HW 4

RL

The rotation axis of a crystal can only be 2, 3, 4, 6-fold.

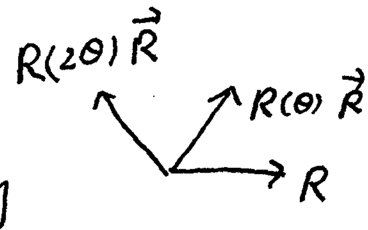
pickup a plane perpendicular to rotation axis, & conside

symmetry

a lattice vector in that plane. Perform rotation $R(\theta)\vec{R}$

primiti $\vec{R}$.

and $R(2\theta)\vec{R}$.



if $\theta = \pi \Rightarrow$ 2- fold

if $\theta \neq \pi \Rightarrow R(\theta)\vec{R}$ and $\vec{R}$ are linearly independent.

within the plane, there're only 2 - primitive vecters

$$\Rightarrow R(2\theta)\vec{R} = m R(\theta)\vec{R} + n\vec{R} \quad (m, n, \text{ integers})$$

$$\Rightarrow \begin{cases} \cos 2\theta = m\cos\theta + n \\ \sin 2\theta = n\sin\theta \end{cases} \Rightarrow 2\sin\theta\cos\theta = n\sin\theta$$

$$\Rightarrow \sin\theta\left(\cos\theta - \frac{n}{2}\right) = 0 \quad \text{for } \theta \neq \pi, 0 \Rightarrow$$

$$\cos\theta = \frac{n}{2}. \Rightarrow n = 0, \pm 1, \pm 2$$

$$\theta = \pm\frac{\pi}{2}, \pm\frac{\pi}{3}, \pm\pi, 0$$

$$\pm\frac{2}{3}\pi$$

take $0 < \theta \leq \pi \Rightarrow \theta = \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$

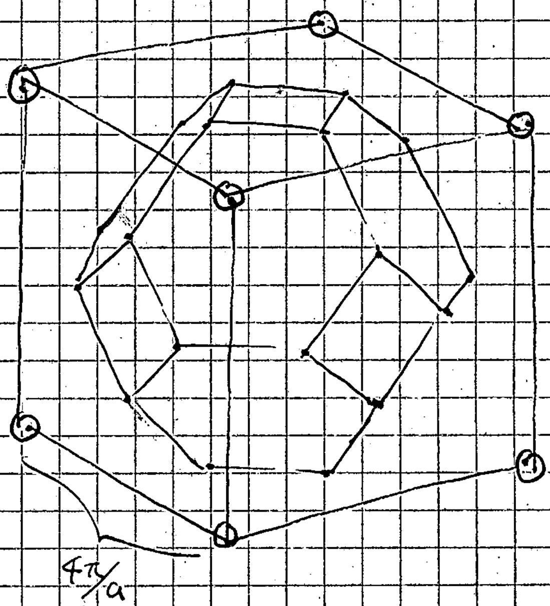
$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ 6 & 4 & 3 & 2 \end{array}$$

you can check $\cos 2\theta = m\cos\theta + n$ can also be satisfied!

2. First BZ for fcc and bcc lattice.

First BZ for fcc is the Wigner-Seitz cell of the reciprocal lattice to fcc, which has the same shape as the W-S cell of bcc lattice.

There are 6 squares and 8 hexagons.



The coordinate of each vertex

$(\pm\frac{\pi}{a}, 0, \pm\frac{2\pi}{a})$

$(0, \pm\frac{\pi}{a}, \pm\frac{2\pi}{a})$

$(\pm\frac{\pi}{a}, \pm\frac{2\pi}{a}, 0)$

$(0, \pm\frac{2\pi}{a}, \pm\frac{\pi}{a})$

$(\pm\frac{2\pi}{a}, \pm\frac{\pi}{a}, 0)$

$(\pm\frac{2\pi}{a}, 0, \pm\frac{\pi}{a})$

The coordinate of ~~ecentral~~ central points of each face:

Squares: $(0, 0, \pm\frac{2\pi}{a})$ $(0, \pm\frac{2\pi}{a}, 0)$ $(\pm\frac{2\pi}{a}, 0, 0)$

hexgons: $(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, \pm\frac{\pi}{a})$

First BZ for bcc is the W-S cell of the reciprocal lattice of bcc, which has the same shape as the W-S cell of fcc lattice.

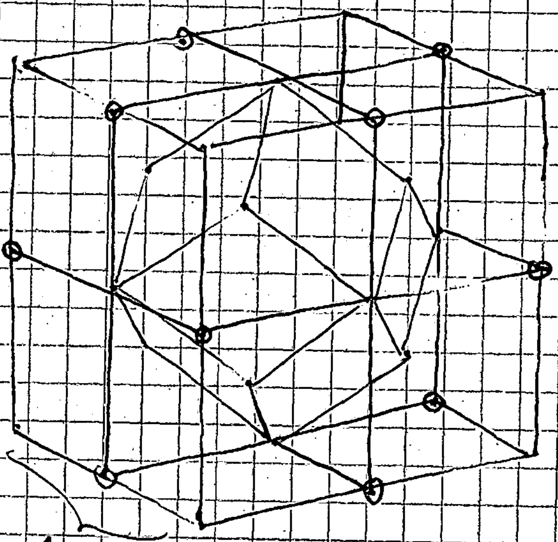
coordinate of vertex

$(0, 0, \pm\frac{2\pi}{a})$

$(0, \pm\frac{2\pi}{a}, 0)$

$(\pm\frac{2\pi}{a}, 0, 0)$

$(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, \pm\frac{\pi}{a})$



$\frac{4\pi}{a}$

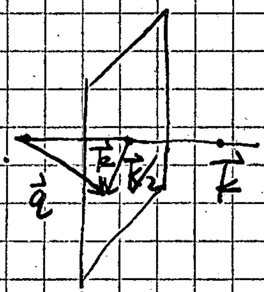
coordinate of the central points of each face

$(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, 0)$

$(\pm\frac{\pi}{a}, 0, \pm\frac{\pi}{a})$

$(0, \pm\frac{\pi}{a}, \pm\frac{\pi}{a})$

3. A&M 9.1



$\vec{q} = \frac{1}{2}\vec{K} + \vec{k}$

$$\varepsilon^0_{\vec{q}} = \frac{\hbar^2 (\frac{\vec{K}}{2} + \vec{k}_{\parallel})^2 + \vec{k}_{\perp}^2}{2m}$$

$$\varepsilon^0_{\vec{q}-\vec{K}} = \frac{\hbar^2 (\frac{\vec{K}}{2} - \vec{k}_{\parallel})^2 + \vec{k}_{\perp}^2}{2m}$$

$$\varepsilon = \frac{1}{2}(\varepsilon^0_{\vec{q}} + \varepsilon^0_{\vec{q}-\vec{K}}) \pm \left[\left(\frac{\varepsilon^0_{\vec{q}} - \varepsilon^0_{\vec{q}-\vec{K}}}{2}\right)^2 + |U_K|^2\right]^{1/2}$$

$$= \frac{\hbar^2 (\frac{\vec{K}}{2})^2}{2m} + \frac{\hbar^2(\vec{k}_{\parallel}^2 + \vec{k}_{\perp}^2)}{2m} \pm \left[\left(\frac{\vec{K}\vec{k}_{\parallel}}{2m}\right)^2 + |U_K|^2\right]^{1/2}$$

$$= \varepsilon^0_{\vec{K}/2} + \frac{\hbar^2 \vec{k}^2}{2m} \pm \left[4\varepsilon^0_{\vec{K}/2}\frac{\hbar^2 \vec{k}_{\parallel}^2}{2m} + |U_K|^2\right]^{1/2}$$

(a)

$\varepsilon_F = \varepsilon^0_{\vec{K}/2} \mp |U_K| + \Delta$

lowest energy of uper band is $\varepsilon^0_{\vec{K}/2} + |U_K|$

so when $0 < \Delta < 2|U_K|$ ε_F will not reach the lowest energy of higher. so in this condition Fermi surface lies in lower band.

when $\vec{k}_{\parallel} = 0$

$$\varepsilon_F = \varepsilon^0_{\vec{K}/2} + \frac{\hbar^2 k_\perp^2}{2m} - |U_K| \quad \text{with } \vec{k}_{\parallel} = 0$$

$$= \varepsilon^0_{\vec{K}/2} + \frac{\hbar^2 \rho^2}{2m} - |U_K| \quad \text{with } \vec{k}_{\parallel} = 0$$

so $\frac{\hbar^2 \rho^2}{2m} = \Delta \qquad \rho = \sqrt{\frac{2m\Delta}{\hbar^2}}$

(b) When $\Delta > 2|U_K|$ Fermi surface can enter the higher band

For higher band : ρ_1

$$\varepsilon_F = \varepsilon^0_{\vec{K}/2} + |U_K| + \frac{\hbar^2 \rho_1^2}{2m}$$

For lower band : ρ_2

$$\varepsilon_F = \varepsilon^0_{\vec{K}/2} - |U_K| + \frac{\hbar^2 \rho_2^2}{2m}$$

$\therefore \frac{\hbar^2(\rho_2^2 - \rho_1^2)}{2m} = 2|U_K|$

$\therefore \pi(\rho_2^2 - \rho_1^2) = \frac{4m\pi}{\hbar^2} |U_{\vec{K}}|$