The Dynamical Matrix

Recall: Hamiltonian: $\mathcal{H} = \sum_{\ell} \frac{P_\ell^2}{2M_\ell} + \frac{1}{2}\sum_{\ell,\ell'} \varphi^0(\ell,\ell') u_\ell u_{\ell'}$

Classical eqn's of motion:

1. $\frac{\partial \mathcal{H}}{\partial P_\ell} = \dot{R}_\ell = \dot{u}_\ell$ 2. $\frac{\partial \mathcal{H}}{\partial R_\ell} = -\dot{P}_\ell = \frac{\partial \mathcal{H}}{\partial u_\ell}$

1. $\frac{\partial \mathcal{H}}{\partial P_\ell} = \dot{u}_\ell \Rightarrow P_\ell = M_\ell \dot{u}_\ell$

2. $\frac{\partial \mathcal{H}}{\partial R_\ell} = -\dot{P}_\ell = \frac{\partial \mathcal{H}}{\partial u_\ell} \Rightarrow \frac{\partial \mathcal{H}}{\partial u_\ell} = \frac{1}{2}\frac{\partial}{\partial u_\ell}\left\{\sum_{\ell'\ell''} \varphi^0(\ell',\ell'') u_{\ell'} u_{\ell''}\right\}$

Note ℓ, ℓ', ℓ'' are just indices

$$= \frac{1}{2}\left\{\sum_{\ell'} \varphi^0(\ell',\ell) u_{\ell'} + \sum_{\ell''} \varphi^0(\ell,\ell'') u_{\ell''}\right\}$$

$$= \sum_{\ell'} \varphi^0(\ell,\ell') u_{\ell'}$$

and: $\dot{P}_\ell = M_\ell \ddot{u}_\ell$

$$\boxed{\begin{aligned} &\therefore \quad M_\ell \ddot{u}_\ell = -\sum_{\ell'} \varphi^0(\ell,\ell') u_{\ell'} \\ &\text{OR} \quad M_\ell \ddot{u}_\ell + \sum_{\ell'} \varphi^0(\ell,\ell') u_{\ell'} = 0 \end{aligned}}$$

This is valid in general for an interaction potential energy function which is dependent on the ion positions.

$$M_\ell \ddot{u}_\ell + \sum_{\ell'} \varphi^0(\ell,\ell') u_{\ell'} = 0$$

→ leads to set of N coupled diff. eqn's.

e.g. $M_1 \ddot{u}_1 + \varphi^0(1,1)u_1 + \varphi^0(1,2)u_2 + \cdots \varphi^0(1,N)u_N = 0$

$\vdots$

$M_N \ddot{u}_N + \varphi^0(N,1)u_1 + \varphi^0(N,2)u_2 + \cdots \varphi^0(N,N)u_N = 0$

Assume solutions of the form:

$$u_\ell(t) = u^0_\ell \underbrace{e^{\pm i\omega t}}$$

amp. of oscillation

$$\Rightarrow -M_\ell \omega^2 u^0_\ell + \sum_{\ell'} \varphi^0(\ell,\ell') u^0_{\ell'} = 0$$

<u>or</u>

$$\sum_{\ell'} \underbrace{\left[-M_\ell \omega^2 \delta_{\ell\ell'} + \varphi^0(\ell,\ell')\right]}_{N \times N \text{ matrix. } \equiv L} u^0_{\ell'} = 0$$

define: $-L_{\ell\ell'} \equiv -M_\ell \omega^2 \delta_{\ell\ell'} + \varphi^0(\ell,\ell')$

$$\Rightarrow \underbrace{L}_{N\times N \text{ matrix}} \underbrace{u^0}_{\text{vector of } u^0_\ell\text{'s}} = 0$$

Recall: $$\varphi^\circ(\ell,\ell') \equiv \left.\frac{\partial^2 W}{\partial R_{\ell'}\,\partial R_\ell}\right|_0 \quad \rightarrow \text{real}$$

$$\varphi^\circ(\ell,\ell') = \varphi^\circ(\ell',\ell)$$

$$L_{\ell,\ell'} = M_\ell \omega^2 \delta_{\ell\ell'} - \varphi^\circ(\ell,\ell')$$

→ elements are real & symmetric

∴ Matrix L is Hermitian

Our set of equations: $\sum_{\ell'} L_{\ell\ell'} u^\circ_{\ell'} = 0$

has (nontrivial) solutions provided $|L| = 0$

→ Results in solution of N roots for ω^2

→ Since L is Hermitian, the roots i.e. ω^2 are real

→ while this corresponds to $2N$ soln for ω $(\pm\sqrt{\omega^2})$

$$u_\ell(t) \propto e^{i\omega t} + e^{-i\omega t}$$

∴ still just N soln's. ⟶ 1D

For N degrees of freedom, N roots

i.e. 1D → N roots
2D → $2N$
3D → $3N$

→ each value of ω^2 represents a phonon frequency or normal mode of vibration

Assume solutions:

$$u_\ell^\circ(k) = A(k)\frac{e^{ik\cdot R_\ell^\circ}}{\sqrt{M_\ell}}$$

in 1D $R_\ell^\circ = a\ell$.

amplitude of mode k

normalization

→ apply periodic boundary conditions: $u_\ell = u_{\ell+N}$

$$k = \frac{2\pi}{aN} m \quad , m \text{ integer}$$

→ for 1D but sim. expressions for 2 → 3D.

Recall, there are N modes, i.e. # of m's. By convention, limit m to:

$$m \in \left(-\frac{N}{2}+1 \; , \; \frac{N}{2}\right)$$

⇒ total N modes

Verify Solutions

$$\sum_{\ell'} L_{\ell\ell'} u_{\ell'}^\circ = 0 = \sum_{\ell'}\left(M_\ell \omega^2(k)\,\delta_{\ell\ell'} - \varphi^\circ(\ell,\ell')\right)A(k)\frac{e^{ikR_{\ell'}^\circ}}{\sqrt{M_{\ell'}}}$$

$$= M_\ell \omega^2(k) A(k)\frac{e^{ikR_\ell^\circ}}{\sqrt{M_\ell}} - \sum_{\ell'}\frac{e^{ikR_\ell^\circ}}{\sqrt{M_{\ell'}}}A(k)\varphi^\circ(\ell,\ell')\underbrace{e^{ik(R_{\ell'}^\circ - R_\ell^\circ)}}_{=1 \text{ when } \ell'=\ell}$$

$$0 = \sqrt{M_\ell}\, A(k)\, e^{ikR_\ell^0} \underbrace{\left[\omega^2(k) - \sum_{\ell'} \frac{\varphi^0(\ell,\ell')}{\sqrt{M_\ell M_{\ell'}}} e^{ik(R_{\ell'}^0 - R_\ell^0)} \right]}$$

$\therefore$ $\qquad = 0$

$$\therefore \quad \omega^2(k) = \sum_{\ell'} \frac{\varphi^0(\ell,\ell')}{\sqrt{M_\ell M_{\ell'}}} e^{ik(R_{\ell'}^0 - R_\ell^0)}$$

$$\equiv D(k) \rightarrow \text{Dynamical Matrix.}$$

$$\boxed{\omega^2(k) = D(k)}$$

$$\boxed{D(k) \equiv \sum_{\ell'} \frac{\varphi^0(\ell,\ell')}{\sqrt{M_\ell M_{\ell'}}} e^{ik(R_{\ell'}^0 - R_\ell^0)}}$$

Note that $D(k)$ does not depend on ℓ:

→ take $M_{\ell'} = M_\ell = M$

→ R_ℓ^0 are lattice vectors $\therefore$ $R_{\ell'}^0 - R_\ell^0 \equiv R_{\ell'-\ell}^0$ is a lattice vector

→ $\varphi_\ell^0(\ell,\ell')$ depends on separation of ℓ & ℓ'

Let $\ell' - \ell \equiv m$

$$\boxed{D(k) = \frac{1}{M} \sum_m e^{ikR_m^0} \varphi^0(m)}$$

$$D(k) = \underbrace{\frac{1}{M}}_{\text{mass}} \sum_m \underbrace{e^{ikR_m^0}}_{\text{geometric phase factor}} \underbrace{\varphi^0(m)}_{\text{Force constants}} = \omega^2(k)$$

generalization of:

$$\omega^2 = \frac{K}{m}$$

One more note:

$$\sum_{\ell \ell'} \varphi^0(\ell, \ell') = 0 \quad \rightarrow \text{think Newton's 3}^{\text{rd}} \text{ Law.}$$

i.e. $\sum_m \varphi^0(m) = 0$

$$\Rightarrow \varphi^0(0) + \sum_{m \neq 0} \varphi^0(m) = 0$$

↳ separate self interaction

$$\therefore \; D(k) = \frac{1}{M} \sum_{m \neq 0} e^{ikR_m^0} \varphi^0(m) + \frac{1}{M} \underbrace{\varphi^0(0)}_{= -\sum_{m \neq 0} \varphi^0(m)}$$

$$\boxed{D(k) = \frac{1}{M} \sum_{m \neq 0} \left(e^{ikR_m^0} - 1\right) \varphi^0(m)}$$

geometric factor depends only on lattice

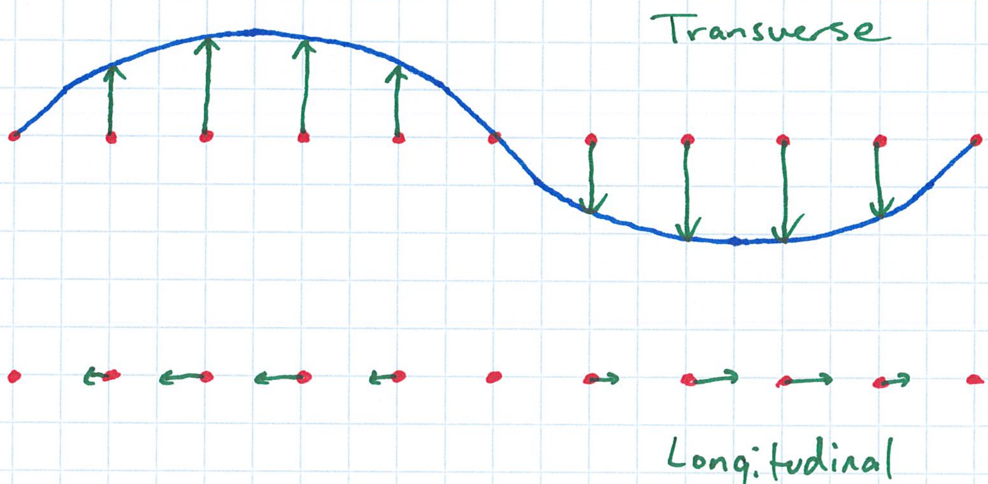
"self-force" components removed

Physical Interpretation of Solutions

$$u_\ell(k,t) = \frac{\epsilon(k)}{\sqrt{M}} e^{ikR_\ell^0} e^{-i\omega(k)t}$$

↳ displacement of ion ℓ vibrating in mode k

- Normal modes are collective vibrations.



- sound waves are low frequency longitudinal & trans. phonons (20 Hz – 20 KHz)

largest λ? : $k = \frac{2\pi}{\lambda} = \frac{2\pi}{Na} m \Rightarrow m = 1 \Rightarrow \lambda = Na$

size of crystal

smallest λ? : $m = \frac{N}{2} \Rightarrow \lambda = 2a$

↳ 2 unit cells