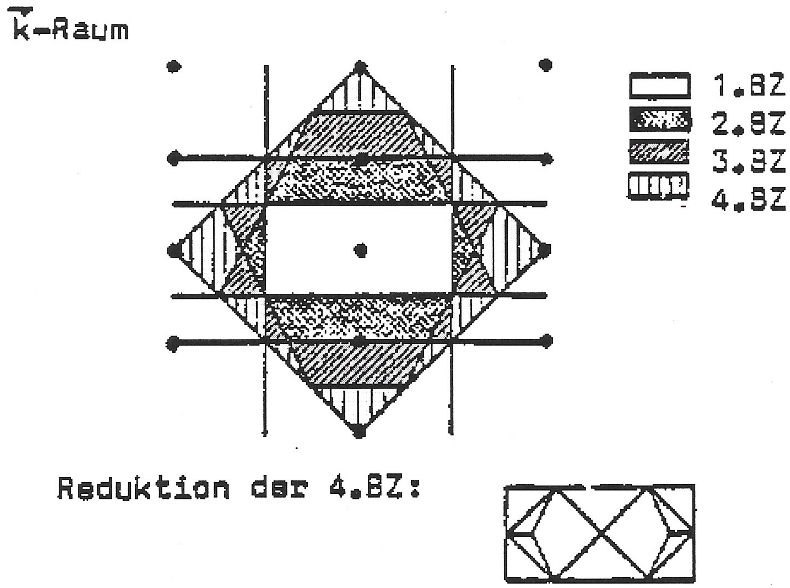
Σ PHY 140 HW 7.

1.

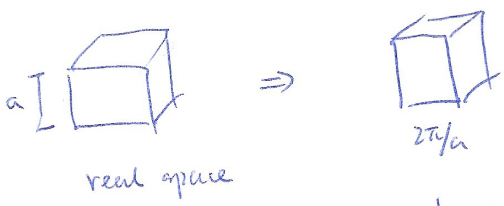


First three BZ for 2D rectangular lattice with a/b =2

Source: http://www.uni-ulm.de/fkp/lehre/gl5/ComKurs1/question/k-space/sol3.htm

Easy to follow guide:
http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php

4. SC lattice



allowed k values

$$k_x = n\frac{2\pi}{L} \quad (= k_y = k_z)$$

So allowed # of states:

$$(2\pi/a)^3 / (2\pi/L) = \frac{L^3}{a^3} = \underline{\underline{N}}$$

← i.e. # of unit cells.

Total volume in first BZ

each $\vec{k}$ state takes this volume

5. FCC lattice

FCC lattice in real space ⇒ BCC in k space

volume of conventional unit cell in k space (of first BZ)

$$= 4 \cdot \left(\frac{2\pi}{a}\right)^3$$

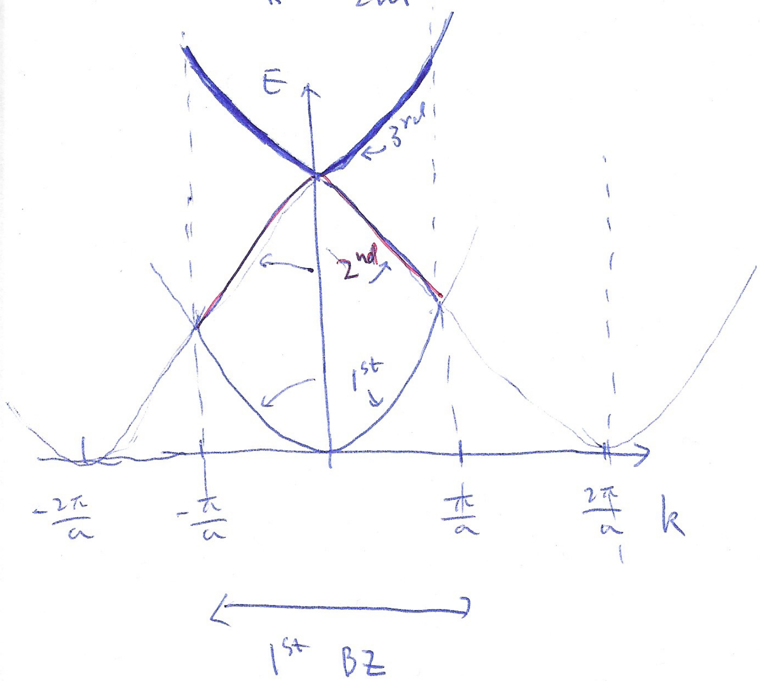
So # of allowed states

$$4 \cdot \left(\frac{2\pi}{a}\right)^3 / (2\pi/L)^3 = 4 \cdot \frac{L^3}{a^3} = \underline{\underline{4 \cdot N}}$$

There are 4 primitive unit cells in 1 conventional FCC cell so each primitive unit cell contributes $\underline{N}$ states in 1st BZ.

7. In empty lattice model, $\bar{e}$'s are free, energy is just KE.

$$E_k = \frac{\hbar^2 k^2}{2m}$$

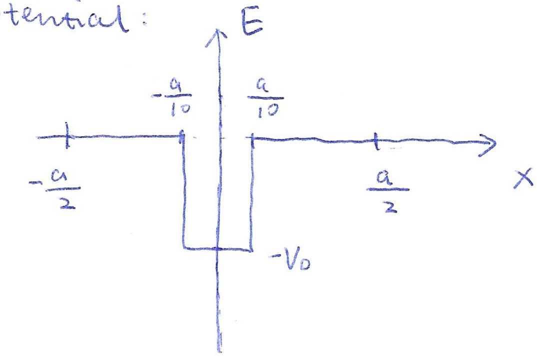


So First band: $0 \leq E_1 \leq \frac{\hbar^2 (\frac{\pi}{a})^2}{2m} \Rightarrow 0 \leq E_1 \leq \frac{\hbar^2 \pi^2}{2ma^2}$

Second band: $\frac{\hbar^2 (\frac{\pi}{a})^2}{2m} \leq E_2 \leq \frac{\hbar^2 (\frac{2\pi}{a})^2}{2m} \Rightarrow \frac{\hbar^2 \pi^2}{2ma} \leq E_2 \leq \frac{2\pi^2 \hbar^2}{ma^2}$

Third band: $\frac{\hbar (\frac{2\pi}{a})^2}{2m} \leq E_3 \leq \frac{\hbar^2 (\frac{3\pi}{a})^2}{2m} \Rightarrow \frac{2\pi^2 \hbar^2}{ma^2} \leq E_3 \leq \frac{9\pi^2 \hbar^2}{2ma^2}$

9. Potential:



a) Calculate the values of first 3 energy gaps in NFE model:

Use (5.20) from Omar book for 1^{st} gap

$$E_g = |V_{-2\pi/a}| \cdot 2 \qquad \text{where} \qquad V_{2\pi/a} = \frac{1}{a}\int_{-a/2}^{a/2} V(x)\, e^{i\frac{2\pi}{a}x}\, dx$$

$$V_{-\frac{2\pi}{a}} = \frac{1}{a}\int_{-\frac{a}{10}}^{\frac{a}{10}} -V_0\, e^{i\frac{2\pi}{a}x}\, dx$$

$$= -V_0 \cdot \frac{1}{a} \cdot \frac{a}{i2\pi}\, e^{i\frac{2\pi}{a}x}\Big|_{-a/10}^{a/10}$$

$$= -\frac{V_0}{i2\pi} \cdot \left(e^{i\frac{2\pi}{10}} - e^{-i\frac{2\pi}{10}}\right) = \frac{V_0}{\pi}\sin\left(\frac{\pi}{5}\right)$$

$$\Rightarrow \cancel{V}\ E_g^{(1)} = |V_{-\frac{2\pi}{a}}| \cdot 2 = \frac{2V_0}{\pi}\sin\left(\frac{\pi}{5}\right) = \frac{2V_0}{5}\operatorname{sinc}\left(\frac{\pi}{5}\right) \simeq 0.374\, V_0$$

Similarly, $E_g^{(2)} = |V_{-\frac{4\pi}{a}}| \cdot 2 = \frac{2V_0}{5}\operatorname{sinc}\left(\frac{2\pi}{5}\right) \simeq 0.303\, V_0$

$$E_g^{(3)} = |V_{-\frac{6\pi}{a}}| \cdot 2 = \frac{2V_0}{5}\operatorname{sinc}\left(\frac{3\pi}{5}\right) \simeq 0.202\, V_0$$

b) Put in $V_0 = 5eV$,

$E_g^{(1)} = 1.87\ eV$, $E_g^{(2)} = 1.52\ eV$, $E_g^{(3)} = 1.01\ eV$.

10. Prove (5.27) is normalized

$$\langle \psi_k | \psi_k \rangle = \frac{1}{N} \int \sum_{j=1}^{N} \sum_{i=1}^{N} e^{-ikx_j} \phi_v^*(x-x_j) \phi_v(x-x_i) e^{ikx_i} d^3r$$

$$= \frac{1}{N} \sum_{j=1}^{N} \sum_{i=1}^{N} e^{ik(x_i-x_j)} \int \phi_v^*(x-x_j) \phi_v(x-x_i) d^3r$$

$$= \frac{1}{N} \sum_{j=1}^{N} \sum_{i=1}^{N} e^{ik(x_i-x_j)} \cdot \delta_{ij}$$

$$= \frac{1}{N} \sum_{i=1}^{N} e^{ik\cdot 0} = \frac{1}{N}\left(\sum_{i=1}^{N} 1\right) = \frac{1}{N} \cdot N = \underline{\underline{1}}$$

as required.

Note: In tight binding Model, No overlapping between adjacent (different) sites, therefore

$$\int \underbrace{\phi_v^*(x-x_i)}_{\text{orbital on } i^{th} \text{ site}} \underbrace{\phi_v(x-x_j)}_{\text{orbital on } j^{th} \text{ site.}} dr^3 = 0 \quad \text{if } x_i \neq x_j \text{ (or } i \neq j)$$

So the integral will produce a delta function δ_{ij}, which just set $i=j$ in the $\sum_i \sum_j$ sum.