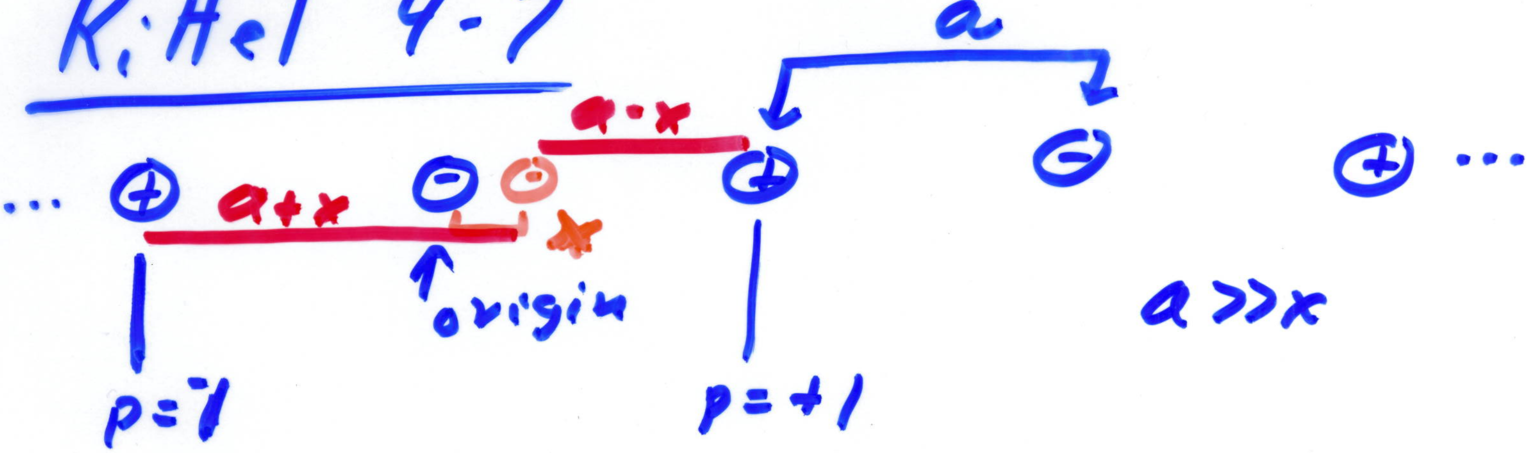
Kittel 4-7



$$F_1 = \frac{+e^2}{(a-x)^2} - \frac{e^2}{(a+x)^2} = \frac{e^2}{a^2(1-\frac{x}{a})^2} - \frac{e^2}{a^2(1+\frac{x}{a})^2}$$

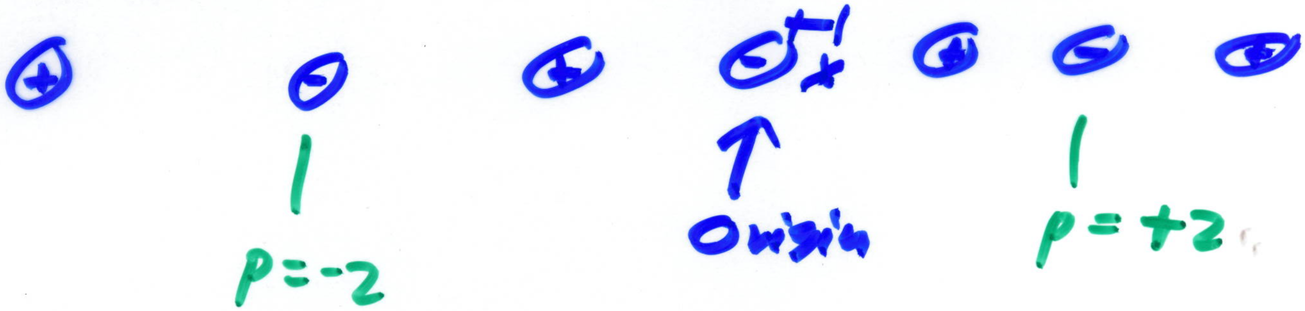
$$= \frac{e^2}{a^2}\left[\left(1-\frac{x}{a}\right)^{-2} - \left(1+\frac{x}{a}\right)^{-2}\right]$$

dipole

$$\approx \frac{e^2}{a^2}\left[\left(1+\frac{2x}{a}+\dots\right) - \left(1-\frac{2x}{a}+\dots\right)\right]$$

$$= \frac{e^2}{a^2}\frac{4x}{a} + O\left(\frac{x^3}{a^3}\right), \quad F_1 = -2C_{1c}\,x$$

$$\Rightarrow C_{1c} = \frac{-2e^2}{a^3}$$



$$F_2 = \frac{e^2}{(2a+x)^2} - \frac{e^2}{(2a-x)^2}$$

$$\approx \frac{e^2}{(2a)^2}\left[\left(1-\frac{2x}{2a}+\cdots\right)-\left(1+\frac{2x}{2a}+\cdots\right)\right]$$

$$= \frac{e^2}{(2a)^2}\left(\frac{-4x}{2a}\right) + O\left(\frac{x^3}{a^3}\right) \; ; \quad F_2 = -2C_{2c}\,x$$

$$\Rightarrow C_{2c} = +\frac{2e^2}{(2a)^3}$$

$$C_{pc} = (-1)^p \frac{2e^2}{(pa)^3}$$

Eq 16-a)

$$\omega^2 = \frac{2}{M} \sum_{p>0} C_p \left[1 - \cos(pka)\right]$$

$$C_1 = C_{1R} + C_{1c} \qquad , \qquad C_2 = C_{2c}$$
$$= \gamma - \frac{2e^2}{a^3} \qquad\qquad C_3 = C_{3c}$$

$$\omega^2 = \frac{2}{M} \gamma \left[1 - \cos(ka)\right] + \frac{2}{M} \sum_{p>0} \frac{(-1)^p 2e^2}{(pa)^3} \left[1 - \cos(pka)\right]$$

$$\omega^2 = \underbrace{\frac{4\gamma}{M}}_{\omega_0^2} \sin^2\left(\frac{ka}{2}\right) + \underbrace{\frac{4\gamma}{M}}_{\omega_0^2} \underbrace{\frac{e^2}{\gamma a^3}}_{\sigma} \sum_{p>0} (-1)^p \frac{\left[1 - \cos(pka)\right]}{p^3}$$

c) Brillouin zone boundary: $k = \frac{\pi}{a}$

$\omega^2 = 0$

$$\frac{\omega^2}{\omega_0^2} = 0 = \sin^2\left(\frac{\pi}{2}\right) + \sigma \sum_{p>0} (-1)^p \frac{[1-\cos(p\pi)]}{p^3}$$

$$0 = 1 + \sigma \sum_{p>0} \frac{(-1)^p}{p^3} \underbrace{\left[1-(-1)^p\right]}_{\substack{0 \text{ if } p\text{-even} \\ 2 \text{ if } p\text{-odd}}}$$

$$0 = 1 + \sigma \sum_{\substack{p \\ \text{odd}}} \frac{(-1)2}{p^3} = 1 - 2\sigma \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3}$$

$$\sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3} = \left(\frac{1}{1^3} + \frac{1}{3^3} + \frac{1}{5^3} + \cdots\right)$$

$\zeta(3)$ $\qquad$ $\zeta(s)$ = Riemann zeta function

$$\zeta(3) = \left(\frac{1}{1^3} + \frac{1}{2^3} + \frac{1}{3^3} + \frac{1}{4^3} + \frac{1}{5^3} + \cdots\right) = 1.202$$

$$\zeta(2) = \left(\frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \cdots\right) = \frac{\pi^2}{6}$$

$$\zeta(1) = \left(\frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \cdots\right) \to \infty$$ harmonic series

$$\zeta(3) = \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3} + \sum_{\substack{p \\ \text{even}}} \frac{1}{p^3}$$

$$= \frac{1}{2^3} + \frac{1}{4^3} + \frac{1}{6^3} + \cdots$$

$$= \frac{1}{2^3}\underbrace{\left[\frac{1}{1^3} + \frac{1}{2^3} + \frac{1}{3^3} + \cdots\right]}_{\zeta(3)}$$

$$= \frac{1}{2^3}\left[\sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3} + \sum_{\substack{p \\ \text{even}}} \frac{1}{p^3}\right]$$

$$\zeta(3) = \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3}\left[1 + \frac{1}{8} + \frac{1}{64} + \cdots\right]$$

$$= \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3}\left[\frac{1}{1-\frac{1}{8}}\right] = \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3}\left(\frac{8}{7}\right)$$

$$\Rightarrow \sum_{\substack{p \\ \text{odd}}} \frac{1}{p^3} = \frac{7}{8}\zeta(3)$$

$$0 = 1 - 2\sigma \frac{7}{8} \zeta(3)$$

$$\sigma_{critical} = \frac{4}{7\zeta(3)} \simeq 0.475$$

$\omega^2 < 0$ if $\sigma > \sigma_{critical}$

Kittel 5.2

Eq 3-35 dilation: $\delta = \dfrac{\Delta V}{V}$

Eq 3-53 energy density: $u = \frac{1}{2} B \delta^2$

potential energy
per unit volume

$$u = \frac{1}{2} B \left(\frac{\Delta V}{V}\right)^2$$

$$U = uV = \frac{1}{2} B \frac{(\Delta V)^2}{V}$$

$$\langle U \rangle = \frac{1}{2} \frac{B}{V} \langle (\Delta V)^2 \rangle = \frac{1}{2} k_B T$$

$$\langle (\Delta V)^2 \rangle = \frac{k_B T V}{B}$$

For Na, bcc - 2 atoms / non primitive cubic cell

$a = \cancel{3.66}$ Å or $\underline{4.22 \text{ Å}}$ ✓

$$V = \frac{a^3}{2}$$

$$\langle (\Delta V)^2 \rangle = \frac{k_B T a^3}{2B}$$

$$= \frac{\left(1.38\times10^{-23}\frac{J}{K}\right)(300K)\left(\overset{4.22}{\cancel{3.66}}\times10^{-10}m\right)^3}{(2)\;7\times10^{10}\frac{erg}{cm^3}\left(\frac{10^6 cm^3}{m^3}\right)\frac{1J}{10^7 erg}}$$

$$= \overset{2.2}{\cancel{1.5}}\times10^{-59}\,m^6$$

$$= \overset{2.2}{1.5}\times10^{-47}\,cm^6$$

$$\Delta V_{rms} = \sqrt{\langle(\Delta V)^2\rangle} = \cancel{3.87\times10^{-24}\,cm^3}$$

$$\underline{\text{or}}\quad 4.7\times10^{-24}\,cm^3 \checkmark$$

$$V = \frac{1}{2}a^3$$

$$\frac{\Delta V}{V} = 3\frac{\Delta a}{a}$$

$$\frac{\Delta V_{rms}}{V} = \cancel{0.158}\quad 0.124$$

$$\frac{\Delta a}{a} = \frac{1}{3}(0.158)$$

$$= \cancel{0.053}\quad 0.0416$$