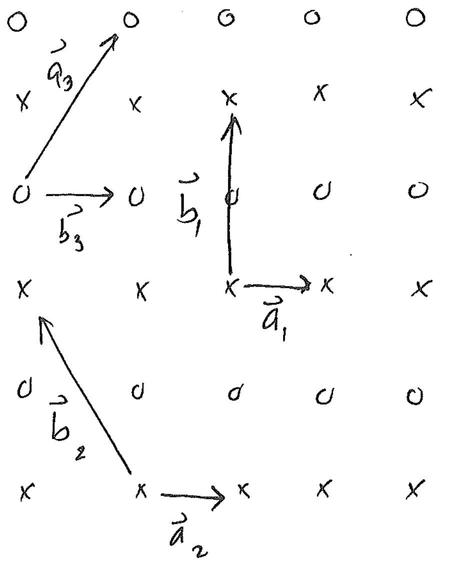
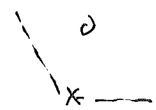
Exam 1 - Solutions

1/ (a) two examples of primitive cells

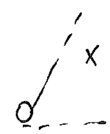


$\vec{a}_1, \vec{b}_1$ has the basis

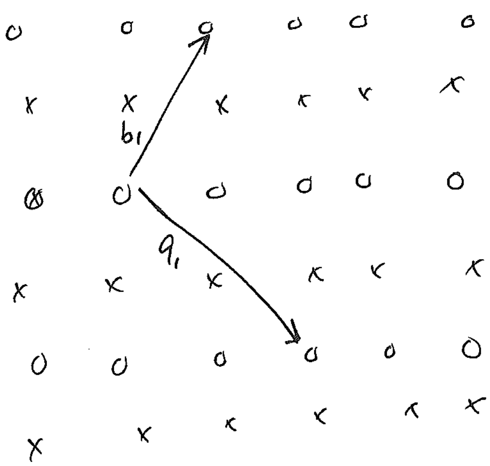
$\vec{a}_2, \vec{b}_2$ has the basis



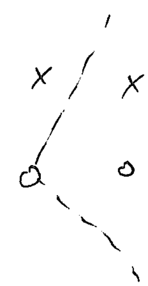
$\vec{a}_3$ $\vec{b}_3$ has the basis



(b) example of non-primitive cells

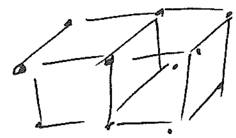


$\vec{a}_1, \vec{b}_1$ has basis



2) (a) Negative (−). Negative energy indicates that energy has to be added to $\underbrace{\text{unbind (or free)}}_{E \geq 0}$ the ion from the crystal

(b) $\dfrac{-6e^2}{4\pi\epsilon_0 a^2}$



6: the 6 nearest neighbours

a: that are a distance a away

$-e^2$: the neighbor has the opposite charge

ex: Na^+ surrounded by 6 Cl^- ions

$\dfrac{+12e^2}{4\pi\epsilon_0 a\sqrt{2}}$

12: the 12 atoms

$a\sqrt{2}$: that are a distance $a\sqrt{2}$ away

$+e^2$: there are the same charge

ex: the 8 closest Na^+ ions to a single Na^+

$\dfrac{-8e^2}{\dots a\sqrt{3}}$

8: the 8 atoms

$a\sqrt{3}$: that are a distance $a\sqrt{3}$ away

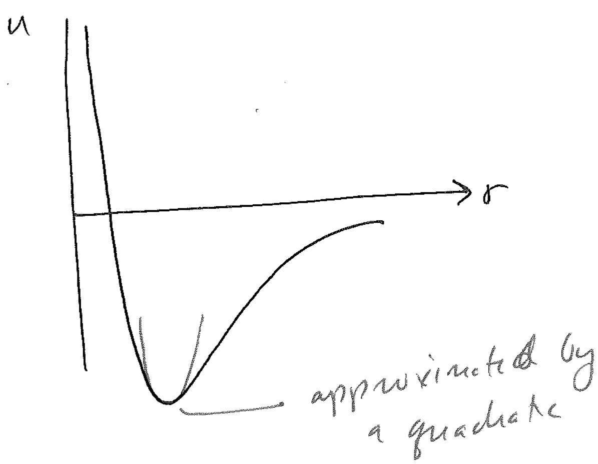
$(-e^2)$: these are opp. charge

Ex: the second closest Cl^- atoms to Na^+

3/ (a) $+\left(\frac{c}{r}\right)^2$ is the repulsion

$-\left(\frac{b}{r}\right)$ attraction.

(b) For a system to exhibit SHO, its $U(x) = \frac{1}{2}kx^2$.
In general, any system with a minimum in potential will show SHO in the limit of small displacements from equilibrium. That is



Show this using a Taylor series expansion around $r = r_m$

$$u(r) \approx \underbrace{u(r_m)}_{\text{offset to potential}} + \underbrace{u'(r_m)(r-r_m)}_{=0 \text{ since } r_m \text{ is the minimum}} + \underbrace{\frac{u''(r_m)(r-r_m)^2}{2!}}_{\text{the SH term.}} + \cdots$$

$$u(r) = a\left[c^2 r^{-2} - b r^{-1}\right]$$

$$u'(r) = a\left[c^2(-2)r^{-3} - b(-1)r^{-2}\right]$$

$$u''(r) = a\left[c^2(-2)(-3)r^{-4} - b(-1)(-2)r^{-3}\right]$$

$$= a\left[6c^2 r^{-4} - 2br^{-3}\right]$$

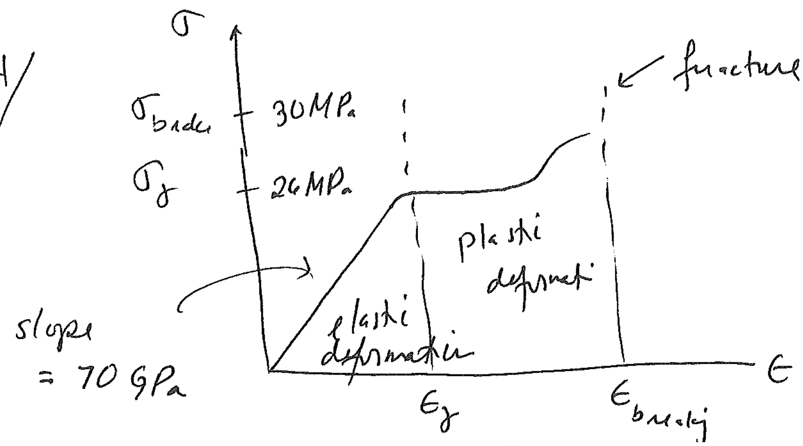
$$u''(r_m) = a2\left[\frac{3c^2}{(2c^2/b)^4} - \frac{b}{(2c^2/b)^3}\right]$$

3 (Cont'd)

$$U''(r_m) = \frac{ab^4}{8c^6}$$

So $$U(r) \simeq U(r_m) + \frac{1}{2}\left[\frac{ab^4}{8c^6}\right][r - r_m]^2$$

4/



$$Y = \frac{\sigma}{\epsilon}$$

$$\epsilon = \frac{\sigma}{Y} = \frac{F/A}{Y} = \frac{8500}{\pi(r_o^2 - r_i^2)} \frac{1}{70 \cdot 10^9}$$

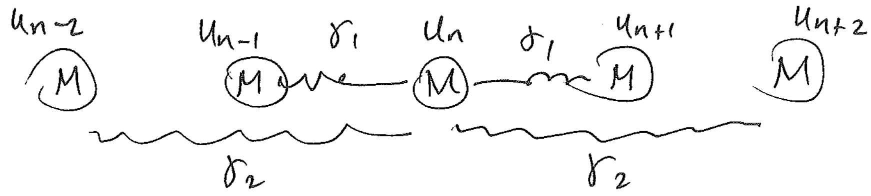
$$\epsilon = \frac{8500}{\pi\left[\left(\frac{0.1625}{2}\right)^2 - \left(\frac{0.16}{2}\right)^2\right]} \frac{1}{70 \cdot 10^9} = 0.19 \cdot 10^{-3}$$

actual compression

$$\frac{\Delta l}{l} = \epsilon$$

$$\Delta l = \epsilon l = 0.6 \text{ mm}$$

5/ Start by applying Newton's 2nd law to the n^{th} atom



$$F = m \frac{d^2 u_n}{dt^2}$$

$$\begin{aligned} -\gamma_1 (u_n - u_{n-1}) + \gamma_1 (u_{n+1} - u_n) \\ -\gamma_2 (u_n - u_{n-2}) + \gamma_2 (u_{n+2} - u_n) \end{aligned} = m \frac{d^2 u_n}{dt} \qquad (1)$$

Propose the following solution

$$u_n(t) = u_0 e^{i(kan - \omega t)} \quad \text{for the } n^{th} \text{ atom} \qquad (2a)$$

$$u_{n-1}(t) = u_0 e^{i(ka(n-1) - \omega t)} \quad (n-1)^{th} \text{ atom} \qquad (2b)$$

and so on.

Sub in (2a), (2b) and similar eqns for $n-2, n+2, n+1$ into (1).

In order for (2) to be a solution of (1),

ω will have to be related to k in some way.

This relationship, $\omega(k)$, is the dispersion relation.

6/ The group velocity $V_G = \frac{d\omega}{dk}$.

(a) In the limit $k \to 0$, we can approximate $\cos ka \approx 1 - \frac{(ka)^2}{2}$

$$\omega^2 \approx \frac{2\gamma}{M}\left[1 - \left(1 - \frac{(ka)^2}{2}\right)\right]$$

$$\omega^2 \approx \frac{2\gamma}{M}\left[\frac{(ka)^2}{4}\right]$$

$$\omega = \sqrt{\frac{\gamma}{2M}}\, ka$$

$$\frac{d\omega}{dk} = \sqrt{\frac{\gamma}{2M}}\, a$$

(b) In the limit $k \to \frac{\pi}{a}$, take the derivative directly

$$\omega = \sqrt{\frac{2\gamma}{M}}\left[1 - \cos(ka)\right]^{1/2}$$

$$\frac{d\omega}{dk} = \sqrt{}\left(\tfrac{1}{2}\right)\left(1 - \cos(ka)\right)^{-1/2}\left(+\sin(ka)\right)(a)$$

$$\frac{d\omega}{dk} = \sqrt{\frac{\gamma}{2M}}\,\frac{a\sin(ka)}{\left[1 - \cos(ka)\right]^{1/2}}$$

$$\left.\frac{d\omega}{dk}\right|_{k=\frac{\pi}{a}} = \sqrt{}\,\frac{a\sin(\pi)}{\left[1 - \cos(\pi)\right]^{1/2}} = 0$$

* note: you can also use this to evaluate $\left.\frac{d\omega}{dk}\right|_{k=0}$, but you'll note that this leads to $\frac{0}{0}$ if you just evaluate at $k=0$. See your calc text on how to do this.

4 cont'd/

(c) since $k = \frac{2\pi}{\lambda}$, $k \to 0$ is the long wavelength limit

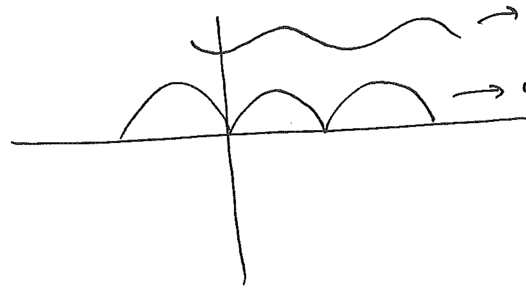
(d) there is <u>no</u> optical branch.

If there are 2+ branches, it means that

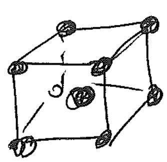
ω has 2+ possible positive values for a given k.

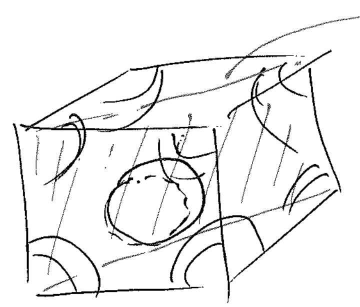
- $\omega = \# \pm \#$

  indicates 2 values of ω

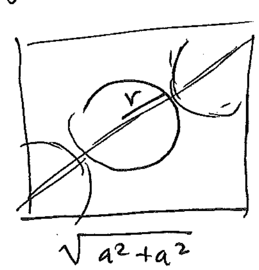
- 

7/ bcc





along the central diagonal



$$\text{packing fraction} = \frac{\text{Volume ions}}{\text{Volume cell}}$$

$$a^2 + a^2 + a^2 = (4r)^2$$

$$3a^2 = 16r^2$$

$$\frac{\sqrt{3}}{4}a = r$$

$$= \frac{\left(1 \times \frac{4}{3}\pi r^3\right) + 8 \times \frac{1}{8}\left(\frac{4}{3}\pi r^3\right)}{a^3}$$

$$= \frac{\frac{8}{3}\pi r^3}{a^3} = \frac{\frac{8}{3}\pi\left[\frac{\sqrt{3}}{4}a\right]^3}{a^3} = \frac{\cancel{8}^{2}\pi\,\cancel{3}\sqrt{3}}{\cancel{3}\,\cancel{4}\cdot 4\cdot \cancel{4}2} = \frac{\sqrt{3}\pi}{8} = 68\%$$

8/ (a) Li, Mg, P - elements in same column have same # valence e^-

increasing # in valence $\longrightarrow$

(b) Be, O, Ne - in general, ionization energy increases w/ column $\longrightarrow$

(c) $1s^6$ - all e^- would be in the gnd state

9/ (a) $2d \sin\theta = m\lambda$

$$d = \frac{m\lambda}{2\sin\theta} = \frac{(1)(0.109\cdot 10^{-9})}{2(\sin 12.6^\circ)} = 0.25 \text{ nm}$$

(b) $E = \frac{p^2}{2m}$ and $\lambda = \frac{h}{p}$

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{6.6\cdot 10^{-34}}{\sqrt{2(9.1\cdot 10^{-31})\left(200\cdot 10^{3}\text{ eV}\,\frac{1.6\cdot 10^{-19}\text{ J}}{\text{eV}}\right)}}$$

$= 2.7\cdot 10^{-12}$ m

$= 0.0027$ nm