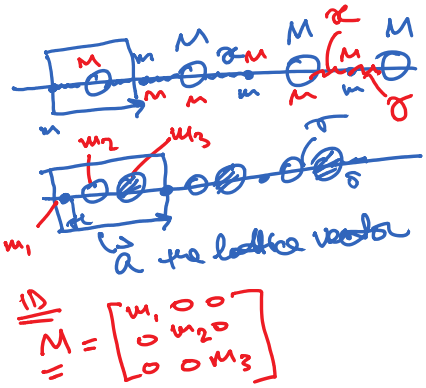
Saturday, March 21, 2020 6:29 PM

$$I_{km} = \frac{4}{8\pi^3}\left[\omega_{km}^4 |M_{km}|^2 + (\omega_{km}+\omega_L)^4 |C_{km}|^2 + \dots\right]$$

↑ Rayleigh scattering!

Lecture 16, Solid State Physics, March 31, 2020

Lattice with a basis: optical modes

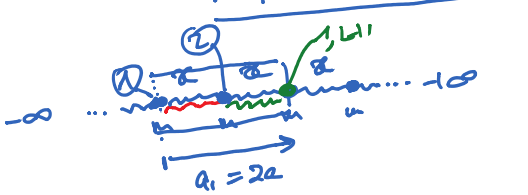


$$M = \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix}$$

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ basis vectors.

in 3D: $M = \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_1 & 0 \\ 0 & 0 & m_1 \end{bmatrix}$ ⊘ ⋮ ⊘ $\begin{bmatrix} m_2 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_2 \end{bmatrix}$ ⊘ ⊘ ⋱

A "fake" problem



$\vec{R} = n\vec{a}_1$, $\{\vec{b}_i\}$ } over the entire crystal (infinite)

$[\vec{b}_1 = 0, \vec{b}_2 = a]$ - basis

potential energy function:

$$V = \frac{\alpha}{2}\sum_{L}\left(u(2,L)-u(1,L)\right)^2 + \left(u(1,L+1)-u(2,L)\right)^2$$

↑ infinite — over entire crystal.

why? because the crystal is ∞!

e.g., $L' = 7a_1 = 7(2a)$

equal! $\frac{\partial^2 V}{\partial^2 V}$ $\frac{\partial^2 V}{\partial^2 V}$

$b_1 = 0, b_2 = \dots$

Hessian: $u(1,l), u(2,l)$

$\frac{\partial^2 V}{\partial u(1,l)\partial u(1,l')}$; $\frac{\partial^2 V}{\partial u(1,l)\partial u(2,l)}$; $\frac{\partial^2 V}{\partial u(2,l)\partial u(1,l')}$; $\frac{\partial^2 V}{\partial u(2,l)\partial u(2,l')}$ (equal!)

$\frac{\partial u(b,l)}{\partial u(b',l')} = \delta_{bb'}\delta_{ll'}$

$\frac{\partial}{\partial x}\frac{\partial}{\partial y} = \frac{\partial}{\partial y}\frac{\partial}{\partial x}$

you form a force constant matrix $\underline{\underline{\Theta}} = \begin{bmatrix} \Theta(11) & \Theta(12) \\ \Theta(21) & \Theta(22) \end{bmatrix}$

$b_1 \to u_1$; $u_1 \to b_2$; $b_2 \to u_2$

$$V' = \frac{\partial V}{\partial u(1\acute{l})} = \frac{\alpha}{2}\sum_l \left(-2u(2l)\delta_{l\acute{l}} + 2u(1l)\delta_{l\acute{l}} - 2u(2l)\delta_{l+1,\acute{l}} + 2u(1,l+1)\delta_{l+1,\acute{l}} \right) =$$

$$= -u(2\acute{l}) + u(1\acute{l}) - u(2\acute{l}-1) + u(1,\acute{l})$$

any cell, you can call it $l' \equiv 0$, then you take a derivative w.r.t. $\frac{\partial u(1,0)}{}$ atom 1 in central cell

$\frac{\partial}{\partial u(2,l)} V' = -2\alpha\delta_{\acute{l}l} = \Theta(11)$

got to rest of matrix elements Θ.

And now the lattice Fourier transform. $L = la_1 = l2a$ original interatomic distance.

$$\Theta_{11} = -2\alpha\delta_{l\acute{l}}$$

$$D_{11} = \sum_l -\frac{2\alpha}{m}\delta_{ll'} e^{i\vec{k}(\vec{L}-\vec{L}')} = \sum_l -\frac{2\alpha}{m}\delta_{l\acute{l}} e^{i\vec{k}2a(l-\acute{l})} = -\frac{2\alpha}{m} = D_{11}$$

force const.!

wave vector $\frac{2\pi}{\lambda} = k$

$$\left[\underline{\underline{D}} - \omega_+^2 \underline{\underline{M}}\right]\chi = \phi \Rightarrow M^{-1/2}(\quad) M^{-1/2} = \phi$$

$$\left[\underline{\underline{D}} - \omega_+^2\right]\chi' = \phi$$

regular eigenvalue problem, not a generalized one.

$$\frac{\partial V_1'}{\partial u(2l')} = -\alpha\left[-\delta_{l\acute{l}} - \delta_{l,\acute{l}}\right] = \Theta(1,2)$$

$$D_{12}(\vec{k}) = \sum_l \frac{\alpha}{m}\left[-\delta_{l\acute{l}} - \delta_{l-1,\acute{l}}\right] e^{i\vec{k}2a(l-\acute{l})} = -\frac{\alpha}{m}\left(1 + e^{i\vec{k}\vec{a}_1}\right)$$

$\vec{a}_1$

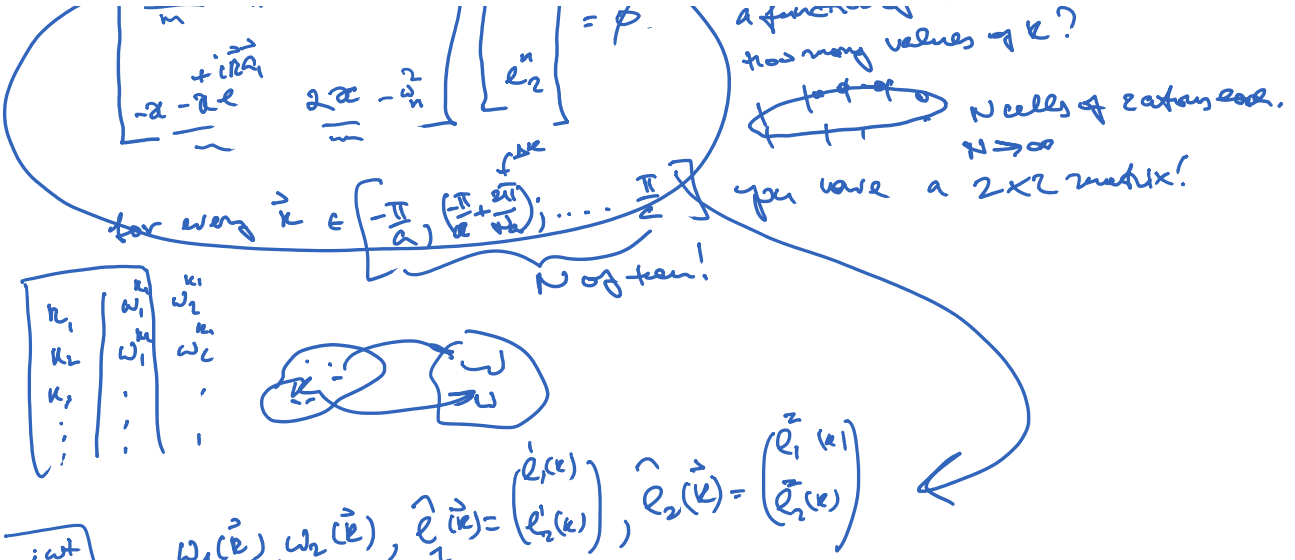
$$\underline{\underline{D}}(\vec{k}) = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$ ← hermitian. (Θ – symmetric)

$i\vec{k}a$; $i\vec{k}a_1$

$$\begin{bmatrix} \frac{2\alpha}{m} - \omega_+^2 & -\frac{\alpha - \alpha e^{\cdots}}{\sim} \\ \cdots & \frac{2\alpha}{\sim} - \omega_+^2 \end{bmatrix} \begin{bmatrix} l_1^n \\ l_2^n \end{bmatrix} = \phi$$

2×2 matrix! But it is a function of $\vec{k}$

how many values of k?



$\omega_1(\vec{k}), \omega_2(\vec{k}), \hat{e}_1(\vec{k}) = \begin{pmatrix} \hat{e}_1^x(k) \\ \hat{e}_1^y(k) \end{pmatrix}, \hat{e}_2(\vec{k}) = \begin{pmatrix} \hat{e}_1^z(k) \\ \hat{e}_2^z(k) \end{pmatrix}$

$e^{i\omega t}$

$\omega^2 < 0 \Rightarrow \omega = i\tilde{\omega}$

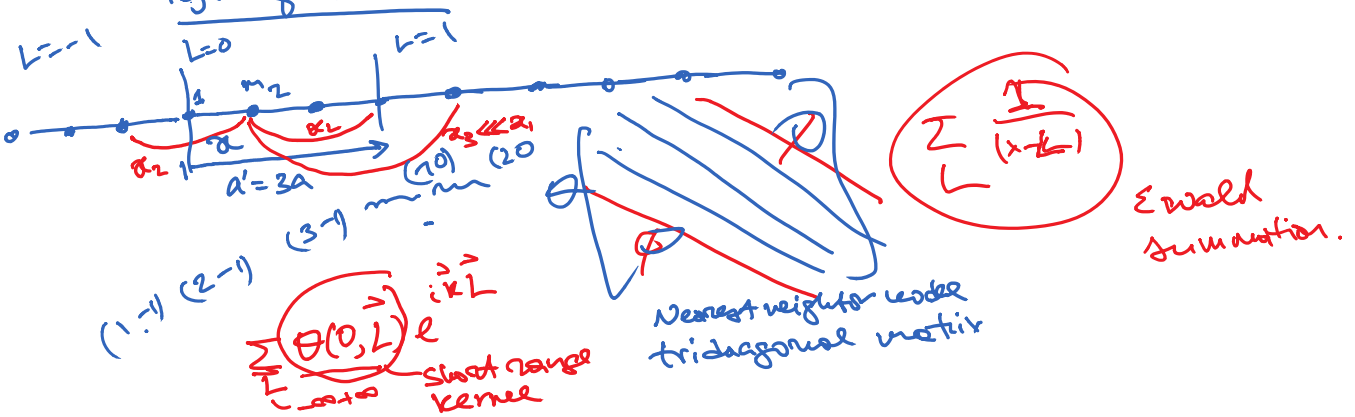
In MATLAB

pick up $\vec{k}$. → D → [U,V] = eig(D)

$\begin{bmatrix} \omega_1^2 & \\ & \omega_2^2 \end{bmatrix} \begin{bmatrix} \hat{e}_1^x & \hat{e}_1^z \\ \hat{e}_2^x & \hat{e}_2^z \end{bmatrix}$

repeat for every k of interest.

Taya's question:

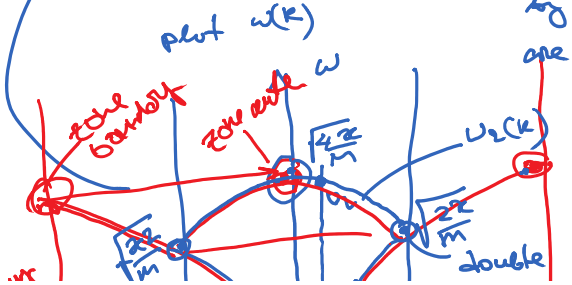


Say we diagonalize $\underline{\underline{D}}(k)$

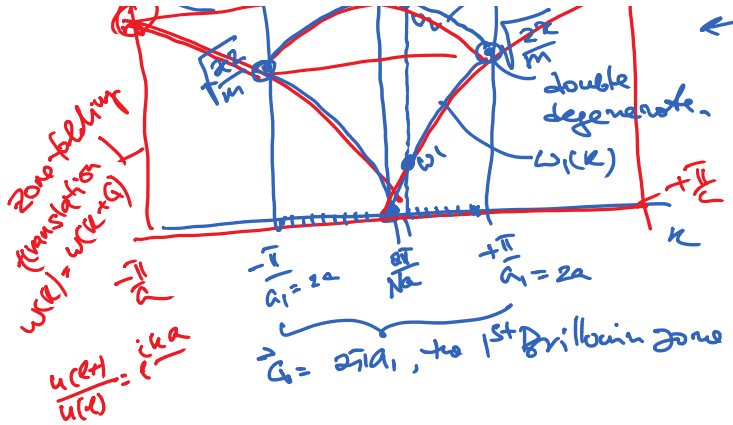
$\omega_{1,2}^2(\vec{k}) = \frac{2\alpha}{m} \pm \frac{\alpha}{m}\sqrt{2 - 2\cos ka_1}$

$a_1 = 2a$

wave vector k, values are governed by the PBC! N! and allowed values are separated by $\frac{2\pi}{N2a}$ ← length of the crystal.



← a real solution to a fake problem.



← a real ... a fake problem.

How to make it real?

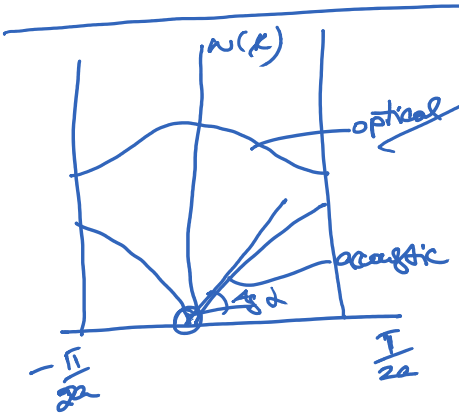
$x \to x_1, x_2$ (ALM)

$m \to M_1, M_2$ (Mandel)

$\vec{G} = 2\pi a_1$, the 1st Brillouin zone of my "real" crystal.

with different masses:

$$\omega^2 = \frac{\alpha}{M_1 M_2}\left(M_1 + M_2 \mp \sqrt{M_1^2 + 2M_1M_2\cos ka + M_2^2}\right)$$



take a limit of $\vec{k} \to 0$

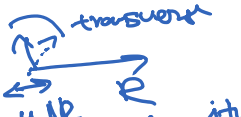
$k = \frac{2\pi}{\lambda}$

$k \to 0$

$\lambda \to \infty$

real vibes are parallel to the line, but I plot them as vertical.

a limit of continuous elastic medium.



for small k:

$$\omega_a = \sqrt{\frac{\alpha}{2(M_1+M_2)}}\,ka$$ — linear function of k — sound wave.

optical frequency $= \omega_0 = \sqrt{\frac{2\alpha(M_1+M_2)}{M_1 M_2}}$ — just a number.

① at zone center $k = 0$

ac. branch | → → | → → |

optical | → ← | → ← |

in the limit of identical masses and springs.

— a zone boundary vibration.

② at zone boundary $k = \frac{\pi}{a}$.

| → → | ← ← | ac.

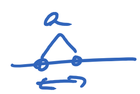
1 → ← k₀ → 1 ... .

Nicholas's question

BT only concerns itself with L, not b!

$e^{i\vec{k}(\ell a - \ell' a)}$ with $\ell \to L$, $\ell' \to L'$

$R(Lb)$, $R'(L'b') \to e^{i\vec{k}(R-R')} = e^{i\vec{k}(L-L'+b-b')} = e^{i\vec{k}(L-L')} e^{i\vec{k}(b-b')}$

in 

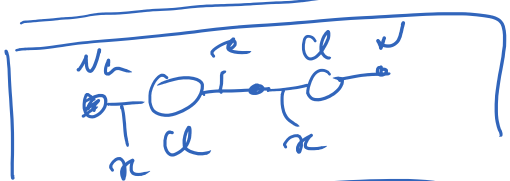
$$\begin{bmatrix} -\frac{\alpha}{m} & -\frac{\alpha}{m}\left(e^{-iqa} - e^{iqa}\right) \\ -\frac{\alpha}{m}\left(e^{ika} - e^{-ika}\right) & -\frac{\alpha}{m} \end{bmatrix}$$

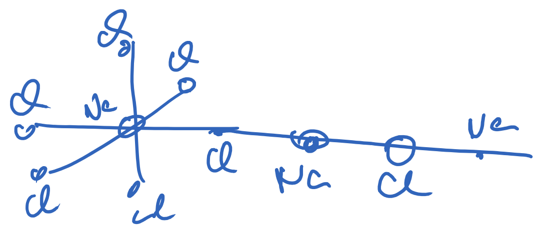
→ has the same eigenvalues but eigenvectors are different

changes $\hat{e}$

in the previous matrix $-\alpha - \alpha e^{-ik(2a)} = D_{12}(k)$

This model in a 1D NaCl (rock salt)





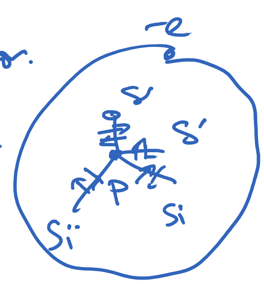
m_{Na}, M_{Cl} Ashkroft-Mermin

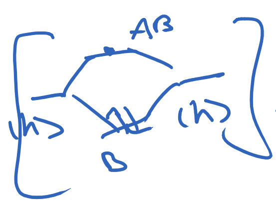
The recipe:

choose the lattice vector.

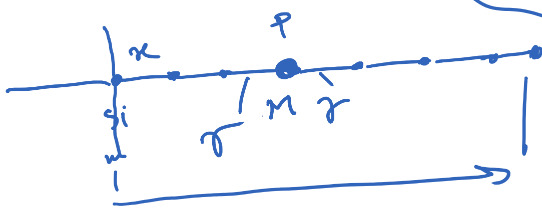
P@Si ⇒ N-type

Si (IV) P (V)





4 times.



double ⇒ 2 branches.

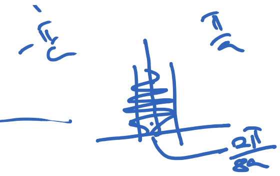
8x8 matrix

$\omega_1, \omega_2 \dots \omega_8 \;\forall \vec{k}$.

... crystal axes $a_1 = 8a$

an ∞ crystal and every 8a there is a P atom!

$a_1 = 8a$



8x8 matrix

$\omega_1, \omega_2 \ldots \omega_8 \; \forall \vec{k}$.

2. Basis

$b_1 = 0$, Si, m_{Si}

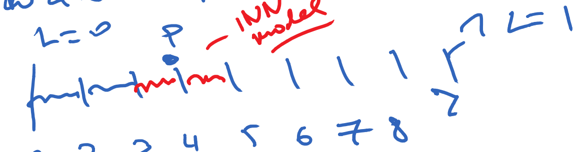
$b_2 = a$ Si, m_{Si}

⋮

$b_4 = 3a$ P — m_P

⋮

3. write the potential energy formula.



$$\sum_L [u(2,0)-(1,0)]^2 \frac{\alpha}{2} + [u(3,0)-u(2,0)]^2 \frac{\alpha}{2} + [u(4,0)-u(3,0)]^2 \frac{\gamma}{2} + [u(5,0)-u(4,0)]^2 \frac{\gamma}{2} + [u(6,0)-u(5,0)]^2 \frac{\alpha}{2} \ldots 7, 8$$

$$\frac{\alpha}{2}[u(1,L+1)-u(8,0)]^2$$

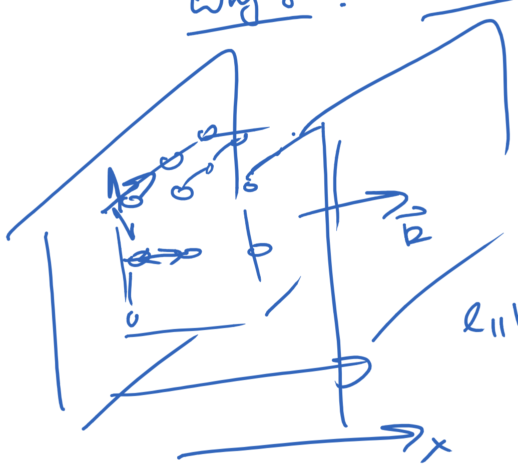
8x8 dynamical matrix

$\Phi \quad \frac{\partial^2 V}{\partial u_i \partial u_j}$ 8x8 $\rightarrow D = \sum_L \Phi(0,L) e^{ikL} \Rightarrow M^{-\frac{1}{2}} D M^{-\frac{1}{2}} = \tilde{D}(k)$.

$\Rightarrow \omega_1, \omega_2, \omega_3 \ldots \omega_8$.

why 8? I don't know.

4, 8, 12, 16. ✓ no difference.



LO/TO splitting

TO LO

∇

$k \cdot E$

$k \parallel E$

$k \perp E = 0$

$e_{\parallel} k$ — longit.

, (y,z) transverse.