How many electrons can be occupied in a band ?

periodic b.c. $\psi(\vec{r}+N_i\vec{a}_i)=\psi(\vec{r})$ $\quad i=1,2,3$ $\quad$ *where* $N_i \to \infty$

$$\psi(\vec{r}+N_i\vec{a}_i)=e^{i\vec{k}\cdot N_i\vec{a}_i}\psi(\vec{r})=\psi(\vec{r}) \qquad \textit{where} \quad \vec{k}=x_1\vec{b}_1+x_2\vec{b}_2+x_3\vec{b}_3$$

$$N_i\vec{k}\cdot\vec{a}_i=2\pi N_i x_i=2\pi m_i \qquad m_i=\text{integer}$$

$$\Rightarrow \quad x_i=\frac{m_i}{N_i} \qquad m_i=0,\pm1,\pm2,....$$

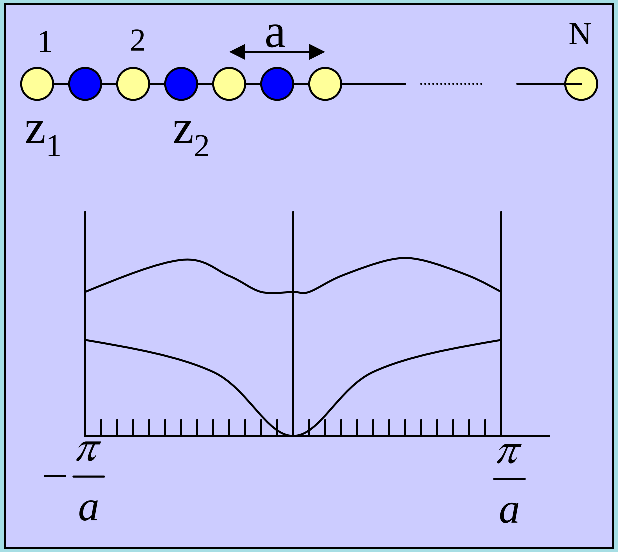
So the allowed Bloch wave vector is $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i$

$$\Delta\vec{k}=\frac{\vec{b}_1}{N_1}\cdot(\frac{\vec{b}_2}{N_2}\times\frac{\vec{b}_3}{N_3})=\frac{1}{N_1N_2N_3}\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)=\frac{1}{N}\frac{(2\pi)^3}{\Omega}=\frac{(2\pi)^3}{V}$$

\# of state in the 1BZ $=\dfrac{vol.\ \ of\ \ 1B.Z.}{\square\vec{k}}=\dfrac{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}{\frac{1}{N}\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}=N$

Each band can occupy 2N electrons per supercell (2 electrons per unit cell).

Example: 1 D



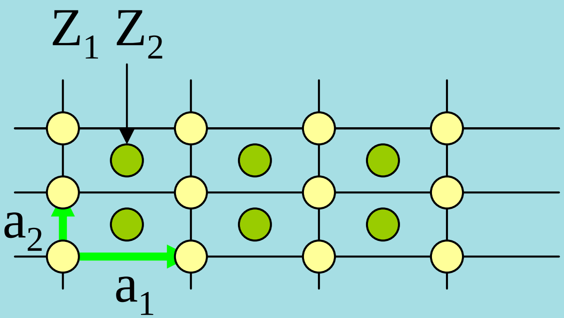
$$k = \frac{m}{N}\frac{2\pi}{a} \qquad where \quad m = 0, \pm 1, \pm 2 \cdots$$

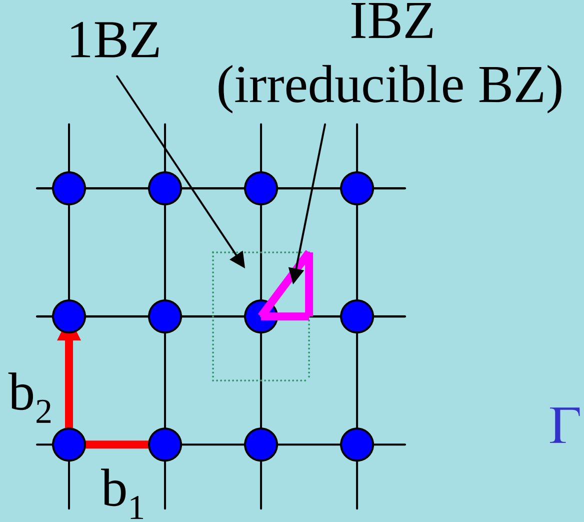
There are *N* states.

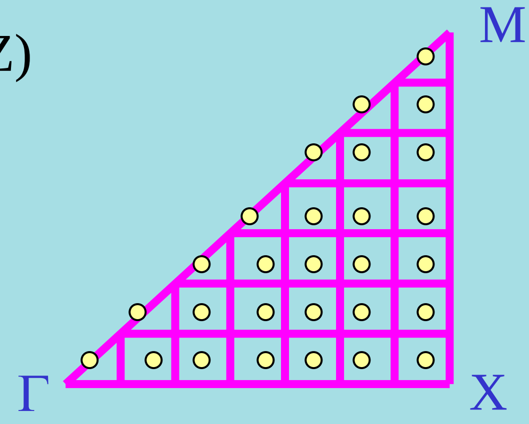
Each band can occupy 2N electrons per supercell
(2 electrons per unit cell).

$\frac{z_1 + z_2}{2}$ bands are filled

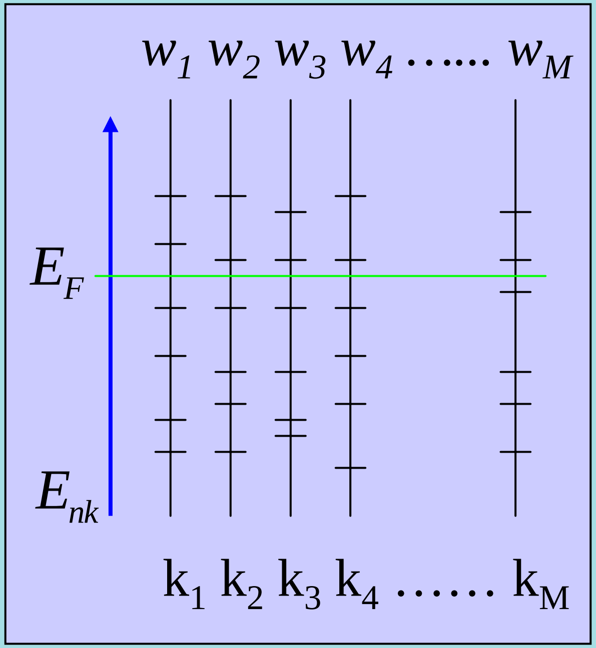
Example: 2 D







IBZ (irreducible BZ)



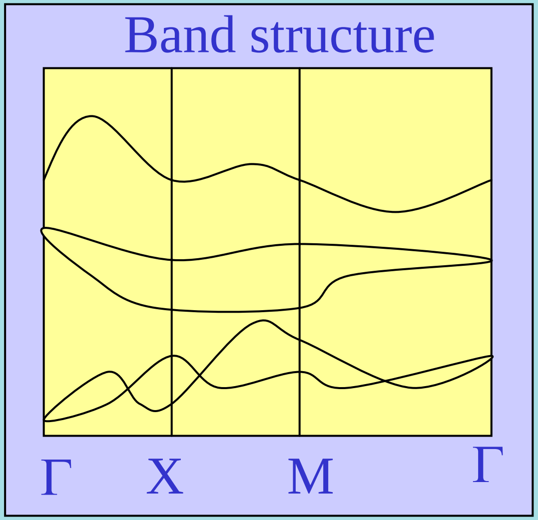
weight of the k points:

$$\omega_k = \frac{2A_k}{\sum_k A_k}$$

$$\sum_{\substack{n \\ E_{nk} \leq E_F}} \sum_k \omega_k = Z_1 + Z_2$$

charge density

$$\rho(\vec{r}) = \sum_{\substack{n \\ E_{nk} \leq E_F}} \sum_k \omega_k \left|\psi_{nk}\right|^2$$



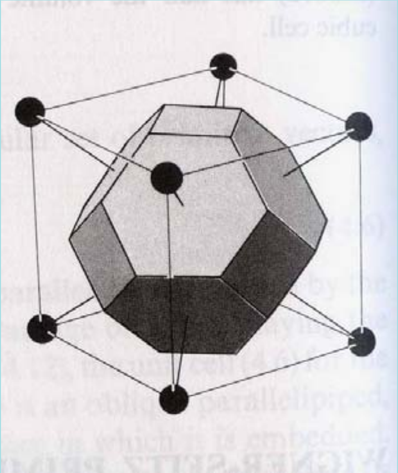
Example: 3 D

Copper (Cu) : fcc structure

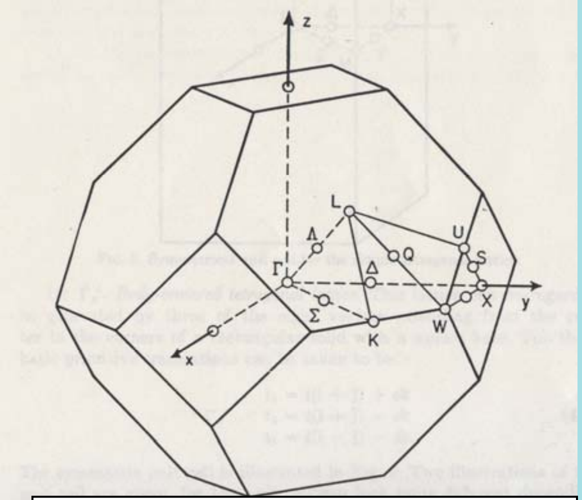
$$\vec{a}_1 = \frac{a}{2}\left(\vec{j} + \vec{k}\right) \qquad \vec{b}_1 = \frac{4\pi}{a}\left(-\vec{i} + \vec{j} + \vec{k}\right)$$

$$\vec{a}_2 = \frac{a}{2}\left(\vec{i} + \vec{k}\right) \qquad \vec{b}_2 = \frac{4\pi}{a}\left(\vec{i} - \vec{j} + \vec{k}\right)$$

$$\vec{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j}\right) \qquad \vec{b}_3 = \frac{4\pi}{a}\left(\vec{i} + \vec{j} - \vec{k}\right)$$



1 BZ of a fcc lattice



IBZ of fcc lattice