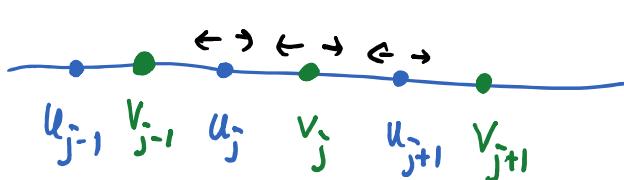


## §1. Lattice dynamics

### \* Classical theory of lattice vibrations

- 1D diatomic chain



equilibrium position:

$$R_j^{(1)} = j a$$

$$R_j^{(2)} = (j + \frac{1}{2}) a$$

Mass:  $M_1$  &  $M_2$

Nearest-neighbor interaction:

$$V(\{u_j\}, \{v_j\}) = V_0 + \frac{1}{2} C \sum_j \left[ (u_j - v_j)^2 + (u_j - v_{j-1})^2 \right]$$

$$M_1 \ddot{u}_j = F_j = -\frac{\partial V}{\partial u_j} = -C (2u_j - v_j - v_{j-1})$$

$$M_2 \ddot{v}_j = F'_j = -\frac{\partial V}{\partial v_j} = -C (2v_j - u_j - u_{j+1})$$

$$\begin{cases} u_j(t) = A_1 e^{i(q_j a - \omega t)} \\ v_j(t) = A_2 e^{i[q(j+\frac{1}{2})a - \omega t]} \end{cases}$$

$$M_1 \omega^2 A_1 e^{i(q_j a - \omega t)} = (2A_1 - A_2 e^{iq\frac{a}{2}} - A_2 e^{-iq\frac{a}{2}}) \times e^{i(q_j a - \omega t)}$$

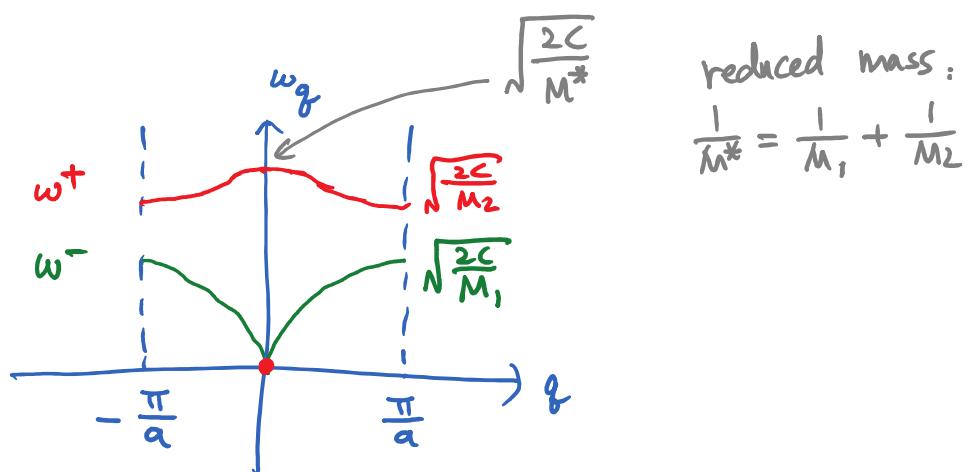
To have a nontrivial solution:

$$\begin{pmatrix} 2C - M_1 \omega^2 & -2C \cos \frac{qa}{2} \\ -2C \cos \frac{qa}{2} & 2C - M_2 \omega^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0$$

$$\Rightarrow \det \begin{pmatrix} 2C - M_1 \omega^2 & -2C \cos \frac{qa}{2} \\ -2C \cos \frac{qa}{2} & 2C - M_2 \omega^2 \end{pmatrix} = 0$$

**Exercise:** Determine dispersion relations  $\omega_q^\pm$  and  $\frac{A_1}{A_2}$  for two vibration modes!

Assume  $M_1 > M_2$ :



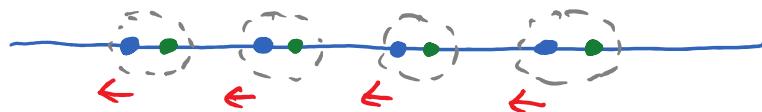
$M_1 = M_2 \Rightarrow 1D$  monoatomic chain

upper branch  $\omega_q^+$  disappears (check!)

Long wavelength limit ( $q \rightarrow 0$ ):

1) acoustic mode  $\omega_q^-$ :

$$\left\{ \begin{array}{l} \omega_q^- \approx v_s |q|, \\ A_1 \approx A_2 \end{array} \right. \quad v_s = \sqrt{\frac{C}{2(M_1 + M_2)}} a \quad \xrightarrow{\text{total mass}}$$

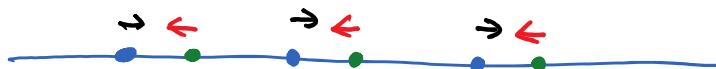


"move together"

(low-energy mode)

2) optical mode  $\omega_q^+$ :

$$\left\{ \begin{array}{l} \omega_q^+ \approx \frac{2C}{M^*} + O(q^3) \\ \frac{A_1}{A_2} \approx -\frac{M_2}{M_1} \end{array} \right.$$



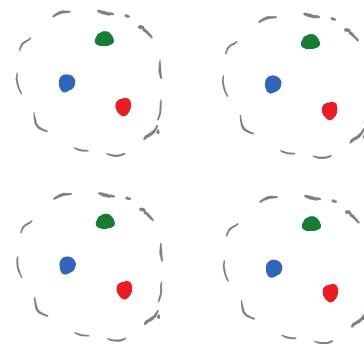
"move against each other"

(relative motion)

— General 3D crystal

$N$  unit cells labeled by

position  $\vec{R}_\mu$  ( $\mu=1, \dots, N$ )



$\alpha$ -th atom within the  $\mu$ -th unit cell:

$$\vec{x}_{\mu\alpha} = \vec{R}_\mu + \vec{d}_\alpha \quad (\vec{x}_{\mu\alpha}: \text{equilibrium position})$$

relative positions for atoms  
within the same unit cell

$$\vec{u}_{\mu\alpha} : u_{\mu\alpha i} \quad (i=x, y, z) \quad (\text{displacement})$$

potential energy:

$$V(\{u_{\mu\alpha i}\}) = V_0 + \frac{1}{2} \sum_{\mu\alpha i, \nu\beta j} D_{\mu\alpha i; \nu\beta j} \underbrace{u_{\mu\alpha i} u_{\nu\beta j}}$$



dynamical matrix

E.D.M.:

$$M_{\alpha} \ddot{u}_{\mu\alpha i} = F_{\mu\alpha i} = - \frac{\partial V}{\partial u_{\mu\alpha i}} = - \sum_{\nu\beta j} D_{\mu\alpha i; \nu\beta j} u_{\nu\beta j}$$

$3 \times N \times r$  equations  
 $i=x, y, z$        $\mu=1, \dots, N$        $\alpha=1, \dots, r$

$$u_{\mu\alpha j}(t) = A_{\alpha j} e^{i(\vec{q} \cdot \vec{R}_\mu - \omega t)}$$

$$M_\alpha \omega^2 A_{\alpha j} e^{i(\vec{q} \cdot \vec{R}_\mu - \omega t)} = \sum_{\nu\beta l} D_{\mu\alpha j; \nu\beta l} A_{\beta l} e^{i(\vec{q} \cdot \vec{R}_\nu - \omega t)}$$

$$\text{Define } D_{\alpha j; \beta l}(\vec{q}) \equiv \sum_\nu D_{\mu\alpha j; \nu\beta l} e^{-i\vec{q} \cdot (\vec{R}_\mu - \vec{R}_\nu)}$$

↓  
dynamical matrix in reciprocal space (3r × 3r)  
(translation symmetry used!)

$$\Rightarrow M_\alpha \omega^2 A_{\alpha j} = \sum_{\beta l} D_{\alpha j; \beta l}(\vec{q}) A_{\beta l}$$

$$\sum_{\beta l} \left[ M_\alpha \omega^2 \delta_{\alpha\beta} \delta_{jl} - D_{\alpha j; \beta l}(\vec{q}) \right] A_{\beta l} = 0$$

Non trivial solution:

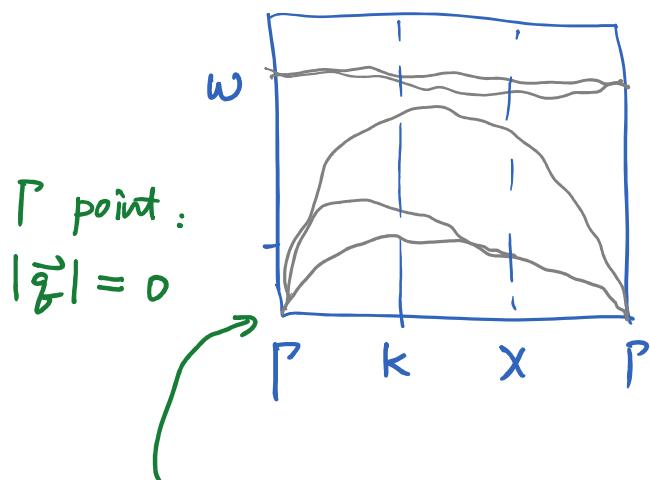
$$\det Q(\omega, \vec{q}) = 0$$

3r × 3r matrix:

$$Q_{\alpha j; \beta l}(\omega, \vec{q}) = M_\alpha \omega^2 \delta_{\alpha\beta} \delta_{jl} - D_{\alpha j; \beta l}(\vec{q})$$

Plot dispersion relation  $\omega_{\vec{q}}$  in the FBZ:

Example: GaAs



See, e.g., theory vs. experiment

Giannozzi et al.,

Phys. Rev. B 43, 7231 (1991)

3 acoustic modes + (3r-3) optical modes !

"Mathematical" reason why  $\omega_{\text{acoustic}} \rightarrow 0$  at P point:

$$\sum_{\beta l} \left[ M_\alpha \omega^2 \delta_{\alpha\beta} \delta_{jl} - D_{\alpha j; \beta l}(\vec{q}) \right] \underline{A_{\beta l}} = 0$$

acoustic modes :  $A_{\beta l} = A_l$   
("move together")

$$\Rightarrow \sum_l \left[ M_\alpha \omega^2 \delta_{jl} - \sum_{\beta} D_{\alpha j; \beta l}(\vec{q}) \right] \underline{A_l} = 0$$

||

0 for  $\vec{q} = 0$  (global shift: no force,  
Similar to  $\sum_l D_{jjl} = 0$   
in 1D monoatomic chain)

$$\Rightarrow \omega \rightarrow 0 \text{ for } \vec{q} = 0$$

## \* Quantum theory of lattice vibrations

- Review: quantum harmonic oscillator

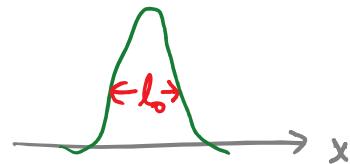
$$H = \frac{1}{2M} P_x^2 + \frac{1}{2} M \omega^2 x^2 \quad [x, p_x] = i\hbar$$

$$= \frac{1}{2} \hbar \omega \left( \frac{1}{M \hbar \omega} P_x^2 + \frac{M \omega}{\hbar} x^2 \right) \quad \text{length unit:}$$

$$= \frac{1}{2} \hbar \omega \left( \frac{l_0^2}{\hbar^2} P_x^2 + \frac{1}{l_0^2} x^2 \right) \quad l_0 = \sqrt{\frac{\hbar}{M \omega}}$$

Ground state in real space:

(Gaussian wave packet)



$\Rightarrow$  Atoms will "vibrate" even at  $T=0$ !

(zero-point motion due to uncertainty principle)

Boson realization: convenient approach for harmonic oscillators

Bosonic creation and annihilation operators:

$$a^+, a \quad [a, a^+] = 1$$

Hilbert space:  $|0\rangle$  ("vacuum",  $a|0\rangle = 0$ )

$$|n\rangle = \frac{1}{n!} (a^+)^n |0\rangle, \quad n=0, 1, 2, \dots$$

$$\langle n | n' \rangle = \delta_{nn'}$$

number of bosons :  $n = a^\dagger a$

$$\begin{aligned}
 n|m\rangle &= a^\dagger a \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle \\
 &= a^\dagger \frac{1}{\sqrt{n!}} [a, (a^\dagger)^n] |0\rangle \\
 &= m \frac{1}{\sqrt{n!}} (a^\dagger)^m |0\rangle \\
 &= m|m\rangle
 \end{aligned}$$