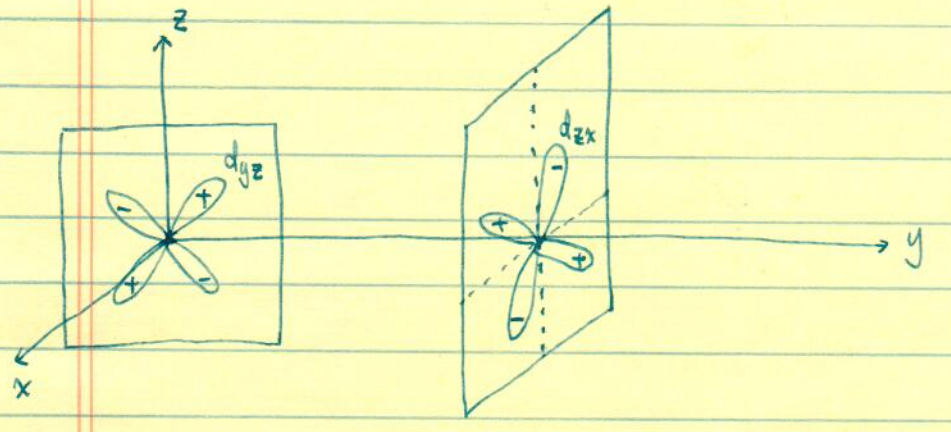
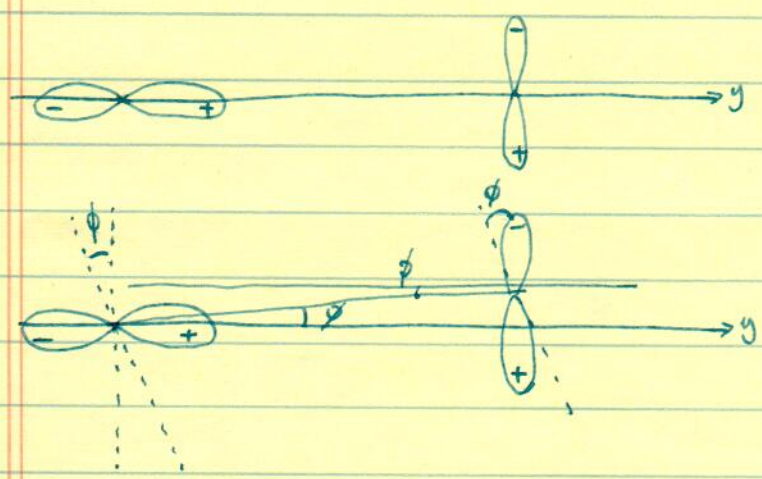
2016 / 9 / 27 (화) (1)

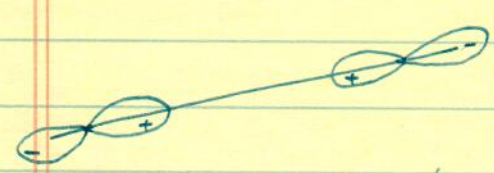
지금 할일은 $E_{yz,zx}$ 와 $E_{zx,yz}$ 를 구하는 것이다.



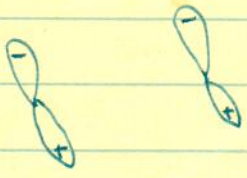


$$-V_{dd\pi}\cos\phi\sin\phi + \sin\phi\cos\phi\, V_{dd\delta}$$

$$\therefore (V_{dd\delta} - V_{dd\pi})\cos\phi\sin\phi$$



$-V_{dd\pi}\cos\phi\sin\phi$

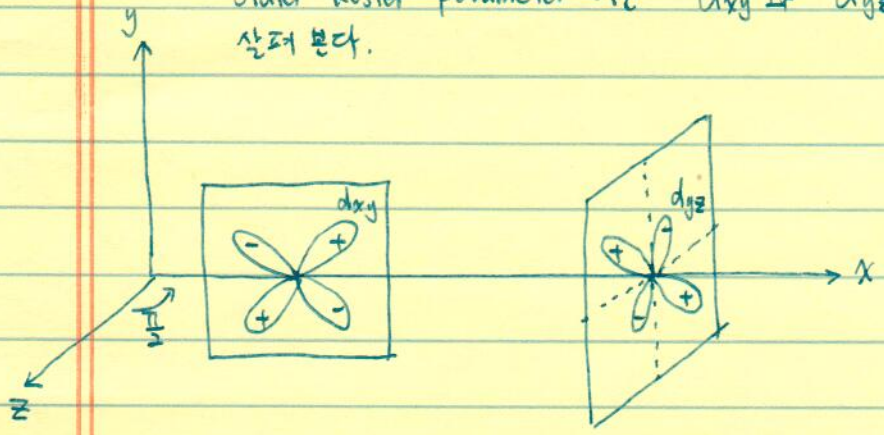


$+V_{dd\delta}\cos\phi\sin\phi$

이것은 내가 schematic 계산
이제 Slater-Koster parameter 와 비교해봐야.

2016 / 9 / 27 (화) (2)

Slater-Koster parameter 에는 d_{xy} 와 d_{yz} 의 값이 나와 있으므로 $E_{xy,yz}$ 를 살펴 본다.



$$E_{xy,yz} = 3lm^2n\,V_{dd\sigma} + ln(1-4m^2)\,V_{dd\pi} + ln(m^2-1)\,V_{dd\delta}$$

$$\begin{cases} l = \cos\phi \sin\theta \\ m = \sin\phi \sin\theta \\ n = \cos\theta \end{cases}$$

$$= \cos\theta\cos\phi\sin\theta\left(-1+\sin^2\theta\sin^2\phi\right)V_{dd\delta}$$

$$+ \cos\theta\cos\phi\sin\theta\left(1-4\sin^2\theta\sin^2\phi\right)V_{dd\pi}$$

$$+ 3\cos\theta\cos\phi\sin\theta\sin^2\theta\sin^2\phi\;V_{dd\sigma}$$

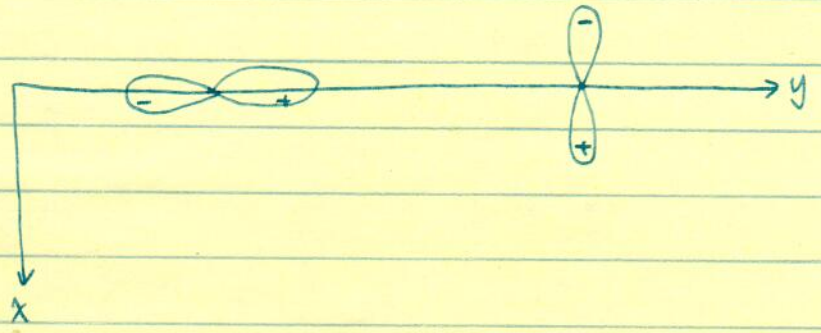
at $\phi = 0$ $\quad \cos\theta\sin\theta\left(V_{dd\pi} - V_{dd\delta}\right)$

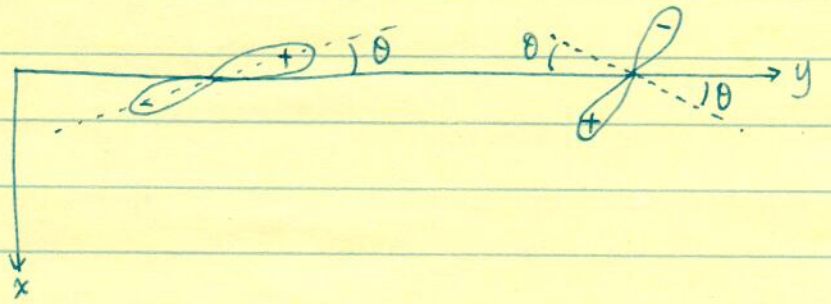
$\theta \to \theta + \frac{\pi}{2}$ $\quad \cos\theta\sin\theta\left(V_{dd\delta} - V_{dd\pi}\right)$

즉, Slater-Koster parameter 는 대략 schematic 개념과 같다.

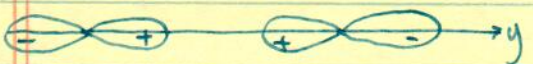
2016 / 9 / 27 (3)

그 다음은 rotation 에 대한 Slater-Koster parameter 를 구해보자.

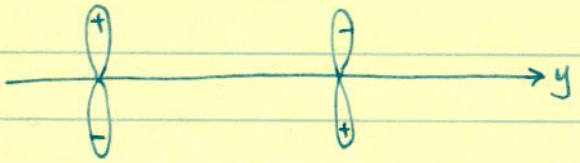




$$\cos\theta \sin\theta \left(-V_{dd\pi} - V_{dd\delta}\right) = -\cos\theta \sin\theta \left(V_{dd\pi} + V_{dd\delta}\right)$$



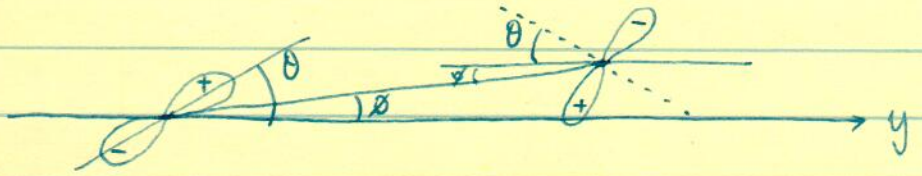
$-V_{dd\pi} \cos\theta \sin\theta$



$-V_{dd\delta} \cos\theta \sin\theta$.

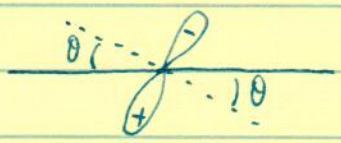
2016 / 9 / 27 (화) (4)

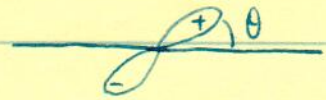
그럼 rotation 과 orbital 이동이 동시에 있을 때는 어떻겠는가?



$$-\cos(\theta-\phi)\sin(\theta+\phi)\,V_{dd\pi} - \cos(\theta+\phi)\sin(\theta-\phi)\,V_{dd\delta} \quad \cdots (*)$$

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





$$-\sin\theta\cos\theta\,V_{dd\pi} - \cos\theta\sin\theta\,V_{dd\delta}$$

$(*)\ (\leftarrow \phi=\frac{1}{2}) \Rightarrow -\cos\theta\sin\theta\,(V_{dd\pi}+V_{dd\delta})$ okay !!

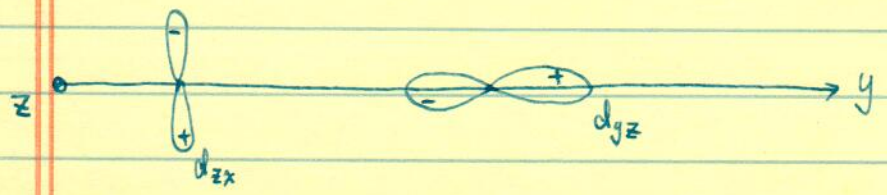
$$\therefore\ E_{yz,zx} = -\cos(\theta-\phi)\sin(\theta+\phi)\,V_{dd\pi} - \cos(\theta+\phi)\sin(\theta-\phi)\,V_{dd\delta}$$

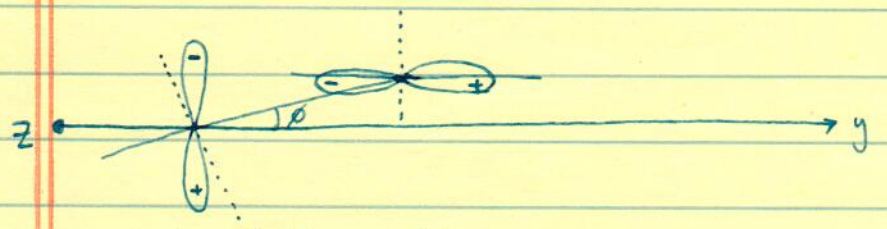
θ : local rotation, ϕ : coordinate angle.

2016/9/27 (화) (5).

그럼 $E_{zx,yz}$ 는 어떻게 될까?

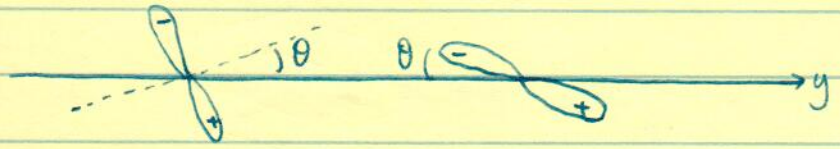
- Pristine slater - Kostar





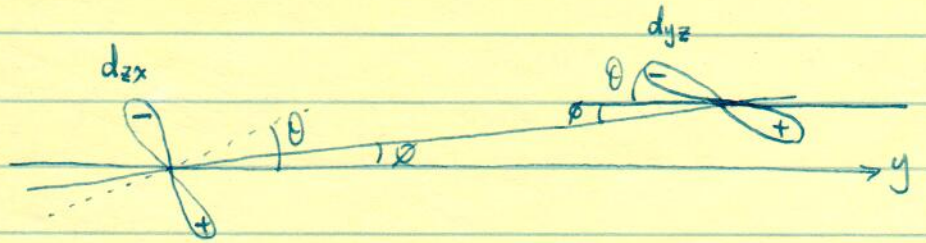
$\cos\phi \sin\phi \, (V_{dd\delta} - V_{dd\pi})$

- rotation Slater-Koster parameters



$\sin\theta\cos\theta \, (V_{dd\delta} + V_{dd\pi})$

- Combination of pristine and rotation Slater-Koster parameter.



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

$E_{yz,zx}(\theta,\phi) \xrightarrow{\theta \to -\theta,\ \phi \to \pi+\phi} E_{zx,yz}(\theta,\phi)$.