Phonon Dispersion Curves

→ The Dynamical matrix tells us about the normal modes of vibration (eigenvalues $\omega^2(k)$)

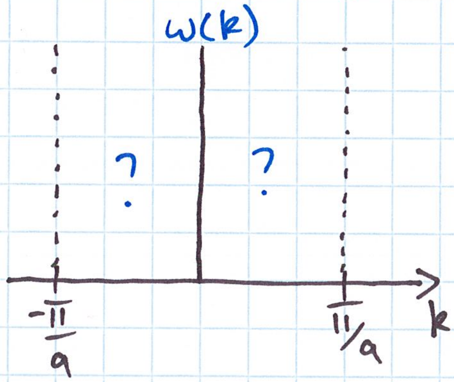
$$D(k) = \omega^2(k) = \sum_{m\neq 0} \left(e^{ikR^o_m} - 1\right) \frac{\varphi^o(m)}{M}$$

Recall: $k = \frac{2\pi}{Na} m$, m = integer **1D**

with N unique values of k (i.e. m)

choose: $m \in \left\{-\frac{N}{2}+1 , \frac{N}{2}\right\}$

i.e. $k = -\frac{\pi}{a} \rightarrow \frac{\pi}{a}$ ⇒ 1st Brillouin Zone



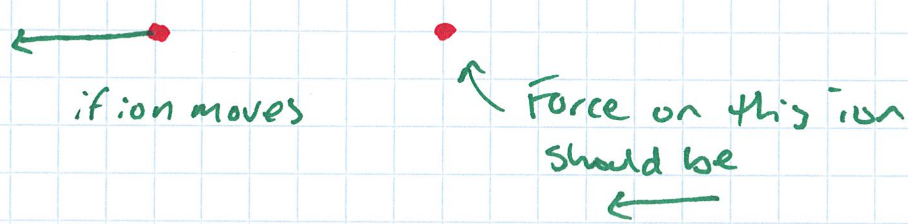
→ Dispersion curves can be plotted in 1st B.Z.

- the nature of $\omega(k)$ depends explicitly on $\varphi^o(m)$ i.e. the interaction potential

Simple model: Nearest Neighbour interactions only

Recall: In SHO model $\varphi^0(m)$ is just the force constant

Nearest Neighbours:



ie. Force should restore displacement

$m = \pm 1$

$$\varphi^0(\pm) \equiv -\gamma$$

$m \neq \pm 1$

$$\varphi^0(m) = 0$$

Dynamical Matrix:

$$D(k) = \omega^2(k) = \sum_{m \neq 0} \left(e^{ikR^0_m} - 1\right) \frac{\varphi^0(m)}{M}$$

In 1D: $R^0_m = ma$

$$\therefore \quad \omega^2(k) = -\frac{\gamma}{M}\left[e^{-ika} - 1 + e^{ika} - 1\right]$$

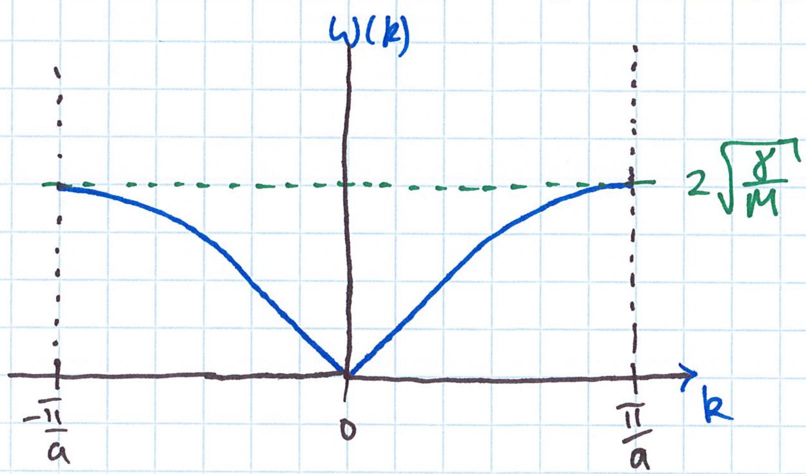
$$\omega^2(k) = \frac{-\gamma}{M}\left[e^{-ika} - 1 + e^{ika} - 1\right]$$

$$= \frac{2\gamma}{M}\left(1 - \cos ka\right)$$

$$= \frac{4\gamma}{M}\sin^2\left(\frac{ka}{2}\right)$$

$$\therefore \quad \boxed{\omega(k) = 2\sqrt{\frac{\gamma}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

1D linear chain $\bar{w}$ n.n. interactions



Low frequency regime (sound, or macroscopic regime)

$k \to 0 \Rightarrow \omega \propto k$ linear @ low freq.

$$\omega(k) \equiv C_s k = 2\sqrt{\frac{\gamma}{M}}\,\frac{ka}{2}$$

speed of sound $\longrightarrow C_s = a\sqrt{\frac{\gamma}{M}}$

Near B.Z. boundary:

$$k \approx \frac{\pi}{a} \qquad \omega \simeq 2\sqrt{\frac{\gamma}{M}} = \text{constant}.$$

Next example: 1^{st} & 2^{nd} N.N. interactions

$$\varphi^0(\pm 1) = -\gamma \quad ; \quad \varphi^0(\pm 2) = -\gamma\alpha$$

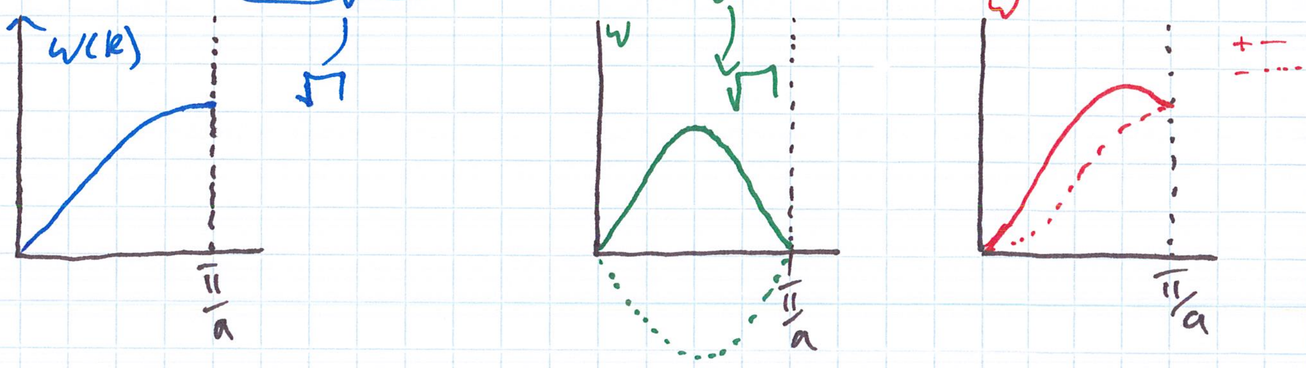
new parameter (presume <1, but not necessarily). Can be $\pm$

$$\omega^2(k) = \frac{-\gamma}{M}\left[(e^{ika}-1)+(e^{-ika}-1)+\alpha\left\{(e^{2ika}-1)+(e^{-2ika}-1)\right\}\right]$$

$$= \frac{2\gamma}{M}\left[1-\cos ka + \alpha(1-\cos 2ka)\right]$$

$$= \frac{4\gamma}{M}\left(\underbrace{\sin^2\left(\frac{ka}{2}\right)}_{\sqrt{}} + \alpha \underbrace{\sin^2(ka)}_{\sqrt{}}\right)$$

$\frac{1}{2}\lambda$ of first term.



→ Including longer range forces, i.e. 3, 4^{th} etc. next nearest neighbors, introduces $\sin^2$ terms $\bar{w}$ shorter wavelengths.

↳ adds modulation, wiggles, to dispersion curve.

Diatomic solid (1D chain)

→ 2 different atoms

↳ unit cell: - 2 atoms
- length $2a$

How can we treat a crystal $\bar{w}$ a basis?

Return to Dynamical Matrix.

$$D(k) = \sum_{\ell'} \frac{\phi(\ell,\ell')}{\sqrt{M_\ell M_{\ell'}}} e^{ik\cdot(R^o_{\ell'} - R^o_\ell)}$$

Sum over all atoms: $\bar{w}$ no basis, equiv. to sum over all unit cells.

Instead, label atom ℓ as: (n, α)

unit cell

atom in basis

atom ℓ is the basis atom α in unit cell n.

$\bar{R}_\ell = \bar{R}^o_n + \bar{R}_\alpha + \bar{u}_\ell$ → $\bar{R}_\alpha$ = position in unit cell

Before, $D(k)$ did not depend on ℓ explicity, ie. is the same for all ℓ.

Now, $D(k)$ does not depend on n, but does depend on α

→ does not depend on unit cell
→ does depend on basis atom.

Intuitively this should make sense.

$D(k)$ now a matrix $N_b \times N_b$ where

N_b is # of basis atoms in unit cell.

Aside

$D(k)$ is actually a square matrix w/ dimension equal to the degrees of freedom of the system.

$$d = N_d + N_b$$

d: dim. of $D(k)$

N_d: system dimension 1D, 2D, 3D

N_b: # basis atoms

Previously we looked @ 1D w/ 1 atom per unit cell
∴ $d=1 \Rightarrow D(k)$ gave 1 solution to $\omega^2(k)$.

Matrix elements of $D_{\alpha\beta}(k)$

$$D_{\alpha\beta}(k) = \sum_n \frac{\phi^{\circ}_{\alpha\beta}(n,n')}{\sqrt{M_\alpha M_\beta}} e^{ik\cdot(R^{\circ}_{n'} - R^{\circ}_{n})}$$

Again we can parameterize $n'-n=m$

$$\boxed{D_{\alpha\beta}(k) = \frac{1}{\sqrt{M_\alpha M_\beta}} \sum_m \varphi^{\circ}_{\alpha\beta}(m)\, e^{ikR^{\circ}_m}}$$

and:

$$\sum_{\beta,m} \varphi^{\circ}_{\alpha\beta}(m) = 0$$

E.V. equation:

$$\boxed{\begin{gathered} \omega^2(k)\,\epsilon_\alpha(k) = \sum_\beta D_{\alpha\beta}(k)\,\epsilon_\beta(k) \\ \omega^2\,\bar{\epsilon} = \hat{D}\,\bar{\epsilon} \end{gathered}}$$

Must solve:

$$|\hat{D} - \omega^2\hat{I}| = 0$$

For nontrivial solutions.

⇒ This is what we've been doing all along but w/ a single DoF!

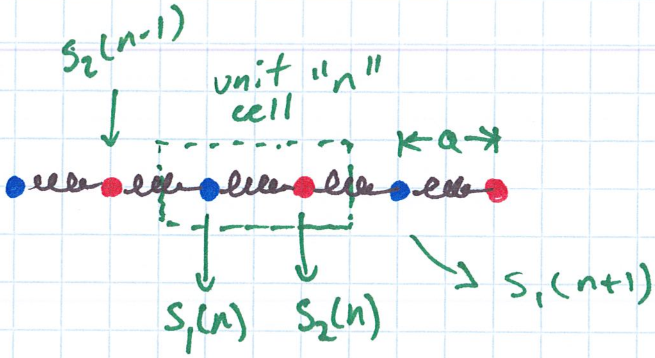
Back to the example.....

$$\bar{R}_\ell = \bar{R}^{\circ}_n + \bar{R}^{\circ}_\alpha + \bar{u}_\ell$$

$$\bar{u}_\ell = \frac{\epsilon_\alpha(k)}{\sqrt{M_\alpha}}\, e^{i\bar{k}\cdot\bar{R}^{\circ}_\alpha}\, e^{i\bar{k}\cdot\bar{R}^{\circ}_n}\, e^{-i\omega t}$$

$\varphi^{\circ}_{\alpha\beta}(m)$ → difference in unit cell

→ two atoms of interaction (atom type α,β in basis)



→ as before, assume interaction between atoms is characterized by the spring constant. γ.
Nearest neighbour interaction only

what are the $\hat{D}(k)$ elements?

$$\text{Between:} \rightarrow S_1(n) \ \& \ S_2(n) \Rightarrow \varphi^0 = -\gamma$$

$$\varphi^0_{12}(0) = -\gamma$$

$$\rightarrow S_1(n) \ \& \ S_2(n-1) \Rightarrow \varphi^0_{12}(-1) = -\gamma$$

all longer $\alpha = S_1$ interactions $\varphi = 0$.

<u>but</u>: $\sum_{\beta,m} \varphi^0_{\alpha\beta}(m) = 0$

$$\therefore \varphi^0_{11}(0) = 2\gamma$$

Likewise: $\varphi^0_{21}(0) = -\gamma$

$$\varphi^0_{21}(+1) = -\gamma$$

$$\varphi^0_{22}(0) = 2\gamma$$

$$D_{\alpha\beta} = \frac{1}{\sqrt{M_\alpha M_\beta}} \sum_m \varphi^0_{\alpha\beta}(m)\, e^{ikR^0_m}$$

e.g. $$D_{11} = \frac{1}{M_1}\, 2\gamma\, e^{ik\cdot 0} = \frac{2\gamma}{M_1}$$

$e^{ik\cdot 0} \to$ only $m=0$ term survives

$$D_{12} = \frac{1}{\sqrt{M_1 M_2}}\,(-\gamma)\Big(\underbrace{1}_{m=0} + \underbrace{e^{-ik(2a)}}_{m=-1}\Big)$$

$\to R^0_{-1} = 2a$, one unit cell

$$\hat{D}(k) = \begin{bmatrix} \dfrac{2\gamma}{M_1} & \dfrac{-\gamma}{\sqrt{M_1 M_2}}\left(1 + e^{-2ika}\right) \\ \dfrac{-\gamma}{\sqrt{M_1 M_2}}\left(1 + e^{2ika}\right) & \dfrac{2\gamma}{M_2} \end{bmatrix}$$

$$\left| \hat{D} - \omega^2 \hat{I} \right| = 0$$ $\Rightarrow$ will give 2 soln's for $\omega^2(k)$

$$\left(\frac{2\gamma}{M_1} - \omega^2\right)\left(\frac{2\gamma}{M_2} - \omega^2\right) - \frac{\gamma^2}{M_1 M_2}\left(1 + e^{2ika}\right)\left(1 + e^{-2ika}\right) = 0$$

$$\Rightarrow \omega^4 - 2\gamma\omega^2\left(\frac{1}{M_1} + \frac{1}{M_2}\right) - \frac{4\gamma^2}{M_1 M_2}\sin^2 ka = 0$$

$\to$ quadratic eqn in ω^2

Solutions:

$$\omega^2 = \gamma\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \gamma\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1M_2}\sin^2 ka}$$

What do these look like?

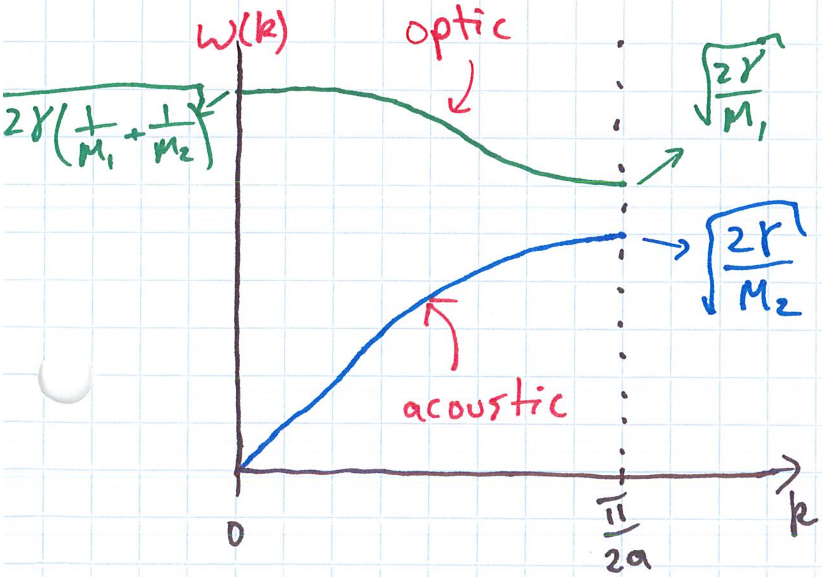
take small k ($ka \ll 1$)

$$\omega_+^2(k) \approx \gamma\left(\frac{1}{M_1} + \frac{1}{M_2}\right)\left(2 - \mathcal{O}(ka)^2\right) \approx 2\gamma\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$$

$$\omega_-^2(k) \approx \frac{2\gamma}{M_1+M_2}(ka)^2$$

$k = \frac{\pi}{2a}$ (zone boundary)

$$\left.\begin{matrix}\omega_+^2 \approx \dfrac{2\gamma}{M_1} & \qquad \omega_-^2 \approx \dfrac{2\gamma}{M_2}\end{matrix}\right\} \text{assumes } M_2 > M_1$$



Optic branch → $\omega \to$ const. @ low k (long wavelengths)

Acoustic branch → ω linear in k @ long wavelengths

Physical difference between Optical & Acoustic branches

Recall: $\hat{D}(k)\,\epsilon(k) = \omega^2 \epsilon(k)$

& $\epsilon(k) = \begin{bmatrix} \epsilon_1(k) \\ \epsilon_2(k) \end{bmatrix}$

where: $u_1 \propto \frac{1}{\sqrt{M_1}} \epsilon_1(k)$

$u_2 \propto \frac{1}{\sqrt{M_2}} \epsilon_2(k)$

From our dynamical matrix & our e.v. problem, we can write:

$$\frac{2\gamma}{M_1}\epsilon_1 - \frac{\gamma}{\sqrt{M_1 M_2}}\left(1 + e^{-2ika}\right)\epsilon_2 = \omega^2 \epsilon_1$$

(and a second similar eqn. but they are redundant)

For the optical branch in the $k \approx 0$ limit:

$$\omega^2 \approx 2\gamma\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$$

$$\therefore 2\left(\frac{1}{M_1} - \frac{1}{M_1} - \frac{1}{M_2}\right)\epsilon_1 = \frac{1}{\sqrt{M_1 M_2}}\left(1 + \underbrace{e^{-2ika}}_{\approx 1}\right)\epsilon_2 \quad k \approx 0$$

$$\therefore \frac{\epsilon_1}{\epsilon_2} \approx -\sqrt{\frac{M_2}{M_1}} \implies \frac{u_1}{u_2} \approx -\frac{M_2}{M_1}$$

Optical branch, small k:

$$\frac{u_1}{u_2} \approx -\frac{M_2}{M_1}$$

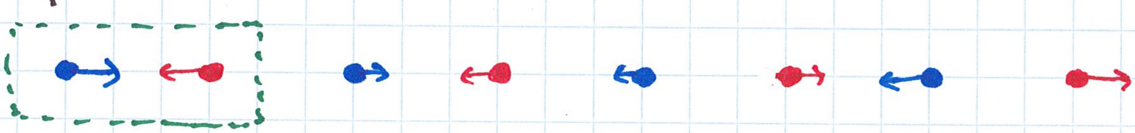
- displacements in opposite directions
- scaled by mass (inverse)

Acoustic branch: small k, $\omega \longrightarrow 0$

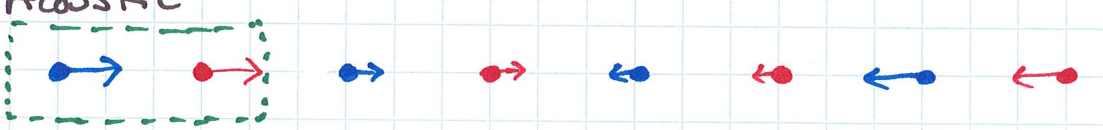
$$\frac{\epsilon_1}{\epsilon_2} \approx +\sqrt{\frac{M_1}{M_2}} \quad ; \quad \frac{u_1}{u_2} \approx +1$$

- displacements in same direction
not scaled by mass

Optical



Acoustic



Acoustic $\longrightarrow$ unit cell vibrates as one = "in phase"

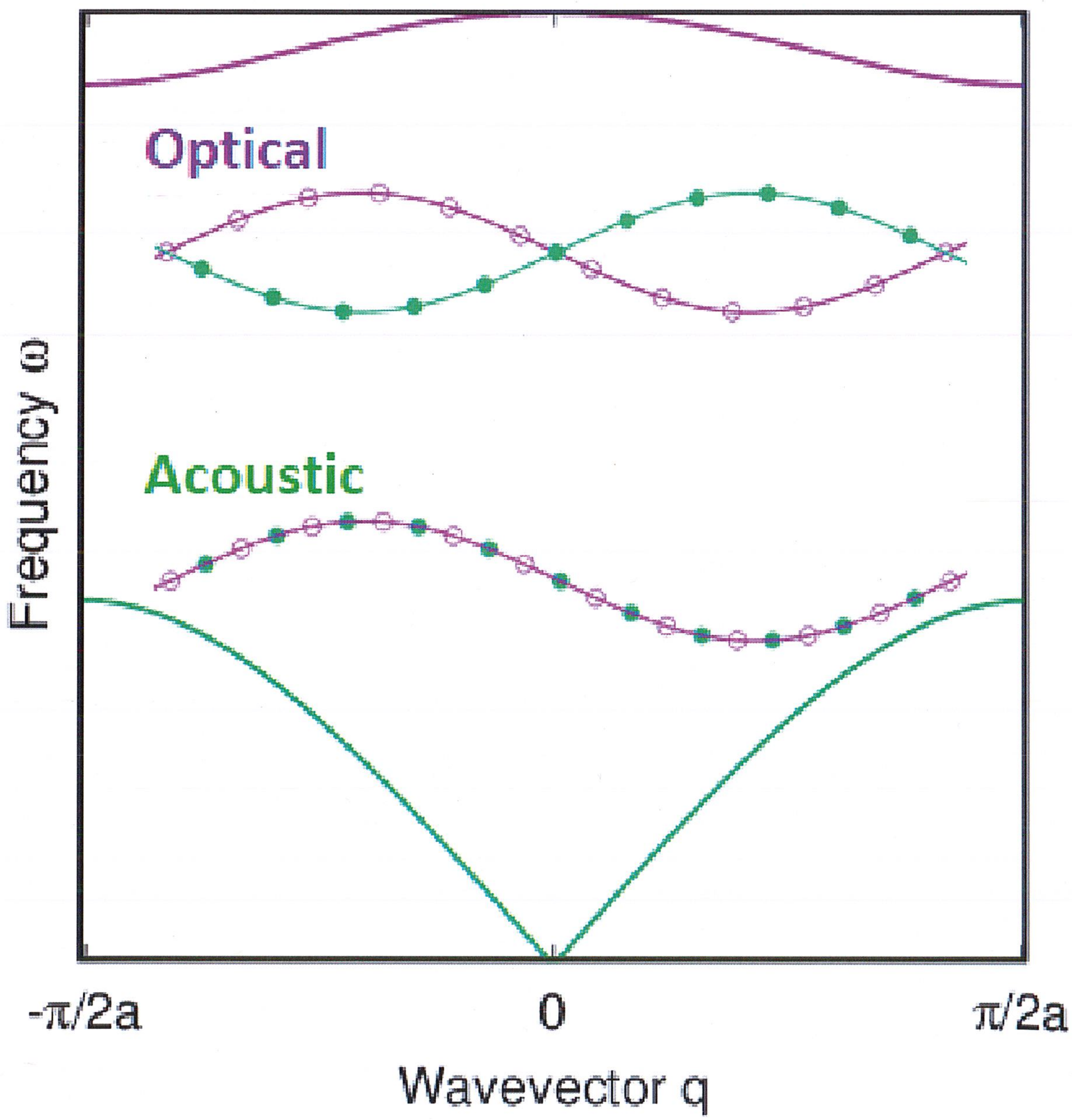
Optical $\rightarrow$ atoms in unit cell vibrate against each other

$\rightarrow$ atoms experience a molecular vibrational mode which couples to the lattice vibration

$\rightarrow$ results in time-varying electric dipole moment

↳ can couple to EM-radiation

$\rightarrow$ i.e. light, ~ IR, can excite optical phonons


Optical
Acoustic
Frequency ω
-π/2a
0
π/2a
Wavevector q