pi}{a}$, we can take $k \in BZ = [-\pi/a, \pi/a)$

. As in the previous chapters: $u_{N+1} = u_1$

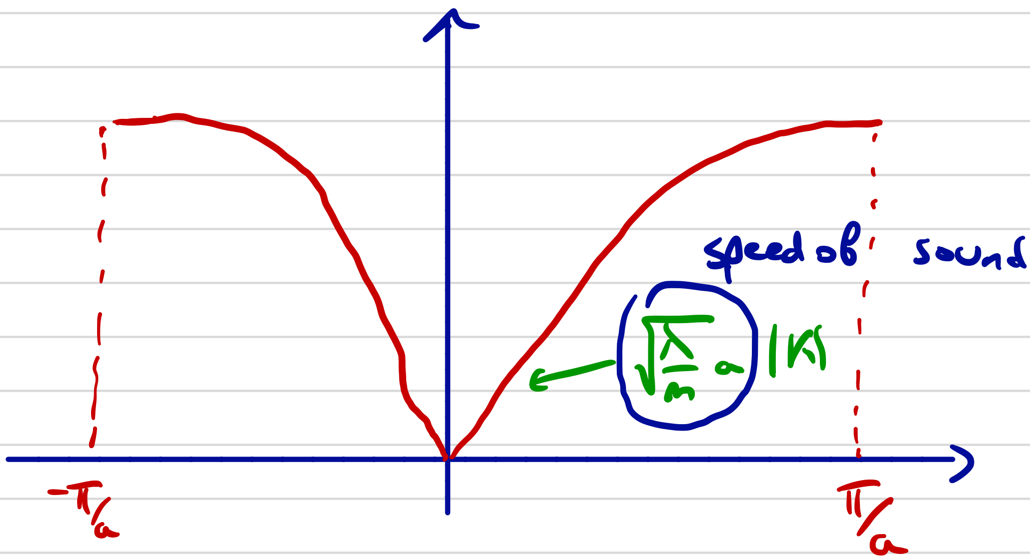
$$\Rightarrow \quad e^{iKNa} = 1 \quad \Rightarrow \quad K = \frac{2\pi}{Na} n \,; \quad n \text{ integer.}$$

(as before: $K$ quantized since $N$ is finite, and $\in BZ$ because of $a$. $K_{max} \sim \frac{1}{a}$ : cf. 1st chapter)

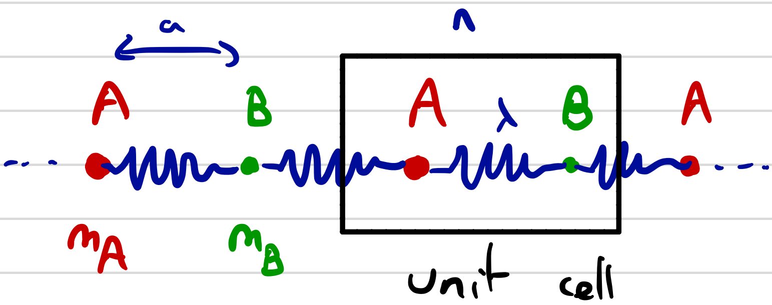
. Plug in e.o.m: $-m\omega^2 = -\lambda(2 - 2\cos Ka)$

$$\Rightarrow \quad m\omega^2 = \lambda\, 4 \sin^2\left(\frac{Ka}{2}\right)$$

$$\Rightarrow \quad \boxed{\omega_K = 2\sqrt{\frac{\lambda}{m}} \left|\sin\left(\frac{Ka}{2}\right)\right|}$$




## ⓑ Diatomic chain



$$m_A \ddot{u}_n^A = -\lambda(u_n^A - u_{n-1}^B) - \lambda(u_n^A - u_n^B)$$
$$= -\lambda\left(2u_n^A - u_{n-1}^B - u_n^B\right)$$
$$m_B \ddot{u}_n^B = -\lambda\left(2u_n^B - u_n^A - u_{n+1}^A\right)$$

<u>Ansatz:</u>
$$u_n^A = C_A e^{-i\omega t + 2iKna}$$
$$u_n^B = C_B e^{-i\omega t + 2iKna}$$

$a' = 2a$. $\quad K \to K + \pi/a \quad \longrightarrow \quad K \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$

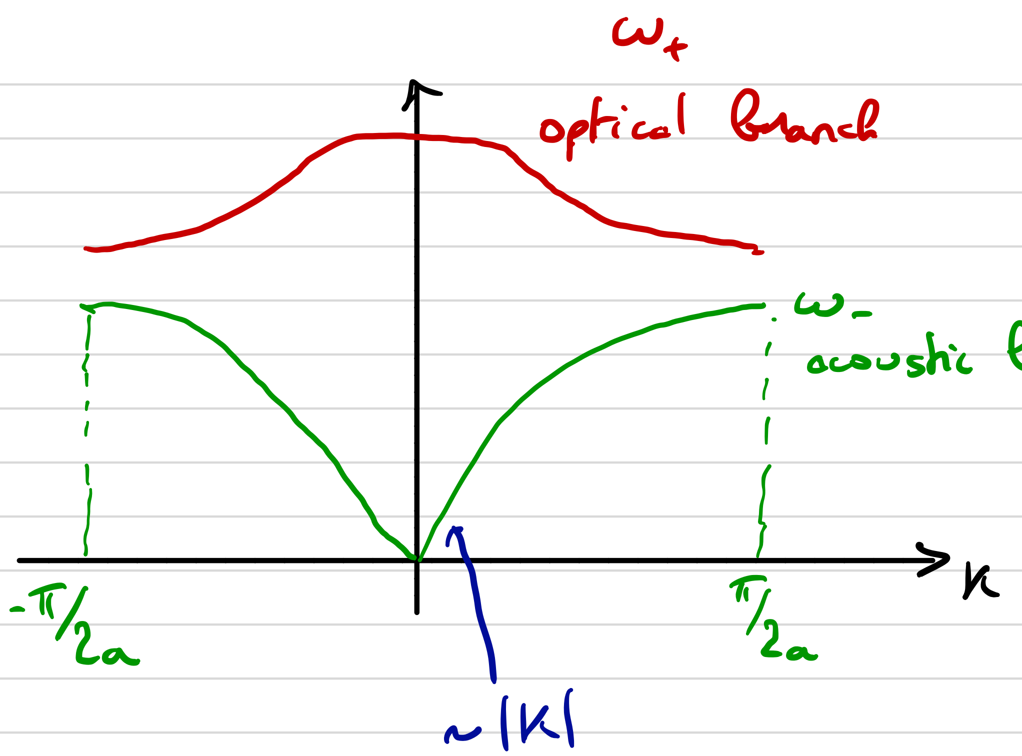
( system invariant under translation by $a' = 2a$ !)

we get:
$$m_A C_A \omega^2 = \lambda\left(2C_A - (1+e^{-2iKa})C_B\right)$$
$$m_B C_B \omega^2 = \lambda\left(2C_B - (1+e^{+2iKa})C_A\right)$$

$$\Rightarrow \underbrace{\begin{pmatrix} m_A\omega^2 - 2\lambda & \lambda(1+e^{-2iKa}) \\ \lambda(1+e^{+2iKa}) & m_B\omega^2 - 2\lambda \end{pmatrix}}_{\hat{M}} \begin{pmatrix} C_A \\ C_B \end{pmatrix} = 0$$

$\hat{M}$ ; $\quad \operatorname{Det}\hat{M} = 0$

$$\boxed{\omega_\pm^2 = \frac{(m_A+m_B)\lambda}{m_A m_B} \pm \frac{\lambda}{m_A m_B}\sqrt{m_A^2 + m_B^2 + 2m_A m_B \cos 2aK}}$$




$\updownarrow$ gap, vanishes for $m_A = m_B$

$$\begin{pmatrix} -2\lambda & 2\lambda \\ 2\lambda & -2\lambda \end{pmatrix}$$

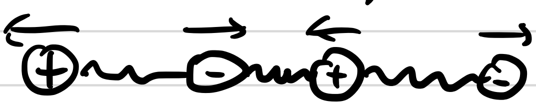
- Eigenvectors in limit $k \to 0$: $\omega_- = 0$: $\hat{M} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0$

  $\Rightarrow \; c_A = c_B$ (in phase)

$$\omega_+^2 = 2\lambda \frac{(m_A + m_B)}{m_A m_B} \quad \Rightarrow \quad \hat{M} = \begin{pmatrix} 2\lambda m_A/m_B & 2\lambda \\ 2\lambda & 2\lambda m_A/m_B \end{pmatrix}$$

eigenvector: $\begin{pmatrix} m_B \\ -m_A \end{pmatrix}$ out of phase.

Name optical: typically A and B have opposite charges.



couples to light

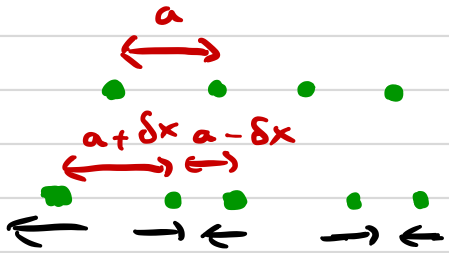
- Those conclusions carry over to $d > 1$.

  linear, acoustic branches: $\omega \sim k$ ("sound waves")

  optical branches: $\omega \underset{k\to 0}{\sim}$ constant

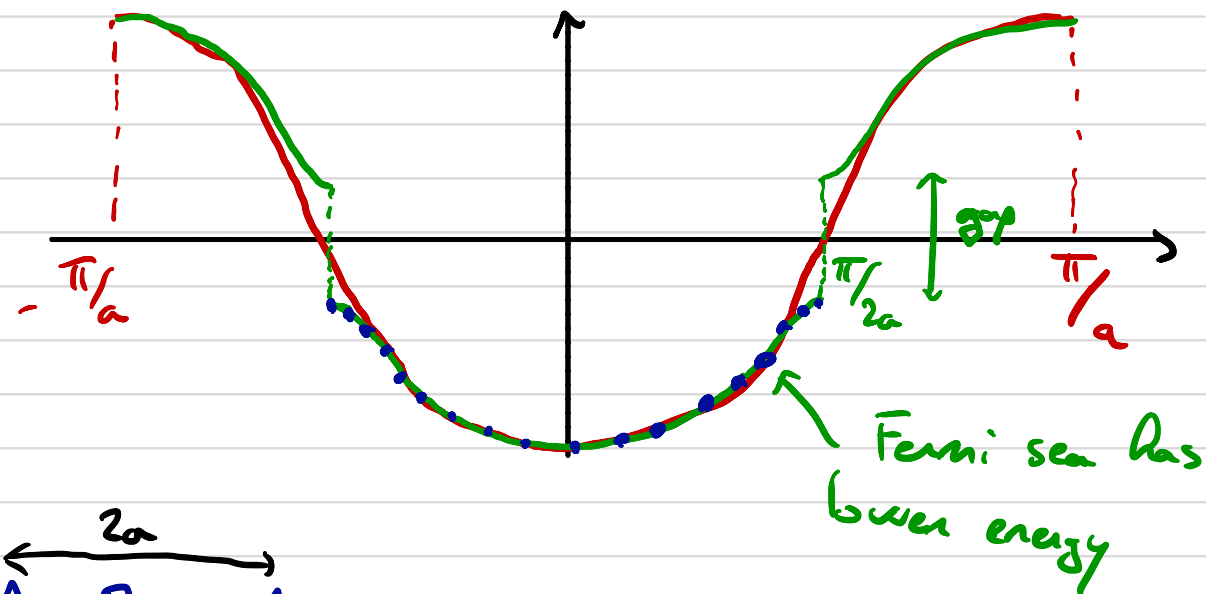
## (c) Peierls transition

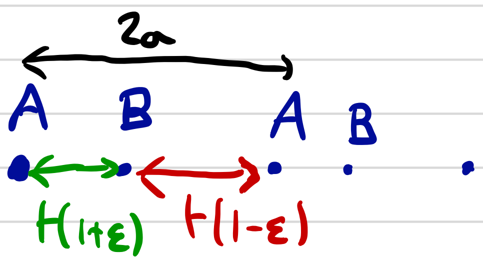
. Spontaneous Dimerization :




. Clearly, this costs an extensive amount of elastic energy : $U/N \sim \frac{1}{2} k (\delta x)^2$ : not favorable.

BUT : contribution from $e^-$ :




New BZ: $\pi/2a$

$$E\phi_n^A = -t(1-\varepsilon)\phi_{n-1}^B - t(1+\varepsilon)\phi_n^B$$
$$E\phi_n^B = -t(1+\varepsilon)\phi_n^A - t(1-\varepsilon)\phi_{n+1}^A$$

$$\begin{pmatrix} \phi_n^A \\ \phi_n^B \end{pmatrix} = \frac{e^{2ikna}}{\sqrt{N}} \begin{pmatrix} C_A \\ C_B \end{pmatrix}$$

$$\begin{pmatrix} 0 & -t(1+\varepsilon) - t(1-\varepsilon)e^{-2iKa} \\ -t(1-\varepsilon) - t(1+\varepsilon)e^{+2iKa} & 0 \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix}$$

$$\Rightarrow \quad E_K^{\pm} = \pm \left| t(1+\varepsilon) + t(1-\varepsilon)e^{-2iKa} \right|$$
$$= \pm 2t \sqrt{\varepsilon^2 + (1-\varepsilon^2)\cos^2 Ka} \qquad (t>0)$$

(2 bands, as expected. if $\varepsilon = 0$: $\varepsilon = -2t \cos K$ "folded" in $\left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$)

Fermi sea: fill $E^-$, energy:

$$E = -2t \sum_{K \in BZ} \sqrt{\varepsilon^2 + (1-\varepsilon^2)\cos^2 Ka}$$
$$= -2tL \int_{-\pi/2a}^{\pi/2a} \frac{dK}{2\pi} \sqrt{\varepsilon^2 + (1-\varepsilon^2)\cos^2 Ka}$$

Set $qa = \frac{\pi}{2} - Ka$ (edge of BZ):

$$\delta E_{e^-} = E(\varepsilon) - E(\varepsilon = 0) = -4tL \int_0^{\pi/2a} \frac{dq}{2\pi} \left( \sqrt{\varepsilon^2 + (1-\varepsilon^2)\sin^2 qa} - \sin qa \right)$$

$\sin qa \simeq qa$ for $q < \Lambda$ cutoff

ignore $q \gtrsim \Lambda$

$$\delta E_{e^-} = -4tL\left[\underbrace{\left(\int_0^{\varepsilon}\frac{dq}{2\pi}\left(\sqrt{\varepsilon^2+(1-\varepsilon^2)q^2a^2}-qa\right)\right)}_{\mathcal{O}(\varepsilon^2)} + \int_{\varepsilon}^{\Lambda}\frac{dq}{2\pi}\underbrace{\left(\sqrt{\varepsilon^2+(1-\varepsilon^2)q^2a^2}-qa\right)}_{\text{Taylor expand: } \underset{\varepsilon \text{ small}}{\simeq} +\frac{\varepsilon^2}{2aq}-\frac{aq\varepsilon^2}{2}+\mathcal{O}(\varepsilon^4)}\right]$$

$$= -4tL\left(\mathcal{O}(\varepsilon^2)+\int_{\varepsilon}^{\Lambda}\frac{dq}{2\pi}\frac{\varepsilon^2}{2aq}\right)$$

$$= -4tL\left(\mathcal{O}(\varepsilon^2)+\frac{\varepsilon^2}{4\pi a}\log\frac{\Lambda}{\varepsilon}\right)$$

$L = Na \quad \Rightarrow \quad \dfrac{\delta E_{e^-}}{N} = \left(\#\,\varepsilon^2 + \varepsilon^2\log\varepsilon\right)$

$$\underset{\varepsilon \text{ small}}{\sim} \varepsilon^2\log\varepsilon \quad (\text{negative})$$

- Compare to $\dfrac{U}{N} \sim \varepsilon^2$ (elastic energy, positive)

$\Rightarrow$ Spontaneous dimerization at $T=0$ (for half filled band)

(→ insulator, energy of $e^-$ "wins").

- At finite $T$: Order destroyed by entropy.

No dimerization

## II Quantization (Focus on monoatomic chain, generalization straightforward)

$$\mathcal{H} = \sum_n \frac{p_n^2}{2m} + \frac{\lambda}{2}\sum_n (u_n - u_{n-1})^2$$

Modes expansion: $\omega_j = 2\sqrt{\frac{\lambda}{m}}\left|\sin\left(\frac{k_j a}{2}\right)\right|$ ; $k_j = \frac{2\pi}{Na} j$

(Classical so far)

$$u_n(t) = \underset{\substack{\uparrow \\ j=0 \text{ mode: C.O.M. motion}}}{x_0(t)} + \sum_{j\neq 0}\left[\alpha_j e^{-i(\omega_j t - k_j n a)} + \underset{\substack{\uparrow \\ \text{make } u_n \in \mathbb{R}}}{h.c.}\right]$$

denote: $\alpha_j^+ = \alpha_j^*$

$$p_n(t) = m\dot{u}_n(t) = \frac{P_0(t)}{N} + \sum_{j\neq 0} m\left[-i\omega_j \alpha_j e^{-i(\omega_j t - k_j n a)} + i\omega_j \alpha_j^+ e^{+i(\dots)}\right]$$

$$(P_0 = M\dot{x}_0 = Nm\dot{x}_0)$$

Quantization : $u_n \longrightarrow \hat{u}_n$ $\qquad [\hat{u}_n, \hat{p}_m] = i\hbar\,\delta_{nm}$

$p_n \longrightarrow \hat{p}_n$

$\alpha_j$ and $\alpha_j^+$ are also operators.

$$\hat{H} = \sum_n \frac{\hat{p}_n}{2m} + \frac{\lambda}{2}\sum_n (\hat{u}_n - \hat{u}_{n-1})^2$$

We have: $$\frac{1}{N}\sum_n e^{+ik_j n a} = \frac{1}{N}\underbrace{\sum_{n=0}^{N-1} e^{i2\pi \frac{jn}{N}}}_{\frac{1 - e^{i2\pi j}}{1 - e^{+i2\pi \frac{j}{N}}}} = \delta_{j,0}$$

$$\Rightarrow \hat{X}_0 = \frac{1}{N}\sum_n \hat{u}_n \quad \text{and} \quad \hat{P}_0 = \sum_n \hat{p}_n$$

$$\Rightarrow [\hat{X}_0, \hat{P}_0] = \frac{1}{N}\sum_{n,m} \underbrace{[\hat{u}_n, \hat{p}_m]}_{i\hbar\delta_{n,m}} = i\hbar$$

. Similarly: $\displaystyle \frac{1}{N}\sum_{n=0}^{N-1} \hat{u}_n e^{-ik_j na} = \hat{\alpha}_j + \hat{\alpha}_{-j}^\dagger$

$$\frac{1}{N}\sum_n \hat{p}_n e^{-ik_j na} = -im\omega_j(\hat{\alpha}_j - \hat{\alpha}_{-j}^\dagger)$$

$\omega_{-j} = \omega_j$

$$\Rightarrow \quad \hat{\alpha}_j = \frac{1}{2m\omega_j N}\sum_n e^{-ik_j na}(m\omega_j \hat{u}_n + i\hat{p}_n)$$

$$\hat{\alpha}_j^\dagger = \frac{1}{2m\omega_j N}\sum_n e^{+ik_j na}(m\omega_j \hat{u}_n - i\hat{p}_n)$$

. Now with some effort, we can get:

$$[\hat{\alpha}_j, \hat{\alpha}_{j'}] = [\hat{\alpha}_j^\dagger, \hat{\alpha}_{j'}^\dagger] = 0$$

$$[\hat{\alpha}_j, \hat{\alpha}_{j'}^\dagger] = \frac{\hbar}{2m\omega_j N}\delta_{j,j'}$$

Suggests rescaling: $\displaystyle \hat{\alpha}_j = \sqrt{\frac{\hbar}{2m\omega_j N}}\,\hat{a}_j$

$$\Rightarrow \boxed{[\hat{a}_j, \hat{a}_{j'}^\dagger] = \delta_{jj'}} \quad \text{(Bosons)}$$

(remember: $j$ labels $k_j = \frac{2\pi}{Na} j$)

Plugging in $\hat{H}$, we get:

decoupled harmonic oscillators

$$\boxed{\hat{H} = \frac{\hat{P}_0^2}{2M} + \sum_{j\neq 0} \hbar\omega_{k_j}\left(\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}\right)}$$

C.O.M: set $\hat{P}_0 = 0$
(no macroscopic motion of lattice)

- Note: Despite the nasty algebra, this calculation is entirely straightforward. Two steps: (1) Diagonalizing the potential $\Rightarrow$ Normal modes, SAME as classical case!, (2) Quantize (same as single harmonic oscillators since normal modes decouple by definition!)

Spectrum: Groundstate $|0\rangle$ s.t. $a_j|0\rangle = 0$

$$E_0 = \sum_{j\neq 0} \frac{\hbar\omega_j}{2}$$

$a_j^\dagger|0\rangle$: phonon mode: energy $E_1 - E_0 = \hbar\omega_j$
(crystal) momentum: $\hbar k_j$

Gapless spectrum since $\hbar\omega_k \xrightarrow[k\to 0]{} 0$ $(N\to\infty)$

# III Field Theory

Focus on sound waves and take continuum limit:

$$u_n = u(x = na)$$

$$u_{n+1} = u(x+a) \simeq u(x) + a\,\partial_x u + \dots$$

$$m\ddot{u}_n = m\,\partial_t^2 u = -\lambda\underbrace{(2u_n - u_{n-1} - u_{n+1})}_{-a^2\partial_x^2 u + \dots}$$

$$\Rightarrow \boxed{\partial_t^2 u - \frac{\lambda a^2}{m}\partial_x^2 u = 0}$$

$c_s = a\sqrt{\frac{\lambda}{m}}$

(consistent with group velocity as $k \to 0$)

**Lagrangian:** $$L = \sum_n \frac{1}{2} m \dot{u}_n^2 - \frac{\lambda}{2}(u_{n+1} - u_n)^2$$

$$= \int_0^L \frac{dx}{a}\left[\frac{1}{2}m(\partial_t u)^2 - \frac{\lambda}{2}a^2(\partial_x u)^2\right]$$

"Classical Field Theory"

## a) Phonons in 3d

Displacement fields: $u_i(\vec{x})$ $\quad i = x, y, z = 1, 2, 3$

Isotropic crystal: Action depends on strain tensor

$$\boxed{\varepsilon_{ij}(\vec{x}) = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i\right)}$$

Strain tensor

$$L = \int d^3\vec{x}\, \underbrace{\left[\frac{1}{2}\rho\left(\partial_t \vec{u}\right)^2 - 2\mu \sum_{ij} \varepsilon_{ij}^2 - \frac{\lambda}{2}\left(\mathrm{tr}\,\varepsilon\right)^2\right]}_{\mathcal{L}}$$

Equation of motion: $\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \partial_t u_i}\right) + \frac{\partial}{\partial \vec{x}} \cdot \left(\frac{\partial \mathcal{L}}{\partial \partial_{\vec{x}} u_i}\right) = 0$

$$\Rightarrow \quad \rho\, \partial_t^2 u_i = \sum_k \partial_k \underbrace{\left[\frac{\partial}{\partial_k u_i} \sum_{nm} \frac{\mu}{2}\left(\partial_n u_m + \partial_m u_n\right)^2\right]}_{\mu\left(\partial_k u_i + \partial_i u_k\right)}$$

$$+ \underbrace{\sum_k \partial_k \left[\frac{\lambda}{2} \frac{\partial}{\partial_k u_i}\left(\sum_n \partial_n u_n\right)^2\right]}_{}$$

$$\sum_k \partial_k \left[\lambda \sum_n \delta_{ki}\, \partial_n u_n\right] = \lambda \sum_n \partial_i \partial_n u_n$$

$$\Rightarrow \quad \boxed{\rho\, \partial_t^2 u_i = (\mu + \lambda)\, \partial_i \partial_j u_j + \mu \sum_j \partial_j^2 u_i}$$

Plane-wave solution: $u_i = u_i^0\, e^{-i\omega t + i\vec{k}\cdot\vec{x}}$

$$\rho\omega^2 u_i^0 = (\mu+\lambda) \underbrace{\sum_j k_j u_j^0}_{\vec{k}\cdot\vec{u}^0} k_i + \mu k^2 u_i^0$$

(= 1)

longitudinal waves : $\omega^2 = \frac{2\mu+\lambda}{\rho} k^2$

$\vec{k} \sim \vec{u}^0$

transverse waves: $\omega^2 = \frac{\mu}{\rho} k^2$

$\vec{k} \cdot \vec{u}^0 = 0$

(= 2)

(gapless. low k only = continuum limit)

## General Solution :

$$\vec{u}(x,t) = \sum_{\substack{\sigma = 1,2,3 \\ \text{Polarizations}}} \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\rho\omega_\sigma(\vec{k})} \vec{u}_\sigma^0 \left( a_\sigma(\vec{k}) e^{i(\vec{k}\cdot\vec{x} - \omega_\sigma(\vec{k})t)} + a_\sigma^\dagger(\vec{k}) e^{-i(\dots)} \right)$$

## (e) Quantum Field Theory (QFT)

$$\vec{\pi} = \frac{\partial L}{\partial \dot{\vec{u}}} = \rho \dot{\vec{u}} \; ; \qquad [\hat{u}_i(\vec{x}), \hat{\pi}_j(\vec{x}')] = i\hbar \delta_{ij} \delta(\vec{x} - \vec{x}')$$

then: $[\hat{a}_\sigma(\vec{k}), \hat{a}_{\sigma'}^\dagger(\vec{k}')] = \delta_{\sigma\sigma'} \delta(\vec{k} - \vec{k}')$

$[\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0$

$$\hat{H} = E_0 + \sum_\sigma \int \frac{d^3\vec{k}}{(2\pi)^3} \hbar\omega_\sigma(\vec{k}) \, \hat{a}_\sigma^\dagger(\vec{k}) \, \hat{a}_\sigma(\vec{k})$$

$\Rightarrow$ Similar to our lattice treatment...