Lect 8: Phonon — long-wave length method

The lattice vibration can be ~~treated~~ as coupled harmonic oscilaters

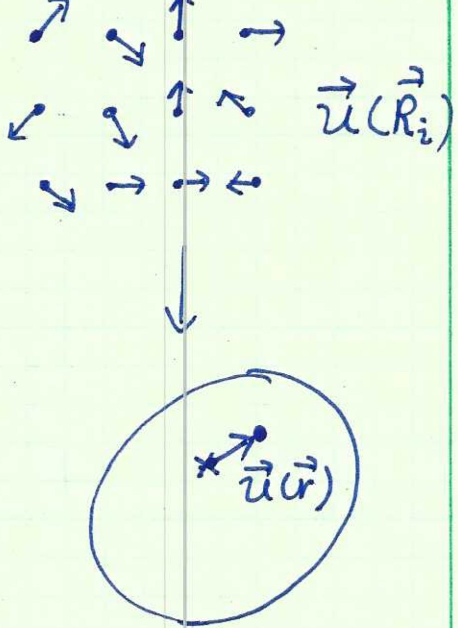
The quantized modes of lattice vibration are phonons. Often the phonons at $k \to 0$ play the leading role. In this limit. we can neglect the discrete nature of lattice and ~~treat~~ the lattice as an elastic media.

Define the displacement field $\vec{u}(\vec{R}_l)$.

$\vec{R}_l$ is the equilibrium position of l- atom.

This atom is away from $\vec{R}_l$ by $\vec{u}(\vec{R}_l)$

$\xrightarrow[\text{continous version}]{}$ $\vec{u}(\vec{r})$.



For later convenience, we define density

$$\rho = \frac{M \leftarrow \text{unit cell mass}}{\Omega \leftarrow \text{unit volum.}}$$

the relation between lattice summation and integral

$$\Omega \sum_l = \int dv$$

Let us construct the Langrange density

$$L = \int dv \, \mathcal{L} = \int dv \, (T - \phi).$$

① $T = \frac{1}{2}\sum_l M |\dot{\vec{u}}_l|^2 \rightarrow \int dv \, \frac{1}{2}\rho |\dot{\vec{u}}(\vec{r})|^2$

$$T = \frac{1}{2}\rho \frac{\partial u_i}{\partial t}\frac{\partial u_i}{\partial t}$$

② $\phi(\vec{r})$ can only depend on derivatives of $\vec{u}(\vec{r})$. because a uniform shift $\vec{u} \rightarrow \vec{u} + \vec{a}$ corresponds to translation. $\nabla \times \vec{u}$ cannot be involved because it corresponds to an overall rotation — only the symmetric part of $\partial_i u_j$ contributes to elastic energy.

Define $u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)$ ← strain tensor

Hooke's law: + requirement of isotropy

$$\phi(r) = \phi_0 + \frac{1}{2}\lambda \underbrace{u_{ii}^2}_{(\mathrm{tr}\, u)^2} + \frac{1}{2}\mu \underbrace{u_{ik}^2}_{\mathrm{tr}(u^2)} .$$

λ, μ: Lame coefficients.

Ex: prove $(\mathrm{tr}\, u)^2$ and $\mathrm{tr}(u^2)$ are the only two invariant quantities under spatial rotation.

$$u_{ik} = \underbrace{\left(u_{ik} - \frac{1}{3}\delta_{ik} u_{ll}\right)}_{\substack{\text{traceless part} \\ \text{pure shear}}} + \underbrace{\frac{1}{3}\delta_{ik} u_{ll}}_{\substack{\text{trace part} \\ \text{hydrostatic compression.}}}$$

$$\Rightarrow \phi(r) - \phi_0 = \frac{1}{2}\lambda u_{ii}^2 + \frac{1}{2}\mu \left[\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right) + \frac{1}{3}\delta_{ik}u_{ll}\right]^2$$

$$= \frac{1}{2}\left(\lambda + \frac{1}{3}\mu\right) u_{ii}^2 + \frac{1}{2}\mu\left[\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right)\right]^2$$ (crossing terms vanish)

$$\phi(r) - \phi_0 = \frac{1}{2}\mu\left[u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right]^2 + \frac{1}{2}K u_{ll}^2 \quad \leftarrow K = \lambda + \frac{2}{3}\mu$$

Shear modulus or modulus of rigidity

bulk modulus or modulus of hydrostatic compression.

$$\Rightarrow \boxed{\mathcal{L} = \frac{1}{2}\rho\frac{\partial u_i}{\partial t}\frac{\partial u_i}{\partial t} - \frac{1}{2}\lambda u_{ii}^2 - \frac{1}{2}\mu u_{ik}^2}$$

$$\delta L = \int dv\ \delta\mathcal{L} = \int dv\ \left[\rho\frac{\partial}{\partial t}\delta u_i \frac{\partial u_i}{\partial t} - \lambda u_{ii}\delta u_{ii} - \mu u_{ik}\delta u_{ik}\right]$$

$$= \int dv\ -\delta u_i\left[\rho\frac{\partial^2 u_i}{\partial t^2} - \lambda\ \partial_i u_{ll} - \mu\ \partial_k u_{ik}\right]$$

$$= -\int dv\ \delta u_i\ \left[\rho\frac{\partial^2 u_i}{\partial t^2} - \lambda\ \partial_i(\nabla\cdot\vec{u}) - \frac{\mu}{2}\left[\partial_i(\vec{\nabla}\cdot\vec{u}) + \partial^2 u_i\right]\right\}$$

$$\Rightarrow \boxed{\rho\frac{\partial^2 u_i}{\partial t^2} = \left(\lambda + \frac{\mu}{2}\right)\partial_i(\nabla\cdot\vec{u}) + \frac{\mu}{2}\partial^2 u_i}$$

① transverse wave : set $\vec{k} = k\hat{e}_z$, $\vec{u} = u\hat{e}_x$ $\Rightarrow \frac{\mu}{2\rho} = C_T^2$

② longitudinal wave $\vec{k} = k\hat{e}_z$, $\vec{u} = u\hat{e}_z$

$$\Rightarrow \rho\frac{\partial^2 u}{\partial t^2} = (\lambda + \mu)\partial_z^2 u \Rightarrow \frac{\lambda + \mu}{\rho} = C_L^2$$

$$\Rightarrow \boxed{\frac{\partial^2 u_i}{\partial t^2} = C_T^2\ \partial^2 u_i + \left(C_L^2 - C_T^2\right)\partial_i(\nabla\cdot\vec{u})}$$

elastic wave equation!

§ Quantization of eigen-mode - phonons

$$P_i = \frac{\partial \mathcal{L}}{\partial \dot{u}_i} = \rho \dot{u}_i \quad \Rightarrow \quad H = \int dv\, \mathcal{H}$$

$$\boxed{\mathcal{H} = P_i \dot{u}_i - \mathcal{L} = \frac{1}{2\rho} P_i^2 + \frac{1}{2}\lambda u_{ii}^2 + \frac{1}{2}\mu u_{ik}^2}$$

$P_i(r)$ is the canonical momentum field conjugate to $u_i(r)$.

Introducing canonical coordinate

$$\vec{u}(\vec{r}) = \frac{1}{\sqrt{NM}} \sum_{k\sigma} \vec{e}_{k\sigma}\, Q_{k\sigma}\, e^{i\vec{k}\cdot\vec{r}} \quad \leftarrow \quad \frac{1}{\sqrt{NM}} = \frac{1}{\sqrt{\rho V}}$$

$$\sqrt{\frac{M}{N}} = \sqrt{\frac{\rho}{V}}\cdot \Omega$$

$$= \frac{1}{\sqrt{\rho V}} \sum_{k\sigma} \vec{e}_{k\sigma}\, Q_{k\sigma}\, e^{i\vec{k}\cdot\vec{r}}$$

$$\vec{p}(r) = \frac{1}{\sqrt{\Omega}}\sqrt{\frac{M}{N}} \sum_{k\sigma} \vec{e}_{k\sigma}\, P_{k\sigma}\, e^{-i\vec{k}\cdot\vec{r}} = \sqrt{\rho/V} \sum_{k\sigma} \vec{e}_{k\sigma}\, P_{k\sigma}\, e^{-i\vec{k}\cdot\vec{r}}$$

we introduce
$$\begin{cases} \sum_\sigma e^i_{k\sigma}\cdot e^j_{k\sigma} = \delta_{ij} \\ [Q_{k\sigma}, P_{k'\sigma'}] = i\,\delta_{kk'}\,\delta_{\sigma\sigma'} \end{cases}$$

$$\Rightarrow [u_i(\vec{r}), P_j(\vec{r}')] = \frac{1}{V}\sum_{k\sigma} e^i_{k\sigma}\cdot e^j_{k\sigma}\, e^{i\vec{k}(\vec{r}-\vec{r}')}$$

$$= i\int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\cdot \delta_{ij} = i\,\delta(\vec{r}-\vec{r}')\,\delta_{ij}$$

or $$\boxed{[u_i(\vec{r}), P_j(\vec{r}')] = i\,\delta(\vec{r}-\vec{r}')\,\delta_{ij}}$$

$$P^2(\vec{r}) = \frac{\rho}{V} \sum_{\substack{k\sigma \\ k'\sigma'}} \mathbb{P}_{k\sigma} \mathbb{P}_{-k'\sigma'} \, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \quad \vec{e}_{k\sigma} \cdot \vec{e}_{-k'\sigma'}$$

$$u_{ii}(\vec{r}) = \frac{1}{\sqrt{\rho V}} \sum_{k\sigma} (i\vec{k}\cdot\vec{e}_{k\sigma}) \, Q_{k\sigma} \, e^{i\vec{k}\cdot\vec{r}}$$

$$u_{ii}^2(\vec{r}) = \frac{1}{\rho V} \sum_{\substack{k\sigma, \\ k'\sigma'}} (i\vec{k}\cdot\vec{e}_{k\sigma})(-i\vec{k}'\cdot\vec{e}_{-k'\sigma}) \, Q_{k\sigma} Q_{-k',\sigma'} \, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}$$

$$u_{il}(\vec{r}) = \frac{1}{\sqrt{\rho V}} \sum_{k\sigma} (ik_i e^l_{k\sigma} + ik_l e^i_{k\sigma}) \, Q_{k\sigma} \, e^{i\vec{k}\cdot\vec{r}}$$

$$u_{il}^2(\vec{r}) = \frac{1}{4\rho V} \sum_{\substack{k\sigma \\ k'\sigma'}} (ik_i e^l_{k\sigma} + ik_l e^i_{k\sigma})(-ik'_i e^l_{-k'\sigma'} - ik_l e^i_{-k\sigma'}) \, Q_{k\sigma} Q_{-k'\sigma'} \, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}$$

$$\int dv \, \frac{P^2}{2\rho} = \frac{1}{2} \sum_{k\sigma\sigma'} \mathbb{P}_{k\sigma} \mathbb{P}_{-k\sigma'} \, \vec{e}_{k\sigma} \cdot \vec{e}_{-k\sigma'}$$

$$\int dv \, \frac{\lambda}{2} u_{ii}^2 + \frac{\mu}{2} u_{ik}^2 = \frac{\lambda}{2\rho} \sum_{k\sigma\sigma'} (\vec{k}\cdot\vec{e}_{k\sigma})(\vec{k}\cdot\vec{e}_{-k\sigma}) \, Q_{k\sigma} Q_{-k\sigma'}$$

$$+ \frac{\mu}{2\rho} \frac{1}{4} \sum_{k\sigma\sigma'} (k_i e^l_{k\sigma} + k_l e^i_{k\sigma})(k_i e^l_{-k\sigma'} + k_l e^i_{-k\sigma'}) \, Q_{k\sigma} Q_{-k\sigma'}$$

we need to fix the convention of $\vec{e}_{k\sigma}$ and $\vec{e}_{-k\sigma}$.

Because $u(r)$ is real $\Rightarrow$ $\vec{e}_{k\sigma} Q_{k\sigma} e^{i\vec{k}\cdot\vec{r}} + \vec{e}_{-k\sigma} Q_{-k\sigma} e^{-i\vec{k}\cdot\vec{r}}$ is real

if we choose $\vec{e}_{k\sigma}$ as real, we can set $\vec{e}_{k\sigma} = \vec{e}_{-k\sigma}$ and $Q_{-k\sigma} = Q^*_{k\sigma}$ (linear polarization)

$$\Rightarrow \vec{e}_{k\sigma} \cdot \vec{e}_{-k\sigma'} = \delta_{\sigma\sigma'}$$

$$\Rightarrow \int dv \frac{p^2}{2\rho} = \frac{1}{2} \sum_{k\sigma} \mathbb{P}_{k\sigma} \mathbb{P}_{-k\sigma}$$

$$\int dv \frac{\lambda}{2} u_{ii}^2 + \frac{\mu}{2} u_{ik}^2 = \frac{1}{2\rho} \sum_{k\sigma\sigma'} \lambda [\vec{k}\cdot\vec{e}_{k\sigma}][\vec{k}\cdot\vec{e}_{k\sigma'}] Q_{k\sigma} Q_{-k\sigma'}$$

$$+ \frac{\mu}{2\rho} \sum_{k\sigma} \left[\frac{1}{2} k^2 Q_{k\sigma} Q_{-k\sigma} + \frac{1}{2}(\vec{k}\cdot\vec{e}_{k\sigma})(\vec{k}\cdot\vec{e}_{k\sigma'})\right] Q_{k\sigma} Q_{-k\sigma'}$$

$$= \frac{1}{2\rho} \sum_{k,\sigma\sigma'} (\lambda + \tfrac{1}{2}\mu)(\vec{k}\cdot\vec{e}_{k\sigma})(\vec{k}\cdot\vec{e}_{k\sigma'}) Q_{k\sigma} Q_{-k\sigma'}$$

$$+ \frac{\mu}{2\rho} \sum_{k\sigma} \frac{1}{2} k^2 Q_{k\sigma} Q_{-k\sigma}$$

Now let's us look at the wave equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = (\lambda + \frac{\mu}{2}) \partial_i (\nabla \cdot \vec{u}) + \frac{\mu}{2} \partial^2 u_i$$

plug in $u_i = e^i_{k\sigma} \, e^{i(\vec{k}\cdot\vec{r} - \omega t)} \Rightarrow -\rho\omega^2 e^i_{k\sigma} = (\lambda + \frac{\mu}{2})(-) k^i (\vec{k}\cdot\vec{e}_{k\sigma})$

$$- \frac{\mu}{2} e^i_{k\sigma} k^2$$

$$\Rightarrow \boxed{\rho\omega^2_{k\sigma} \vec{e}_{k\sigma} = (\lambda + \frac{\mu}{2})(\vec{k}\cdot\vec{e}_{k\sigma}) \vec{k} + \frac{\mu}{2} k^2 \vec{e}_{k\sigma}}$$

$$\Rightarrow (\lambda + \frac{\mu}{2})(\vec{k}\cdot\vec{e}_{k\sigma})(\vec{k}\cdot\vec{e}_{k\sigma'}) = (\rho\omega^2_{k\sigma} - \frac{\mu}{2} k^2) \vec{e}_{k\sigma}\cdot\vec{e}_{k\sigma'}$$

$$= (\rho\omega^2_{k\sigma} - \frac{\mu}{2} k^2) \delta_{\sigma\sigma'}$$

$$\boxed{\omega^2_{kL} = k^2 \frac{\lambda + \mu}{\rho} \qquad \omega^2_{kT} = k^2 \frac{\mu}{2\rho}}$$

$$\Rightarrow \boxed{H = \frac{1}{2} \sum_{k\sigma} \left[\mathbb{P}_{k\sigma} \mathbb{P}_{-k\sigma} + \omega^2_{k\sigma} Q_{k\sigma} Q_{-k\sigma} \right]}$$

§ Quantization

Define $Q_{k\sigma} = \sqrt{\frac{\hbar}{2\omega_{k\sigma}}} \left(a_{k\sigma} + a^{+}_{-k\sigma}\right) \Rightarrow Q_{k\sigma} Q_{-k\sigma} = \frac{\hbar}{2\omega_{k\sigma}} \left(a_{k\sigma} a_{-k\sigma} + a_{k\sigma} a^{+}_{k\sigma} + a^{+}_{-k\sigma} a_{-k\sigma} + a^{+}_{-k\sigma} a^{+}_{k\sigma}\right)$

$P_{k\sigma} = \sqrt{\frac{\omega_{k\sigma}\hbar}{2}} \, \frac{a_{k\sigma} - a^{+}_{-k\sigma}}{i}$

$\Rightarrow P_{k\sigma} P_{-k\sigma} = \frac{\hbar\omega_{k\sigma}}{2} \left(-a_{-k\sigma} a_{k\sigma} - a^{+}_{k\sigma} a^{+}_{-k\sigma} + a_{-k\sigma} a^{+}_{-k\sigma} + a^{+}_{k\sigma} a_{k\sigma}\right)$

$$\Rightarrow \boxed{\begin{aligned} H &= \sum_{k\sigma} \frac{\hbar\omega_{k\sigma}}{2} \left(a_{k\sigma} a^{+}_{k\sigma} + a^{+}_{k\sigma} a_{k\sigma}\right) \\ &= \sum_{k\sigma} \hbar\omega_{k\sigma} \left(a^{+}_{k\sigma} a_{k\sigma} + 1/2\right) \end{aligned}}$$

The displacement field

$$\vec{u}(r) = \sum_{k\sigma} \vec{e}_{k\sigma} \sqrt{\frac{\hbar}{2\rho V \omega_{k\sigma}}} \left(a_{k\sigma} + a^{+}_{-k\sigma}\right) e^{i\vec{k}\cdot\vec{r}}$$