Fri. Nov. 02

- before moving on in our current topic, I'd like to discuss #4 on HW#4
- Some have asked about the lack of knowledge of the wavelength, λ, but we do not need it in this problem
- we only want to identify the crystal types not the lattice spacing
- Selection rules:

NaCl	FCC	all h, k, l even or all h, k, l odd
CsCl	SC	all h, k, l
Diamond	diamond	all h, k, l even, $h+k+l=4n$ all h, k, l, odd

- recall Bragg's law, $2d\sin\theta = n\lambda$
- for $n = 1$, we have $d = \dfrac{\lambda}{2\sin\theta}$
- relating to the Miller indices,

$$d_{h,k,l} = \frac{\lambda}{2\sin\theta} = \frac{a}{h^2+k^2+l^2}, \quad a = \text{lattice constant}$$

- we see that $\dfrac{a^2}{d^2} = \underbrace{h^2+k^2+l^2}_{} = \dfrac{\sin^2\theta}{\sin^2\theta_0}$

$= N$

$\updownarrow$

- see $\dfrac{a^2}{d^2} = \dfrac{\left(\dfrac{\lambda}{2\sin\theta_0}\right)^2}{\left(\dfrac{\lambda}{2\sin\theta}\right)} = \dfrac{\sin^2\theta}{\sin^2\theta_0}$

$\boxed{\text{* note that } \lambda \text{ cancels} \quad \text{* if ratio of sines is fraction, multiply until whole \#}}$

- <u>Ex</u>: Sample 1

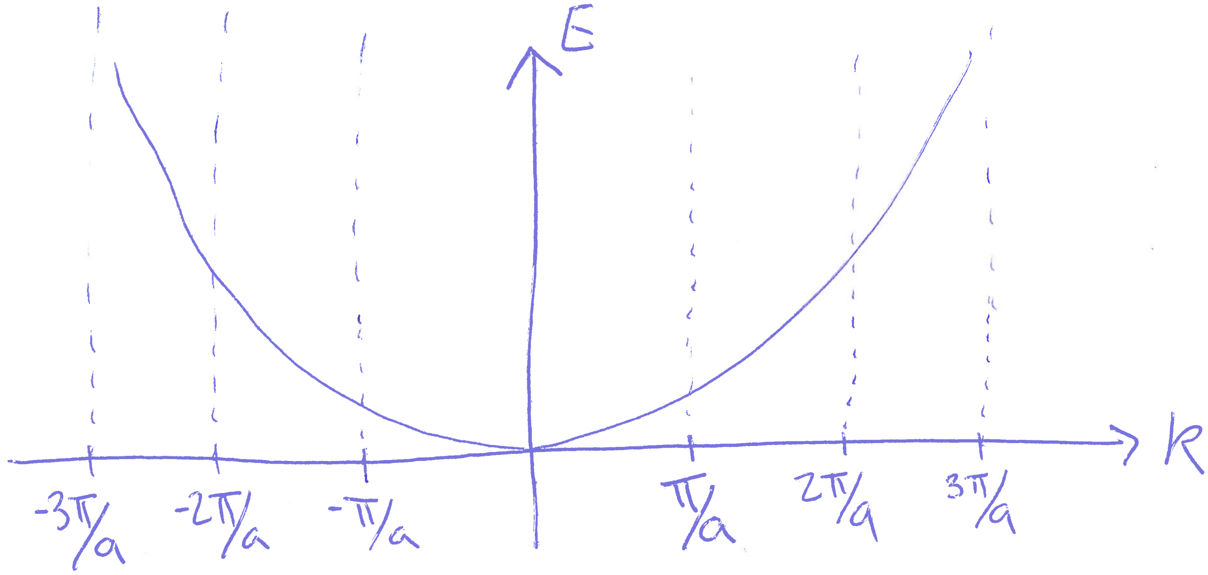
θ	$\dfrac{\sin^2\theta}{\sin^2\theta_0}$	$\{hkl\}$
$\theta_0 = 10.8$	1	100
15.3	~2	110
18.9	~3	111
⋮	~4	200

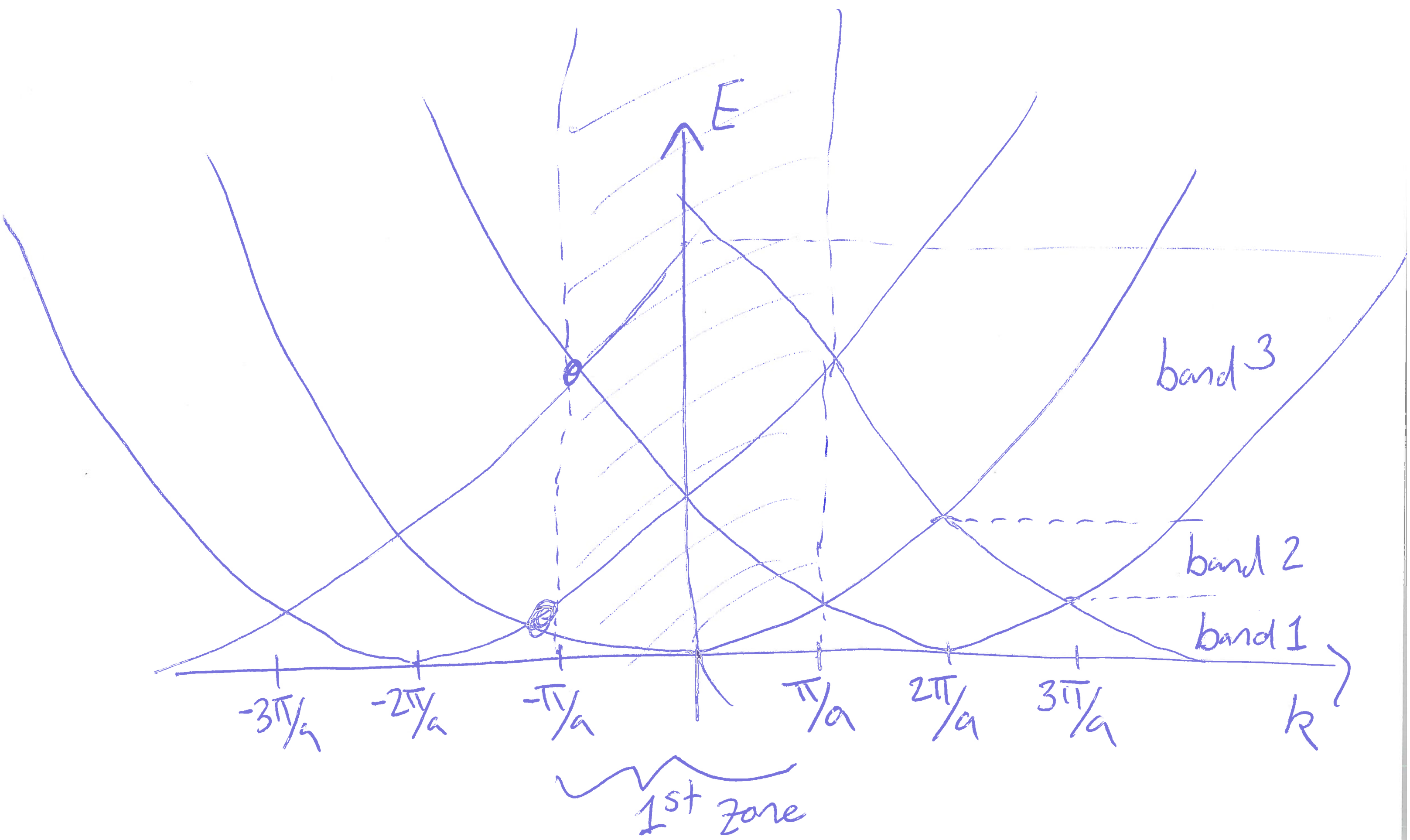
$\Big\}$ SC → all h,k,l

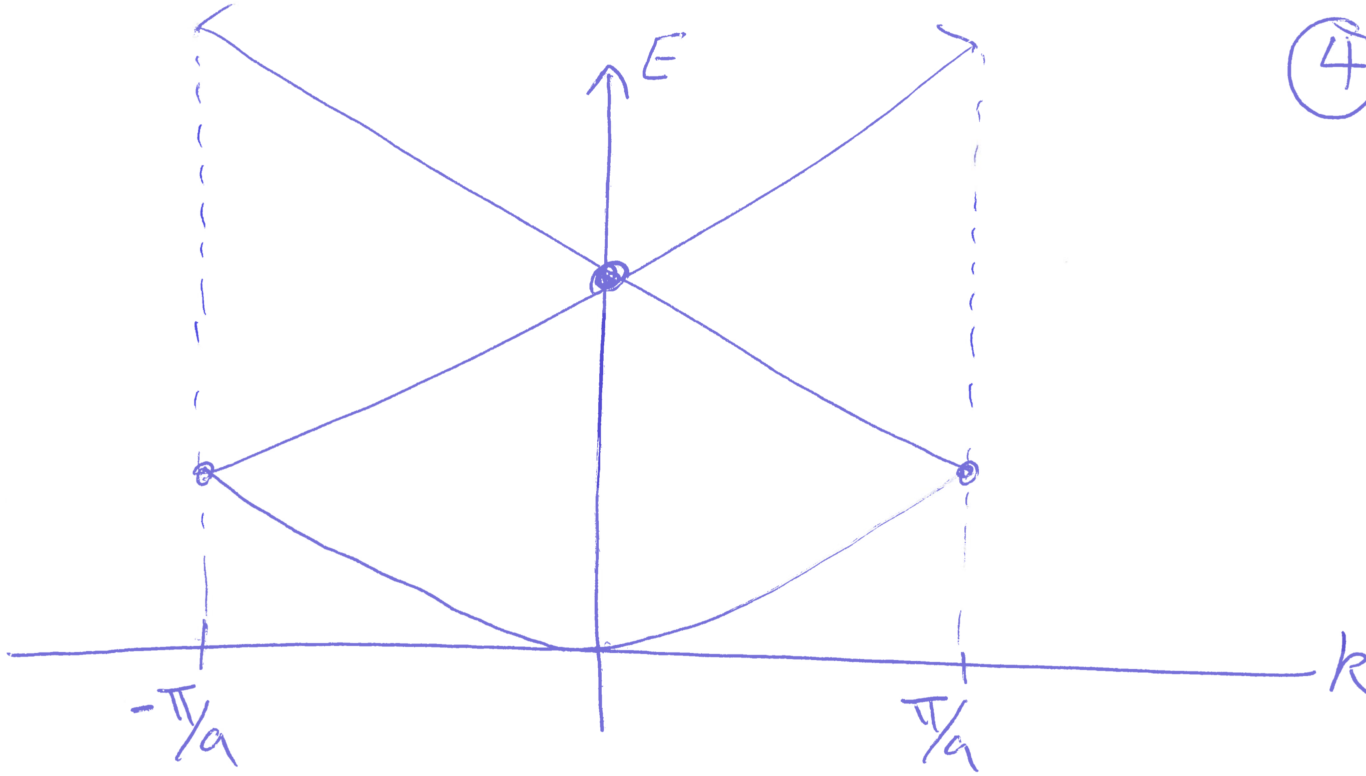
CsCl solid

- Now let's return to band theory for electronic energies within solids

- We start with the "empty lattice model"







- reduced zone scheme dispersion relation (1st Brillouin zone)
- For the 1D case, $\psi_k^{(0)} = \frac{1}{\sqrt{L}} e^{ikx}$

  with energy $E_k^{(0)} = \frac{\hbar^2 k^2}{2m_0}$, where '0' means the wave function is unperturbed

- critically, the periodicity of the lattice leads to periodicity in dispersion curves

→

- let's see what happens when we approach the zone boundary when the electrons interact weakly with the lattice

- the Bragg condition, $n\lambda = 2d\sin\theta$
- for 1D, $\theta = 90°$ & let $n=1$
  - $\lambda = 2d \Rightarrow k = \pi/d$ & $d=a$

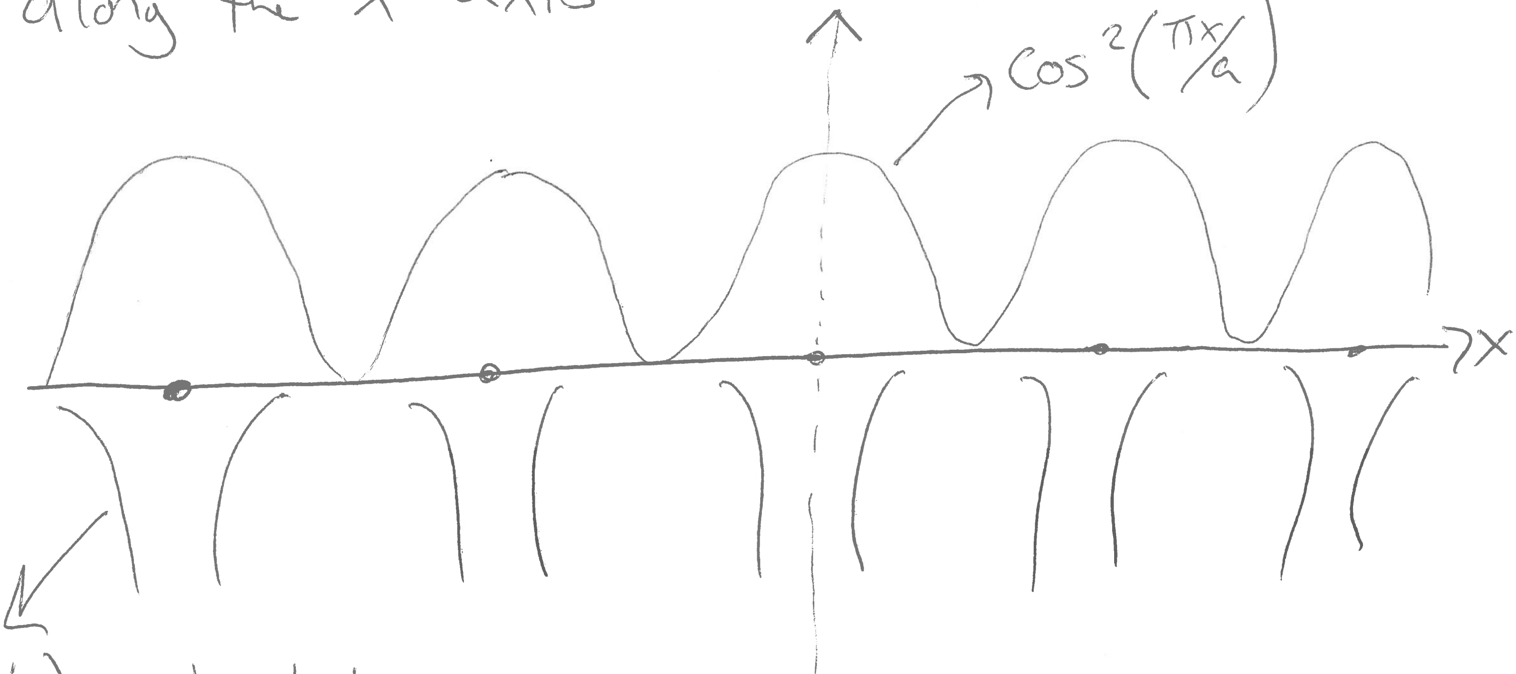
$$\Rightarrow k = \pm\pi/a \quad \text{(first zone boundary)}$$

$$\Rightarrow \psi_k^{(0)} = \frac{e^{ikx}}{\sqrt{L}} = \frac{e^{\pm i\pi x/a}}{\sqrt{L}}$$

$$\psi_\pm(x) = \frac{1}{\sqrt{2L}}\left[e^{i\pi x/a} \pm e^{-i\pi x/a}\right]$$

- the two waves are standing waves, but shifted by a phase factor

- We know $|\psi|^2$ gives a measurable quantity $\rightarrow$ probability of finding an electron along the x-axis



$V(x)$, potential of ions

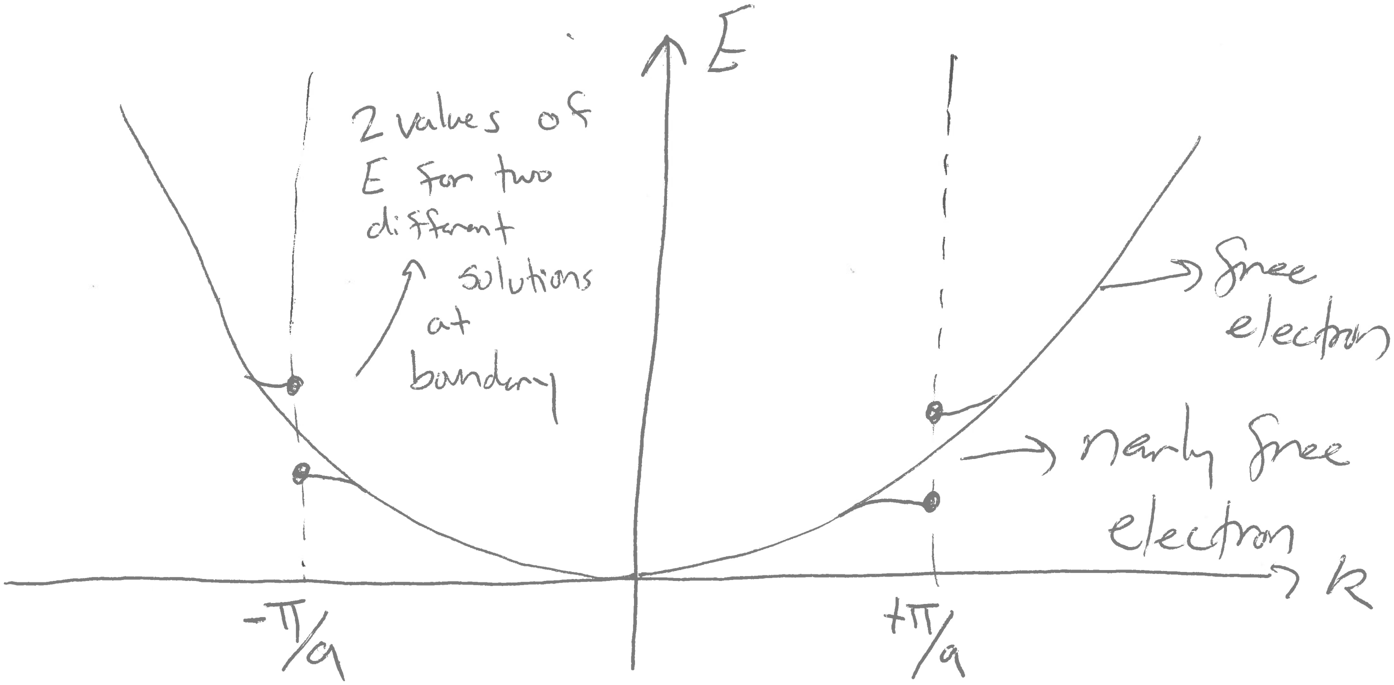
$$|\psi_+(x)|^2 \propto \cos^2(\pi x/a)$$ $\rightarrow$ concentrates electron around ions

- $|\psi_-(x)|^2 \propto \sin^2(\pi x/a)$

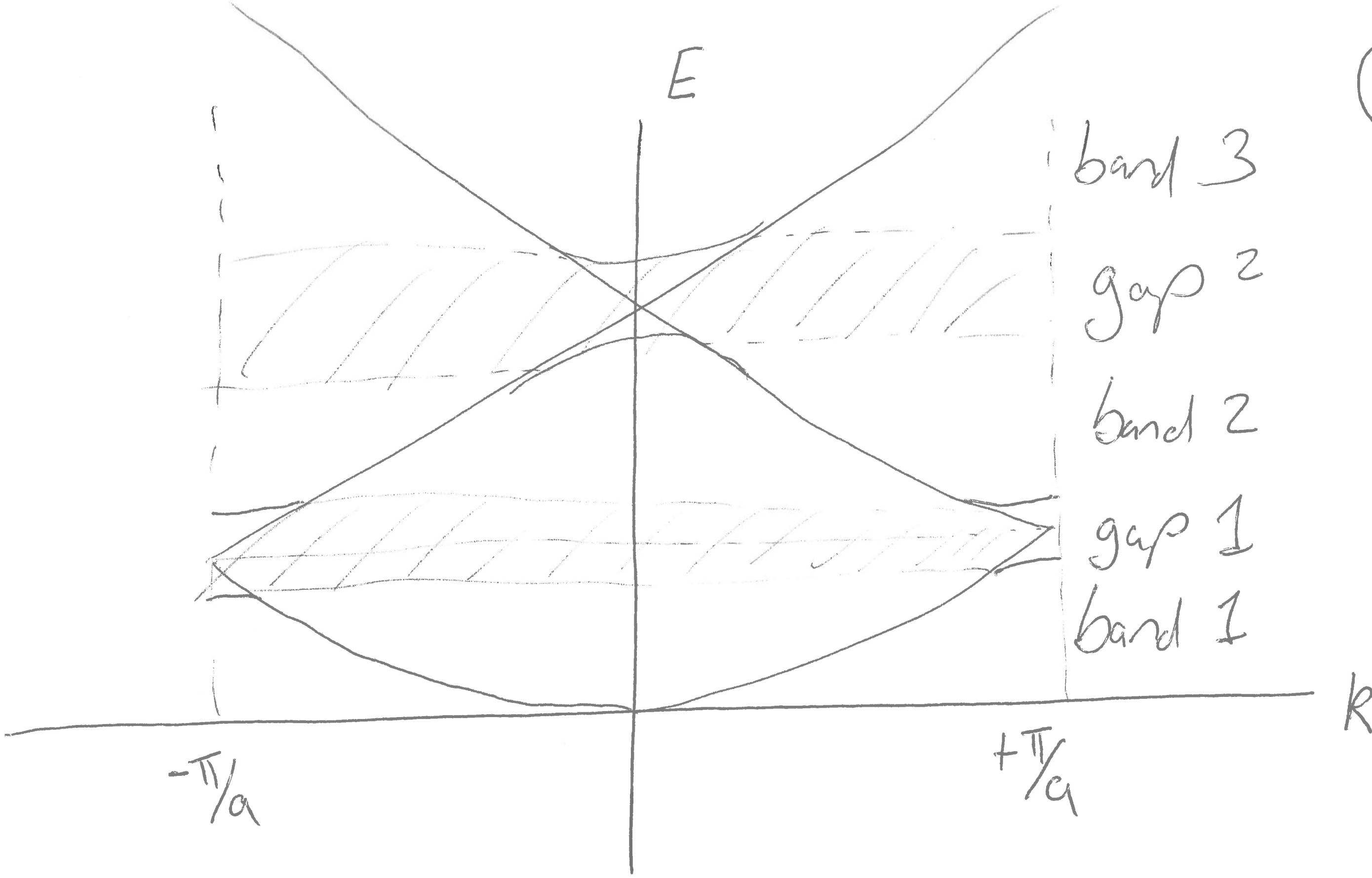
$\rightarrow$ concentrates electrons exactly between ions of solid

- the potential energy is lower for $|\psi_+(x)|^2$ as the + & - charges are closer together

- in other words, at the boundary (e.g. $\pm \pi/a$), we find there are dissimilar values for energy and therefore a gap opens



- the electrons meeting the Bragg condition behave much differently than the free electron → speed = 0 (standing waves)



- reduced zone scheme
- We have a qualitative description of the origin of bands + gaps, but we should make this argument more quantitative
- We will use perturbation theory to describe the "nearly free electron" model
- Weak interactions with lattice