2016 / 10 / 29 (토) (1)

Harrison 책에서 부터

$$E_{xy,xy} = 3l^2m^2 V_{dd\sigma} + (l^2+m^2-4l^2m^2)V_{dd\pi} + (n^2+l^2m^2)V_{dd\delta}$$

$$\begin{aligned} l &= \cos\varphi \sin\theta \\ m &= \sin\varphi\sin\theta \\ n &= \cos\theta \end{aligned} \xrightarrow{\theta=90^\circ} \begin{aligned} l &= \cos\varphi \\ m &= \sin\varphi \\ n &= 0\,. \end{aligned}$$

$$\Rightarrow 3\cos^2\theta\sin^2\theta V_{dd\sigma} + (1-4\cos^2\theta\sin^2\theta)V_{dd\pi}$$

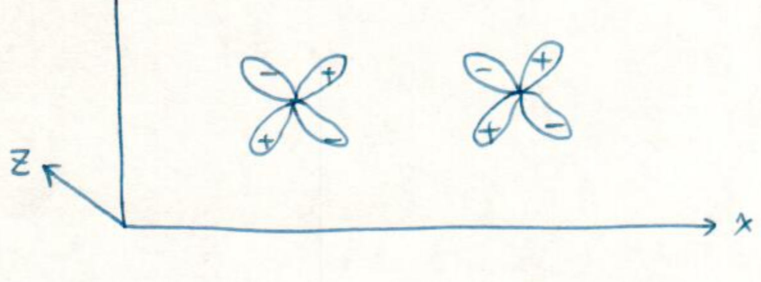
$$+\cos^2\theta\sin^2\theta V_{dd\delta}\,.$$

$$= V_{dd\pi} + \cos^2\theta\sin^2\theta(3V_{dd\sigma}+V_{dd\delta}) - 4\cos^2\theta\sin^2\theta V_{dd\pi}$$

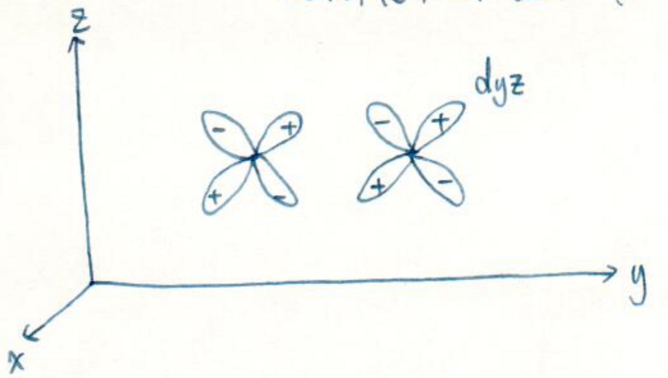
$$= V_{dd\pi} + \cos^2\theta\sin^2\theta(3V_{dd\sigma}+V_{dd\delta}-4V_{dd\pi})$$

$$\Downarrow$$

$$\frac{\sin2\theta}{2}\times\frac{\sin2\theta}{2} = \frac{1}{4}\sin2\theta\sin2\theta\,.$$



2016/10/29 (土) (2)

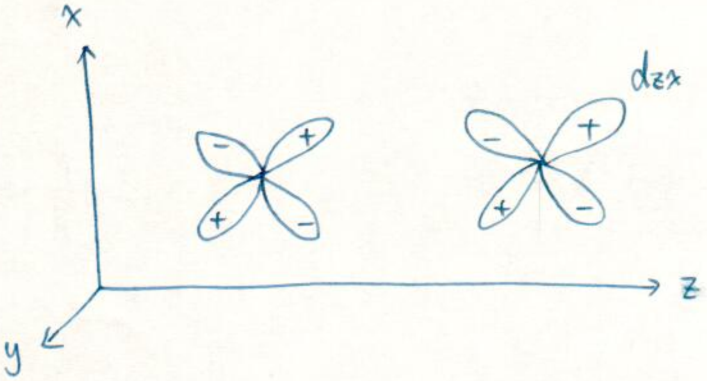


$l = \sin\varphi \sin\theta$

$m = \cos\theta$

$n = \cos\varphi \sin\theta$.

$$E_{yz,yz} = V_{dd\delta} \cos^2\theta + V_{dd\pi} \sin^2\theta$$



$l = \cos\theta$

$m = \cos\varphi \sin\theta$

$n = \sin\varphi \sin\theta$

$$E_{zx,zx} = V_{dd\pi} \cos^2\theta + V_{dd\delta} \sin^2\theta .$$

$$E_{x,x} = l^2 V_{pp\sigma} + (1 - l^2) V_{pp\pi}$$

$$l = \cos\varphi \sin\theta .$$

$$E_{xx} = \cos^2\theta \, V_{pp\sigma} + (1 - \cos^2\theta) V_{pp\pi} \quad l \to x$$

$$= \cos^2\theta \, V_{pp\sigma} + \sin^2\theta \, V_{pp\pi}$$

$$\xrightarrow{\theta = 0} V_{pp\sigma}$$

$$E_{yy} = \sin^2\theta \, V_{pp\sigma} + \cos^2\theta \, V_{pp\pi} \quad l \to y$$

$$\xrightarrow{\theta = 0} V_{pp\pi}$$

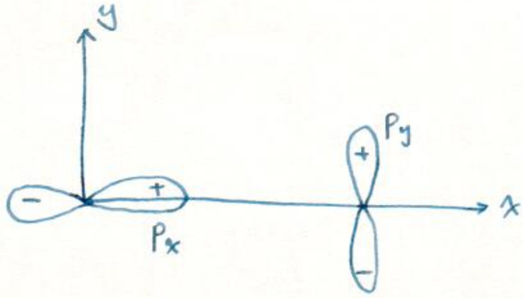
$$E_{x,z} = l n \, V_{pp\sigma} - l n \, V_{pp\pi}$$

$$l \to x, \quad n \to z$$

$$= \cos\varphi \sin\theta \cos\theta \, V_{pp\sigma} - \cos\varphi \sin\theta \cos\theta \, V_{pp\pi}$$

$$= 0.$$

$E_{x,y} = lm\ V_{pp\sigma} - lm\ V_{pp\pi}$



$x \to y \qquad l \to y$

$y \to x \qquad m \to z$

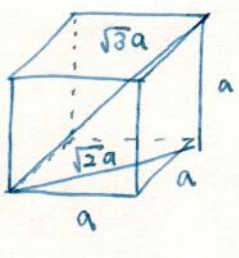
$E_{y,z}$ •

$y \to z \qquad l \to z$

$z \to x \qquad m \to x$

$n \to y$

$E_{zx} = \cos\theta \cos\varphi \sin\theta\ V_{pp\sigma} - \cos\theta \cos\varphi \sin\theta\ V_{pp\pi}$.



$\left(\frac{1}{\sqrt{2}}\right)^5 \qquad 1/\left(\frac{2}{\sqrt{2}}\right)^5 \approx 0.176$.

결론은

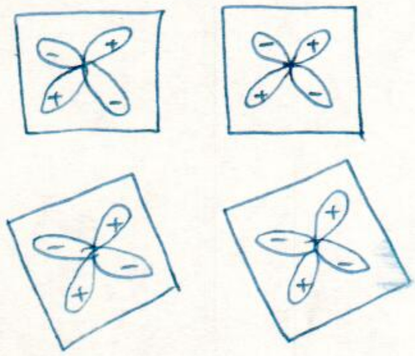
$$\left(d_{xy,0,\tau} \middle| d_{xy,i,\tau} \right) = V_{dd\pi} + \frac{1}{2}\sin(2\theta)\frac{1}{2}\sin(2\theta)\left(3V_{dd\sigma} + V_{dd\delta} - 4V_{dd\pi}\right)$$

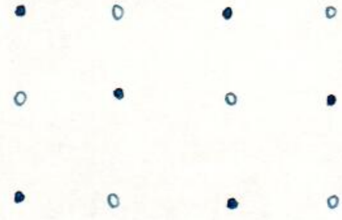
$$\text{or} \quad \frac{1}{4}\left(1 - \cos^2 2\theta\right).$$

$$E_{xy,xy} = V_{dd\pi} + \frac{1}{4}\sin 2\theta \sin 2\theta \left(3V_{dd\sigma} + V_{dd\delta} - 4V_{dd\pi}\right)$$

즉 sublattice 를 도입하면 같은 sublattice 사이에서는

$$V_{dd\pi} + \frac{1}{4}\sin\left(2(\theta-\varphi)\right)\sin\left(2(\theta-\varphi)\right)\left(3V_{dd\sigma} + V_{dd\delta} - 4V_{dd\pi}\right).$$





// 끝.