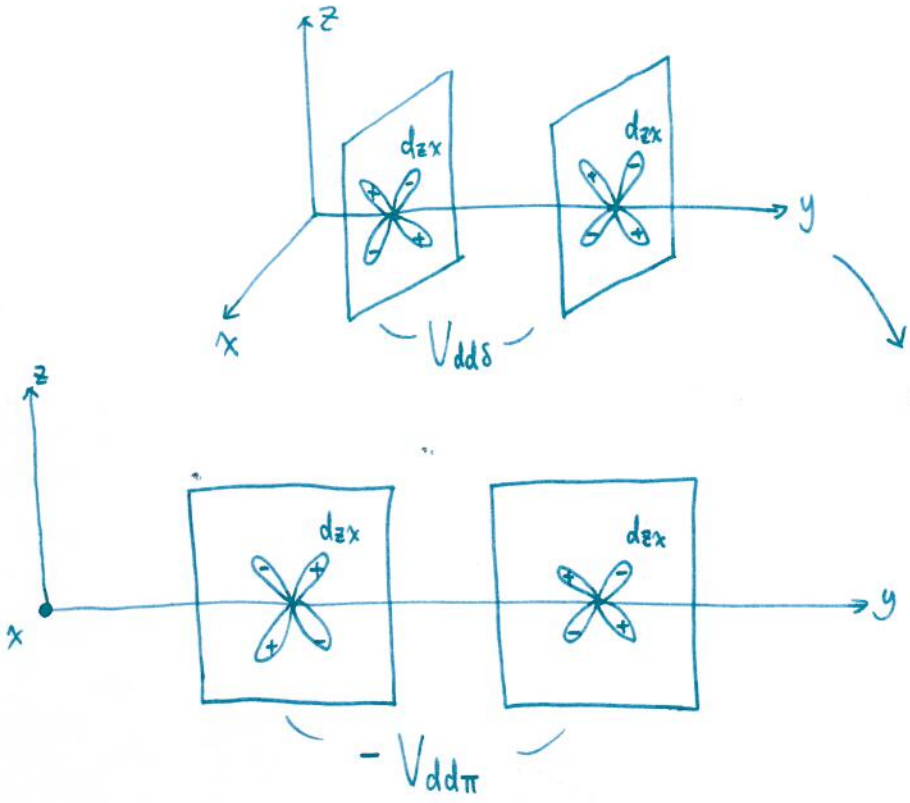
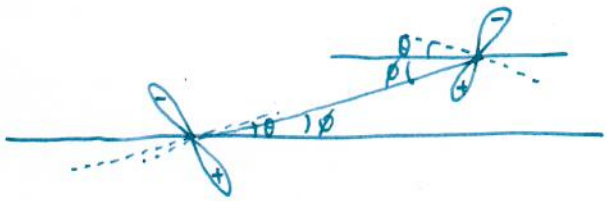
$E_{zx,zx} = \langle d_{zx} | H | d_{zx} \rangle$



$\therefore \; V_{dd\delta}\cos^2\theta - V_{dd\pi}\sin^2\theta$.

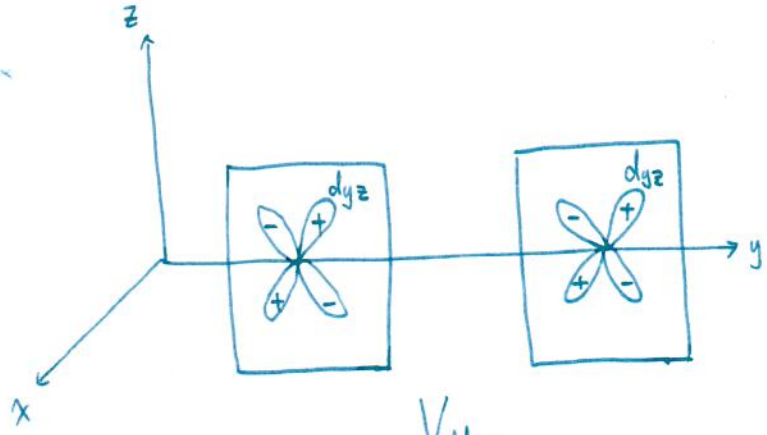


$E_{zx,zx} = V_{dd\delta}\cos(\theta-\phi)\cos(\theta+\phi) - V_{dd\pi}\sin(\theta-\phi)\sin(\theta+\phi)$.

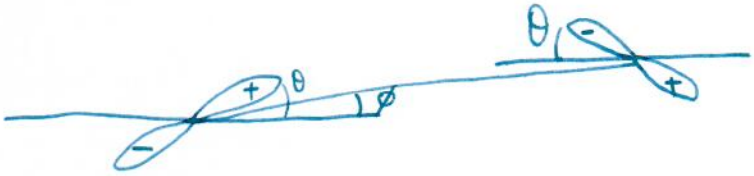
$\phi = \pi$; $V_{dd\delta}\cos^2\theta - V_{dd\pi}\sin^2\theta$. ✓

$\phi = \frac{\pi}{2}$: $V_{dd\pi}\cos^2\theta - V_{dd\delta}\sin^2\theta$ ✓

$E_{yz,yz} = \langle d_{yz} | H | d_{yz}' \rangle$



$V_{dd\pi}$



$\langle d_{yz} | H | d_{yz}' \rangle = V_{dd\pi} \cos(\theta - \phi) \cos(\theta + \phi)$

$- V_{dd\delta} \sin(\theta - \phi) \sin(\theta + \phi)$.

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

$V_{dd\delta} \cos^2\theta - V_{dd\pi} \sin^2\theta$.

according to Harrison's book Slater-Koster parameter for $E_{xy,xy}$ is given by

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

$$(l, m, n) = (\cos\varphi \sin\theta, \sin\theta \sin\varphi, \cos\theta).$$

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

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

위의 notation 은

$\Rightarrow \cos^2 2\phi V_{dd\pi} + \sin^2(2\phi) V_{dd\sigma}$ 로 하기로 한다.

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

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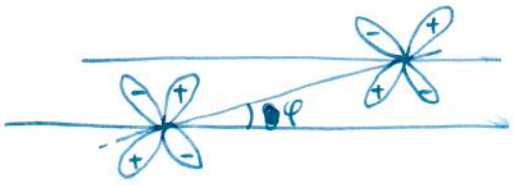


at $\varphi = \frac{\pi}{4} - \frac{\pi}{100}$

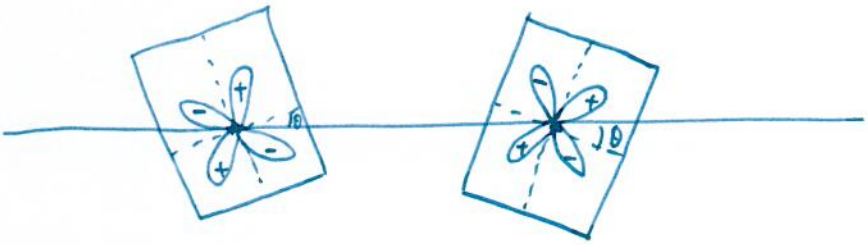
$E_{xy,xy} = 0.00394265\ V_{dd\pi}$

$+ 0.996057\ V_{dd\delta}$

at $\varphi = \frac{\pi}{4} - \frac{\pi}{6}$

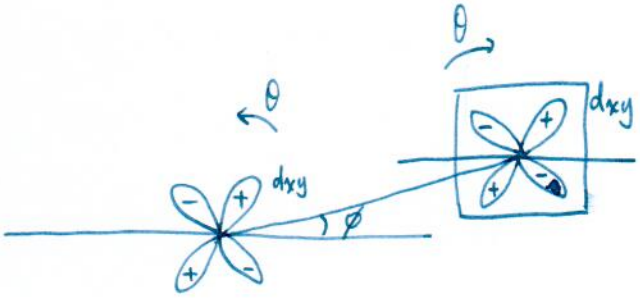
$E_{xy,xy} = 0.75\ V_{dd\pi} + 0.25\ V_{dd\delta}$

Same is true for local rotation of orbital.



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

그럼 다음 한 일은



과정

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

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

일까?