Kittel 3.2

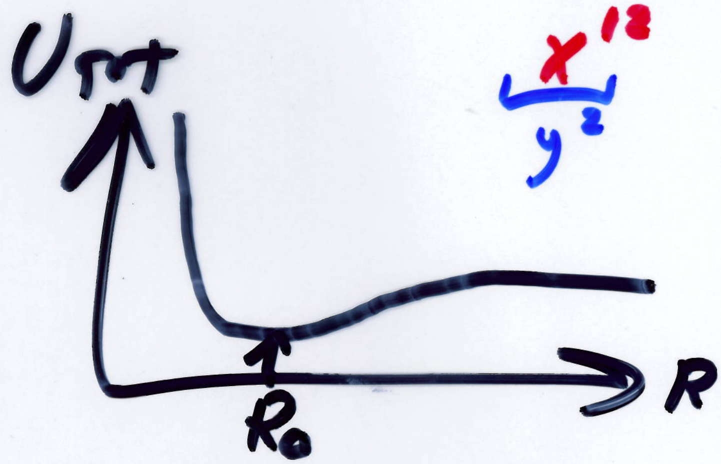
fcc $\frac{R_0}{\sigma} = 1.09$ (3-14) theory

$\frac{R_0}{\sigma} = 1.14$ experimentally.

$$U_{tot} = \frac{1}{2} N 4\epsilon \left[\underbrace{\sum_j{}' \left(\frac{\sigma}{r_{ij}}\right)^{12}}_{\text{repulsive}} - \underbrace{\sum_j{}' \left(\frac{\sigma}{r_{ij}}\right)^{6}}_{\text{attractive}} \right]$$

$r_{ij} \equiv R\, p_{ij}$

$$U_{tot} = \frac{1}{2} N 4\epsilon \left[\underbrace{\underbrace{\left(\frac{\sigma}{R}\right)^{12}}_{x^{12}}}_{y^2} \underbrace{\sum_j{}' p_{ij}^{-12}}_{p12} - \underbrace{\underbrace{\left(\frac{\sigma}{R}\right)^{6}}_{x^{6}}}_{y} \underbrace{\sum_j{}' p_{ij}^{-6}}_{p6} \right]$$



$$0 = \frac{dU_{tot}}{dy} = \frac{d}{dy} \frac{1}{2} N 4\epsilon \left[p12 \cdot y^2 - p6\, y \right]$$

$$= \frac{1}{2} N 4\epsilon \left[2 \cdot p12 \cdot y - p6 \right]$$

$$y = \frac{p6}{2\, p12}$$

$$y = \left(\frac{\sigma}{R}\right)^6 = \frac{p6}{2p12} = \begin{cases} fcc: 0.595700 \\ bcc: 0.6722108 \end{cases}$$

fcc: $p6 = 14.45392$ $\quad p12 = 12.13188$

bcc: $p6 = 12.2533$ $\quad p12 = 9.11418$

$$\frac{R}{\sigma} = \begin{cases} fcc: 1.090173 \\ bcc: 1.06843 \end{cases}$$

$$\frac{U_{tot\ bcc}}{U_{tot\ fcc}} = \frac{(y^2 P_{12} - y P_6)_{bcc}}{(y^2 P_{12} - y P_6)_{fcc}}$$

$$= \frac{(0.672)^2 9.114 - (0.672)\ 12.25}{(0.595)^2 12.131 - (0.595)\ 14.45} = 0.9566$$

$$= \frac{-4.1184\ eV}{-4.305\ eV}$$

$U_{fcc} < U_{bcc}$ $\quad$ fcc more tightly bound.

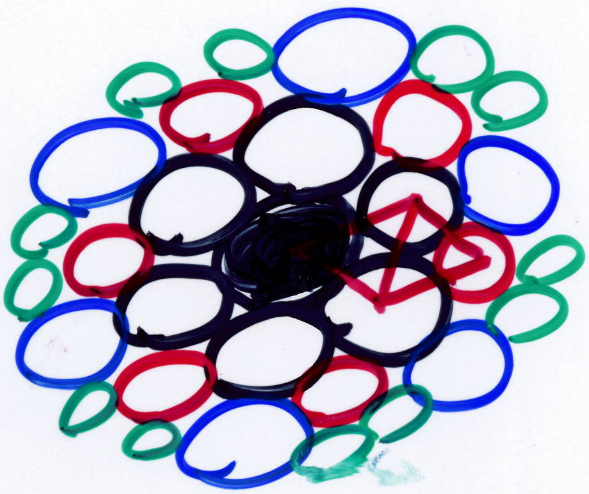
$\rho_{ij} = 1 \quad r_{ij} = d$ — # n.n = 6

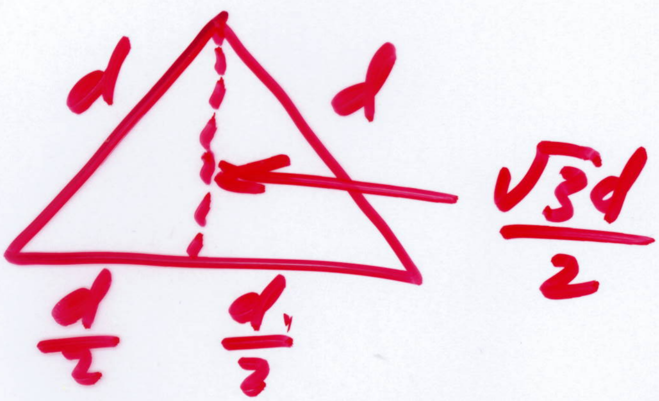
$\rho_{ij} = \sqrt{3} \quad r_{ij} = \sqrt{3}\,d$ # n.n.n. = 6

$\#$ n.n.n.n. 6

$r_{ij} = 2d$

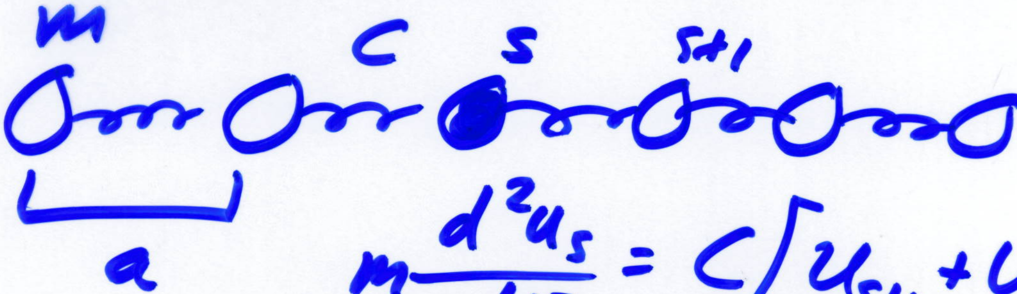
$\rho_{ij} = 2$





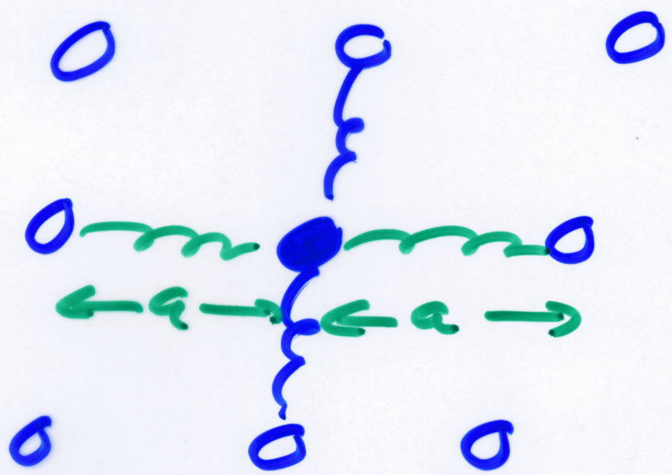
$$P6 = {\sum_j}' \frac{1}{\rho_{ij}^6} = \frac{6}{1^6} + \frac{6}{(\sqrt{3})^6} + \frac{6}{2^6}$$

$$P12 = {\sum_j}' \frac{1}{\rho_{ij}^{12}} = \frac{6}{1^{12}} + \frac{6}{(\sqrt{3})^{12}} + \frac{6}{2^{12}}$$



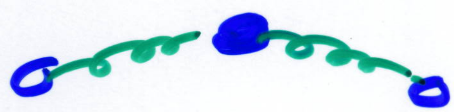
$$m\frac{d^2u_s}{dt^2} = C[u_{s+1} + u_{s-1} - 2u_s]$$

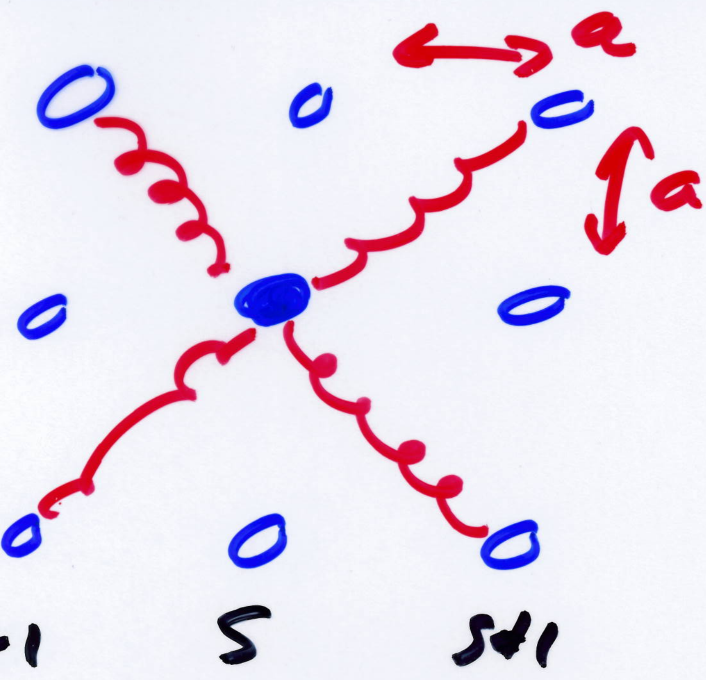
$$= C[u_{s+1} - u_s] + C[u_{s-1} - u_s]$$



Restoring force.

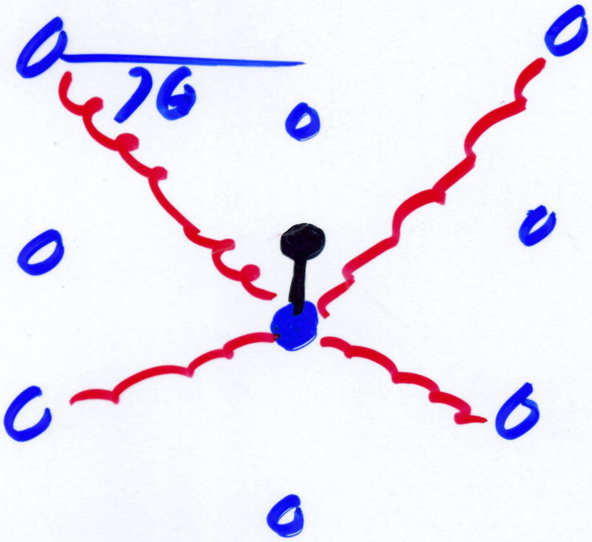
$$F \propto \frac{u^3}{a^2}$$

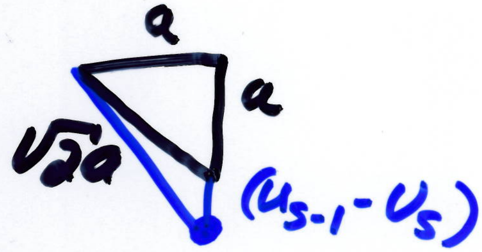




spring was rest length $\sqrt{2}\,a$

Left side





new length of spring is

$$\sqrt{a^2 + [a + (u_{s-1} - u_s)]^2}$$

$$= \sqrt{2a^2 + 2a^2\frac{(u_{s-1} - u_s)}{a} + \cancelto{0}{(u_{s-1} - u_s)^2}}$$

$$= \sqrt{2}\, a \left[1 + \frac{(u_{s-1} - u_s)}{a}\right]^{1/2}$$ binomial theorem

$$(1+x)^n \approx 1 + nx + \ldots O(x^2)$$

$$= \sqrt{2}\, a \left[1 + \frac{(u_{s-1} - u_s)}{2a} + \ldots\right]$$

spring has been stretched $\dfrac{(u_{s-1} - u_s)}{\sqrt{2}}$

force $F = C' \frac{(u_{s-1} - u_s)}{\sqrt{2}}$

vertical component $F_y = F \sin\theta = C' \frac{(u_{s-1} - u_s)}{2}$

Now both left springs

$$F_y = C'(u_{s-1} - u_s)$$

Both right springs

$$F_y = C'(u_{s+1} - u_s)$$

Total force 4 springs $= C'[u_{s+1} + u_{s-1} - 2u_s]$

same form as longitudinal wave

Long. - nearest neighbors

Trans. - <u>next</u> to nearest neighbors

Monatomic basis → 3 modes of vibration
1 longitudinal, 2 transverse.

Polyatomic basis ⇒ new dispersion relation feature

e.g. 2 atom basis ⇒ 2 branches for each mode of vibration.

LO   2TO } 6 total
LA   2TA } 3

L - Longitudinal   T - transverse
O - optical   A - acoustic

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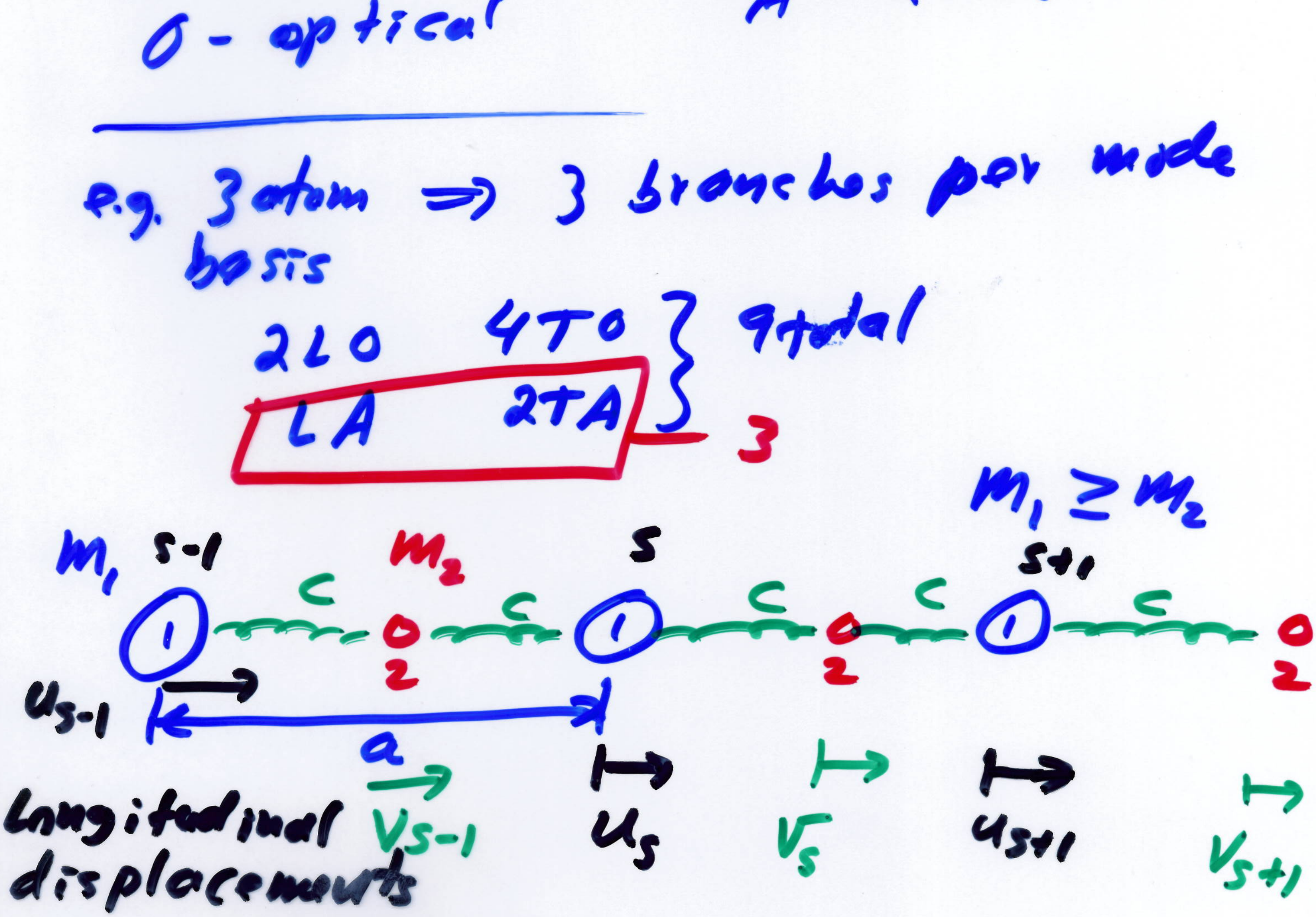
e.g. 3 atom basis ⇒ 3 branches per mode

2LO   4TO } 9 total
LA   2TA } 3

$M_1 \geq M_2$



$$m_1 \frac{d^2 u_s}{dt^2} = C[v_{s-1} - u_s] + C[v_s - u_s]$$

$$= C[v_{s-1} + v_s - 2u_s]$$

$$m_2 \frac{d^2 v_s}{dt^2} = C[u_s - v_s] + C[u_{s+1} - v_s]$$

$$= C[u_s + u_{s+1} - 2v_s]$$

Look for wave-like solutions.
(Take Fourier space and time transforms.)

$a \cdot s = x$

$$u_s = A e^{i(kas - \omega t)}$$

$$v_s = B e^{i(kas - \omega t)}$$

$e^{i(kas - \omega t)} \sim e^{i(kx - \omega t)}$ right moving wave

Look at point in wave with zero phase.