

LATTICE VIBRATIONS, PHONONS

(I) Phonons in one dimension

$$H = \sum_e \frac{p_e^2}{2M} + V(u_1, u_2, \dots)$$

$p_e = -i\hbar \frac{\partial}{\partial u_e}$
 $[u_e, p_{e'}] = i\hbar \delta_{ee'}$
(1)

- The potential V is such that it has a minimum when $u_e = 0$, $\forall e$.
- We expand V in Taylor series around this minimum:

$$\begin{aligned} V(u_1, u_2, \dots) &= V(0, 0, \dots) + \sum_e u_e \left[\frac{\partial V}{\partial u_e} \right]_{u_1=u_2=\dots=0} \\ &\quad + \frac{1}{2!} \sum_{e, e'} u_e u_{e'} \left[\frac{\partial^2 V}{\partial u_e \partial u_{e'}} \right]_{u_1=u_2=\dots=0} \\ &\quad + \frac{1}{3!} \dots \end{aligned} \quad (2)$$

- The first term can be eliminated by suitable choice of zero energy while the second term vanishes by virtue of $u_1 = u_2 = \dots = 0$ being the minimum.

→
$$H \approx \sum_e \frac{p_e^2}{2M} + \frac{1}{2} \sum_{e, e'} u_e V_{ee'} u_{e'} \quad (3)$$

where $V_{ee'} = \left[\frac{\partial^2 V}{\partial u_e \partial u_{e'}} \right]_{u_1=u_2=\dots=0}$ is the DYNAMICAL MATRIX.

- We neglect all higher-order terms in (2) which amounts to "harmonic approximation".

- We next diagonalize the V -term. Define a vector of displacements.

$$Y = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} V_{11} & V_{12} & \dots \\ V_{21} & V_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Then the potential term reads simply $Y^T V Y$

Diagonalize by unitary transformation U : ($U^{-1} = U^*$)

$$Y^T V Y = \underbrace{Y^T U^*}_{\tilde{Y}^+} \underbrace{(U V U^*)}_{\tilde{V}} \underbrace{U Y}_{\tilde{Y}} = \tilde{Y}^+ \tilde{V} \tilde{Y} = \sum_q \tilde{Y}_q^+ \tilde{V}_{qq} \tilde{Y}_q \quad |$$

diagonal

- It is easy to see that this transformation leaves the kinetic energy unchanged:

$$P_e = -i\hbar \frac{\partial}{\partial u_e} = i\hbar \sum_q \frac{\partial \tilde{u}_q}{\partial u_e} \frac{\partial}{\partial \tilde{u}_q} = -i\hbar \sum_q (U)_{eq} \frac{\partial}{\partial \tilde{u}_q} \quad (5)$$

or $\tilde{P} = U^{-1} P$

$$\begin{aligned} \sum_e \tilde{P}_e^+ &= P^+ P = (U \tilde{P})^+ (U \tilde{P}) = \tilde{P}^+ U^+ U \tilde{P} = \tilde{P}^+ \tilde{P} \\ &= \sum_q \tilde{P}_q^+ \tilde{P}_q \end{aligned} \quad (6)$$

- In the new coordinates the Hamiltonian reads

$$H = \sum_q \left(\frac{1}{2M} \tilde{P}_q^+ \tilde{P}_q + \frac{1}{2} M \omega_q^2 \tilde{u}_q^+ \tilde{u}_q \right) \quad (7)$$

where we defined $\omega_q^2 = V_{qq}/M$. Also, the unitary transformation preserves the commutation rules,

$$[u_q, p_{q'}] = i\hbar \delta_{qq'} \quad (8)$$

(check!)

- The Hamiltonian is seen to describe a collection of decoupled harmonic oscillators \rightarrow solve by defining the usual raising/lowering operators:

$$\begin{cases} a_q = \frac{1}{\sqrt{2\hbar\omega_q}} (H\omega_q u_q + i p_q^+) \\ a_q^+ = \frac{1}{\sqrt{2\hbar\omega_q}} (H\omega_q u_q^+ - i p_q) \end{cases} \quad [a_q, a_{q'}^+] = \delta_{qq'} \quad (9)$$

$$\rightarrow H = \sum_q \hbar\omega_q (a_q^+ a_q + \frac{1}{2}) \quad (10)$$

Translation-invariant system

Dynamical matrix depends only on difference $l-l'$:

$$V_{ee'} = V_{e-e'} \quad (11)$$

\rightarrow in this case $U_{ee'}$ is given by Fourier transformation:

$$U_{ee'} = \frac{1}{\sqrt{N}} e^{iqe} \quad (12)$$

$$\begin{aligned} \tilde{V}_{qq'} &= [U^\dagger V U]_{qq'} = \frac{1}{N} \sum_{ee'} e^{-iqe} V_{e-e'} e^{iq'e'} \quad l \rightarrow l+l' \\ &= \frac{1}{N} \sum_{e'} e^{-ie'(q-q')} \underbrace{\sum_e e^{-iqe} V_e}_{V_q} \quad (13) \\ &= \delta_{qq'} V_q \end{aligned}$$

So indeed $U_{ee'}$ diagonalizes the dynamical matrix.

We use periodic boundary conditions.

$$u_{e+Na} = u_e \quad (14)$$

This implies $e^{iql} = e^{iq(e+Na)} \Rightarrow q = \frac{2\pi n}{Na}$

$$u_q = \frac{1}{N} \sum e^{-iql} u_e, \quad p_q = \frac{1}{N} \sum e^{iql} p_e \quad (15)$$

It follows that

$$u_{q+c} = u_q, \quad p_{q+c} = p_q \quad (16)$$

where $c = 2\pi/a$.

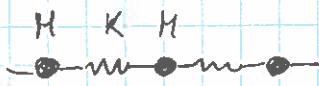
→ Momentum q is only defined in the "1st Brillouin zone" $q \in (-\frac{\pi}{a}, \frac{\pi}{a})$ and there are only N distinct values, $q = 2\pi n/Na$, $n = -\frac{N}{2} + 1, \dots, \frac{N}{2}$

Also, it holds $u_q^+ = u_{-q}$ and $p_q^+ = p_{-q}$. Taking into account $\omega_{-q} = \omega_q$ Eqs. (8) can be inverted as

$$u_q = \sqrt{\frac{k}{2M\omega_q}} (a_{-q}^+ + a_q), \quad p_q = i\sqrt{\frac{M\hbar\omega_q}{2}} (a_q^+ - a_{-q}) \quad (18)$$

and $\omega_q = \sqrt{V_q/M}$.

EXAMPLE 1: "monatomic chain"



masses connected
by springs

$$V = \sum_e \frac{1}{2} K (u_e - u_{e+a})^2$$

$$= \sum_e \frac{1}{2} K (2u_e^2 - 2u_e u_{e+a})$$

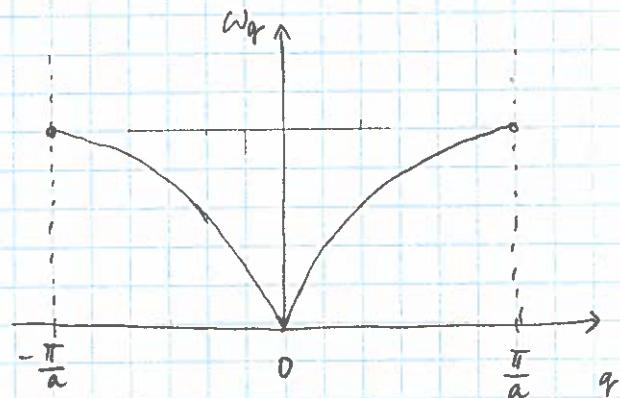
$$\Rightarrow V_{e-e'} = \begin{cases} 2K & \text{if } e=e' \\ -K & \text{if } e=e'+a \\ 0 & \text{otherwise} \end{cases} \quad (19)$$

Fourier transform:

$$\begin{aligned} V_q &= 2K - K(e^{iqa} + e^{-iqa}) \\ &= 2K(1 - \cos qa) \\ &= 4K \sin^2 \frac{qa}{2} \end{aligned} \quad (20)$$

Hence, the spectrum of normal modes reads

$$\begin{aligned} \omega_q &= \sqrt{\frac{V_q}{M}} = 2\sqrt{\frac{K}{M}} \left| \sin \frac{qa}{2} \right| \quad (21) \\ &\approx \sqrt{\frac{K}{M}} |qa| \text{ for } |qa| \ll 1 \end{aligned}$$

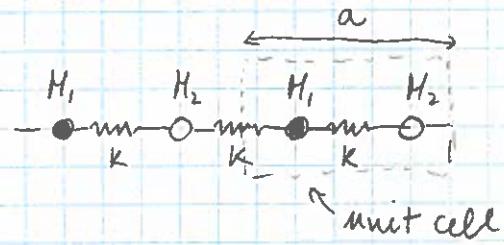


linear dependence signifies a sound-like (acoustic) mode.

EXAMPLE 2: "diatomic chain"

Similar analysis as before gives momentum-space dynamical matrix

$$V_q = \begin{pmatrix} 2K & -K(1+e^{iqa}) \\ -K(1+e^{-iqa}) & 2K \end{pmatrix} \quad (\text{check!}) \quad (22)$$



$$H = \sum_q \left(\frac{p_{q1}^+ p_{q1}^-}{2M_1} + \frac{p_{q2}^+ p_{q2}^-}{2M_2} \right) + \frac{1}{2} \sum_q (u_{q1}^+ u_{q1}^-) V_q \begin{pmatrix} u_{q1} \\ u_{q2} \end{pmatrix} \quad (23)$$

- need to get rid of unequal masses in kinetic energy:

Rescale momenta

$$p_{q1} \rightarrow p_{q1} \left(\frac{M_1}{M_2} \right)^{1/4}, \quad p_{q2} \rightarrow p_{q2} \left(\frac{M_2}{M_1} \right)^{1/4} \quad (24)$$

Because $P_{qz} = -ik \frac{\partial}{\partial u_{qz}}$ we also need to rescale u_{qz} 's!

$$u_{q_1} \rightarrow u_{q_1} \left(\frac{M_2}{M_1} \right)^{1/4}, \quad u_{q_2} \rightarrow u_{q_2} \left(\frac{M_1}{M_2} \right)^{1/4} \quad (25)$$

This finally gives:

$$H = \sum_q \frac{P_{1q}^+ P_{1q}^- + P_{2q}^+ P_{2q}^-}{2\sqrt{H_1 H_2}} + \frac{1}{2} \sum_q (u_{q_1}^+, u_{q_2}^+) \underbrace{\begin{pmatrix} 2K\sqrt{\frac{M_1}{M_2}} & -K(1+e^{iq\alpha}) \\ -K(1+e^{-iq\alpha}) & 2K\sqrt{\frac{M_2}{M_1}} \end{pmatrix}}_{\tilde{V}_q} \begin{pmatrix} u_{q_1} \\ u_{q_2} \end{pmatrix} \quad (26)$$

Now the normal modes are

given by the eigenvalues of \tilde{V}_q :

$$\begin{aligned} 0 &= \det |\tilde{V}_q - \omega \sqrt{H_1 H_2}| \\ &= M_1 M_2 \omega^4 - 2K(M_1 + M_2) \omega^2 + 2K^2(1 - \cos q\alpha) \end{aligned} \quad (27)$$

Solve:

$$\omega_{12}^2 = \frac{2K}{M_1 M_2} \left[(M_1 + M_2) \pm \sqrt{(M_1 + M_2)^2 - 2M_1 M_2 (1 - \cos q\alpha)} \right] \quad (28)$$

