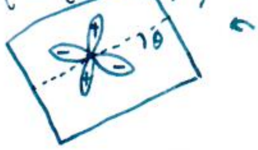
2016/9/27 (화) (1).

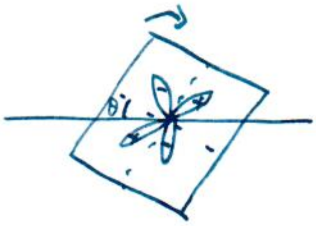
어제에 이어서 다음식이 맞는지 검증해 보자.

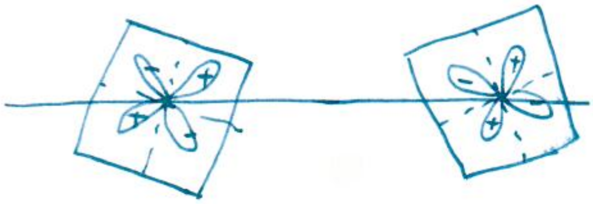
$$E_{xy,xy} = \cos(2(\theta-\phi))\cos(2(\theta+\phi))V_{dd\pi}$$

$$+\sin(2(\theta-\phi))\sin(2(\theta+\phi))V_{dd\sigma}$$



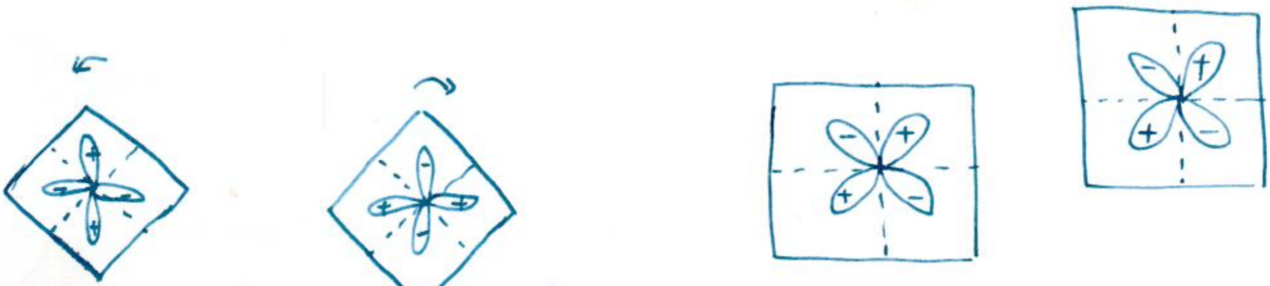
$\phi = \frac{\pi}{2}$





at $\phi=\frac{\pi}{2}$

$$E_{xy,xy} = \cos^2(2\theta)V_{dd\pi} + \sin^2(2\theta)V_{dd\sigma}$$



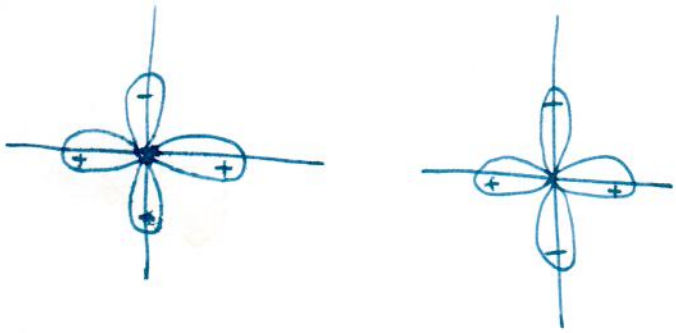
at $\phi=\pi$.

$$E_{xy,xy} = \cos^2(2\theta)V_{dd\pi} \cancel{+} - \sin^2(2\theta)V_{dd\sigma}$$

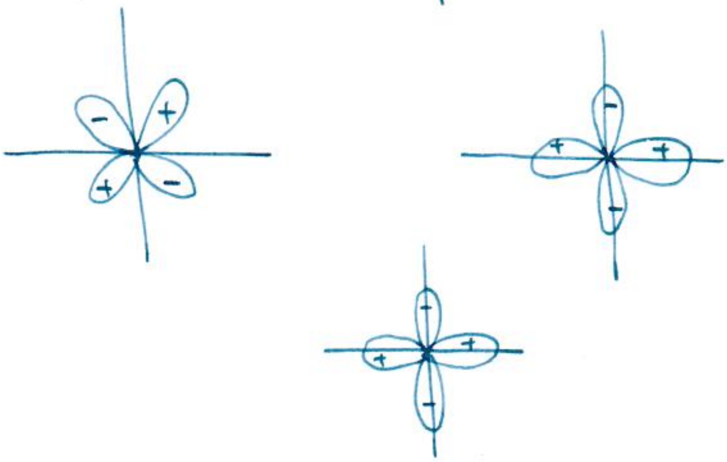
$$\cos^2(2\phi)V_{dd\pi} + \frac{1}{4}\left(\sin^2(2\phi)V_{dd\delta} + 3\sin^2(2\phi)V_{dd\sigma}\right)$$

$\phi = \frac{\pi}{4} + \frac{\pi}{100}$

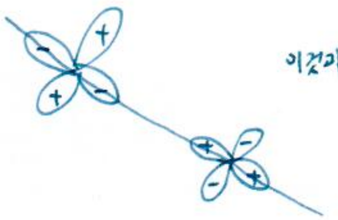
$\phi = \frac{\pi}{4} - \frac{\pi}{100}$



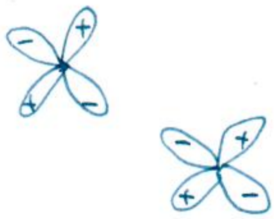
2016/9/27 (화)
(2).



지금 현재 의문점은

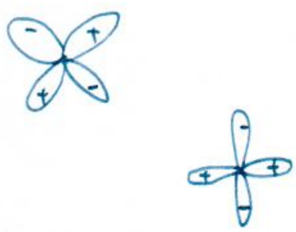


이것과



이 같은 Slater-Koster parameter 를 줄것이냐 하는것이다.

그것을 확인하기 위해서 d_{xy} orbital 과 $d_{x^2-y^2}$ orbital 를 같은 위치에 두고



어떻게 표현되는지 살펴보고 유추해보자.

$$E_{xy,\,x^2-y^2} = \frac{3}{2} lm(l^2-m^2) V_{dd\sigma} + 2lm(m^2-l^2) V_{dd\pi}$$
$$+ \frac{1}{2} lm(l^2-m^2) V_{dd\delta}$$

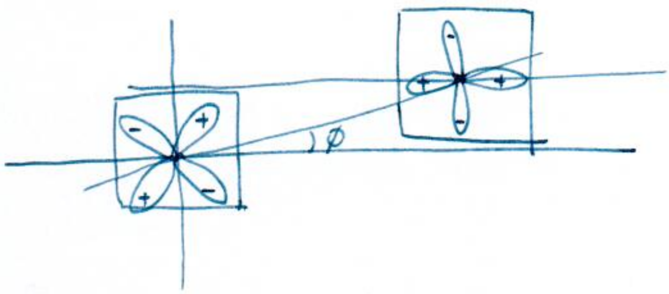
$$\{l, m, n\} = \{\cos\phi \sin\theta,\ \sin\phi \sin\theta,\ \cos\theta\}.$$

$$E_{xy,x^2-y^2} = \frac{1}{8}\sin^4\theta \sin(4\phi)\left(V_{dd\delta} - 4V_{dd\pi} + 3V_{dd\sigma}\right)$$

at $\theta = \frac{\pi}{2}$ $\quad E_{xy,x^2-y^2} = \frac{1}{8}\sin(4\phi)\left(V_{dd\delta} - 4V_{dd\pi} + 3V_{dd\sigma}\right)$

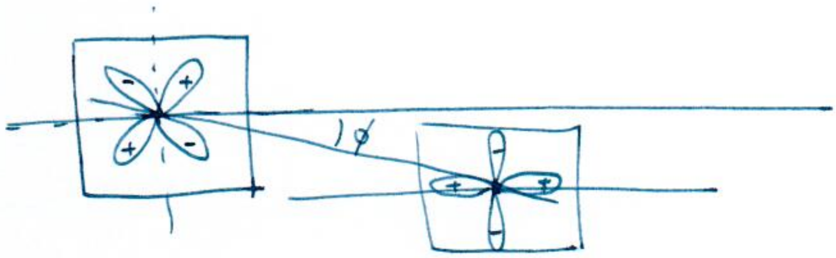
at $\phi = 0$

즉  $E_{xy,x^2-y^2} = 0.$



$$E_{xy,x^2-y^2} = \frac{1}{8}\sin(4\phi)\left(V_{dd\delta} - 4V_{dd\pi} + 3V_{dd\sigma}\right)$$

$=$

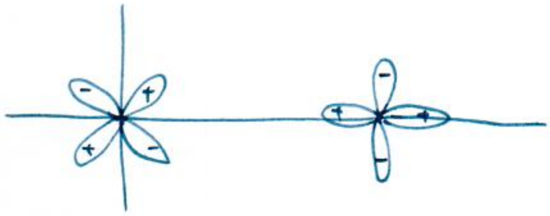


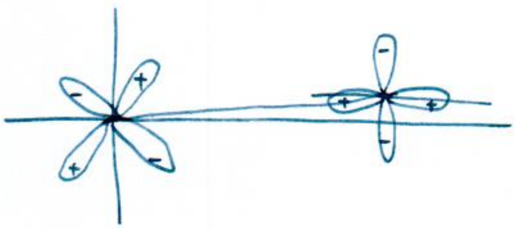
$$E_{xy,x^2-y^2} = -\frac{1}{8}\sin(4\phi)\left(V_{dd\delta} - 4V_{dd\pi} + 3V_{dd\delta}\right).$$

$\sin(2\phi) = 2\sin\phi\cos\phi$

$\sin(4\phi) = 2\sin(2\phi)\cos(2\phi)$.

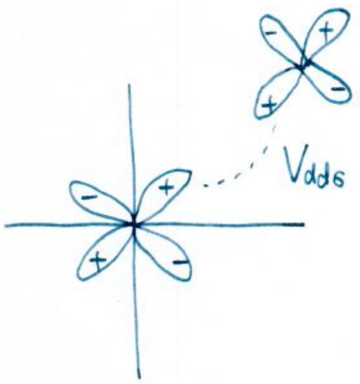
$E_{xy,x^2-y^2} = \frac{1}{4}\sin(2\phi)\cos(2\phi)\left(V_{dd\delta} - 4V_{dd\pi} + 3V_{dd\sigma}\right)$.





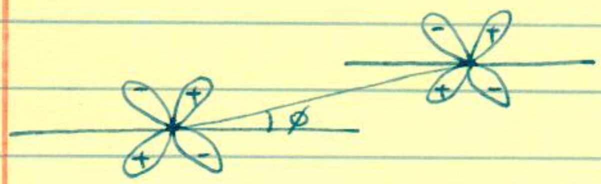
$= -\sin(2\phi)\cos(2\phi)V_{dd\pi} + \sin(2\phi)\cos(2\phi)V_{dd\sigma}$

$V_{dd\sigma}$



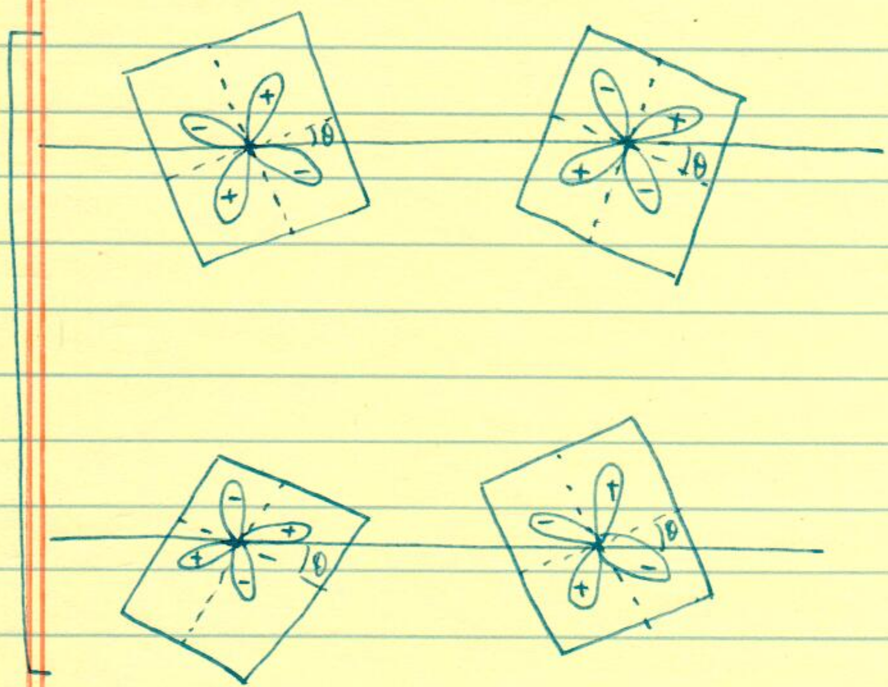
2016/9/27 (화) (5)

그러므로 Slater-Koster parameter



$V_{dd\pi} \cos^2(2\phi) + V_{dd\sigma} \sin^2(2\phi)$

rotation Slater-Koster parameter.



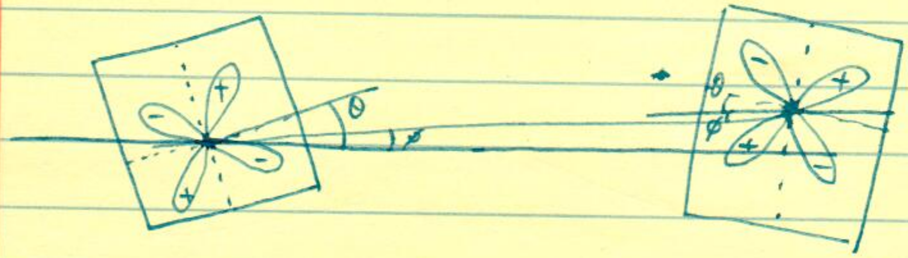
$V_{dd\pi} \cos^2(2\theta) - V_{dd\sigma} \sin^2(2\theta)$

여기에 "−" 이 붙는다.

2016/9/27 (화)

(6)

그럼 공간적인 orbital 이동과 rotation 과의 관계는 어떤것인가?

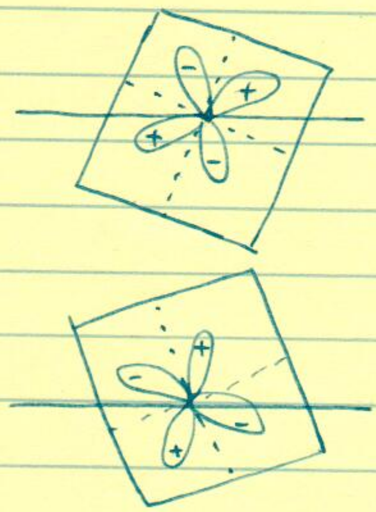


$V_{dd\pi} \cos(2(\theta-\phi)) \cos(2(\theta+\phi))$

$- V_{dd\sigma} \sin(2(\theta-\phi)) \sin(2(\theta+\phi))$

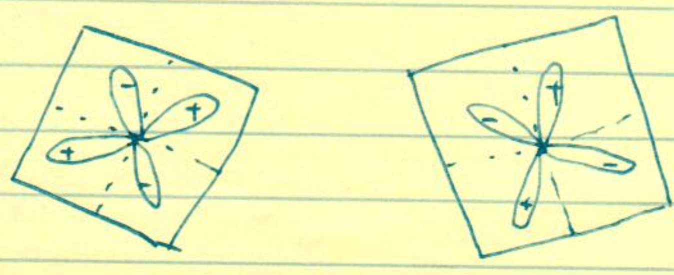
검증을 해보면

$\phi = \frac{\pi}{2}$



$V_{dd\pi}\cos^2(2\theta) - V_{dd\sigma}\sin^2(2\theta)$.

$\phi = \pi$



$V_{dd\pi}\cos^2(2\theta) - V_{dd\sigma}\sin^2(2\theta)$

2016/9/27 (화) (7)

그럼이제 $E_{yz,yz}$, $E_{zx,zx}$, $E_{xy,xy}$ 에 대해서

local rotation과 공간적 orbital 이동에 대해 Slater-Koster Parameter를 구하는것은 완성되었다.

정리하면

$$E_{yz,yz} = V_{dd\pi}\cos(\theta-\phi)\cos(\theta+\phi) - V_{dd\delta}\sin(\theta-\phi)\sin(\theta+\phi)$$

$$E_{zx,zx} = V_{dd\delta}\cos(\theta-\phi)\cos(\theta+\phi) - V_{dd\pi}\sin(\theta-\phi)\sin(\theta+\phi).$$

$$E_{xy,xy} = V_{dd\pi}\cos(2(\theta-\phi))\cos(2(\theta+\phi)) - V_{dd\delta}\sin(2(\theta-\phi))\sin(2(\theta+\phi))$$

다음 할 것은 $E_{yz,zx}$ $E_{zx,yz}$ 가 되겠다.