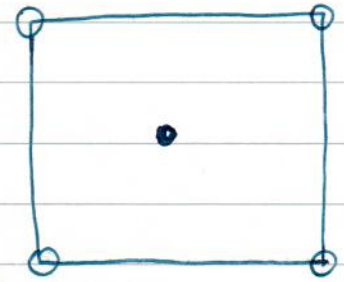
2016 / 9 / 23 (土) (1)

$$H_{\text{bilayer}} = 2t_0 (\cos k_x + \cos k_y)\, \sigma_0 \tau_0 \nu_0$$

$$+ 4t' \cos\frac{k_x}{2} \cos\frac{k_y}{2}\, \sigma_0 \tau_x \nu_0$$

$$+ 4t_{1d} \cos\frac{k_x}{2} \cos\frac{k_y}{2}\, \sigma_z \tau_y \nu_0$$



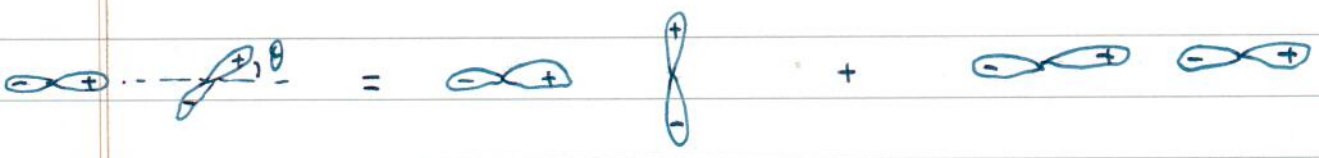
$d_{xy}$
$d_{yz}$
$d_{zx}$

$$|J_z = \tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}} \left( |d_{yz}\downarrow\rangle + i\,|d_{zx}\downarrow\rangle + |d_{xy}\uparrow\rangle \right)$$

$$|J_z = -\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}} \left( |d_{yz}\uparrow\rangle - i\,|d_{zx}\uparrow\rangle - |d_{xy}\downarrow\rangle \right)$$

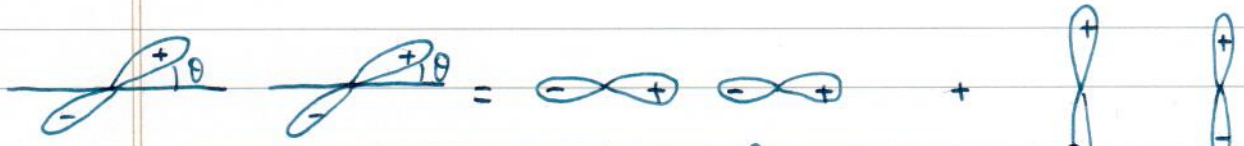
2016/9/23 (금) ~~(3)~~. (2)

Rotation & Slater-Koster parameters.

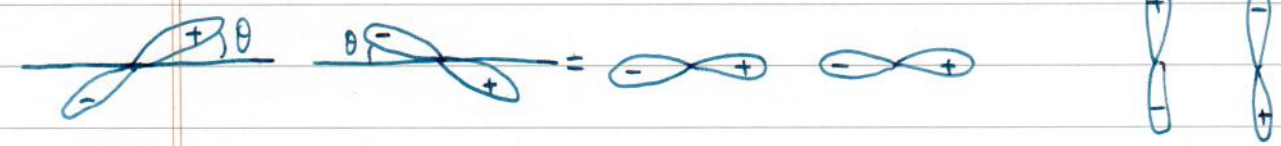


$\langle a | H | b \rangle = 0 \sin\theta + V_{pp\sigma} \cos\theta .$

$= V_{sp\sigma} \cos\theta + 0 \sin\theta$

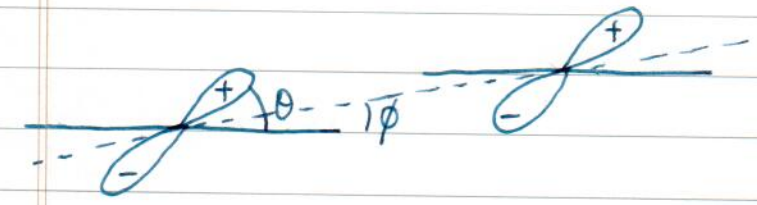


$V_{pp\sigma} \cos^2\theta + V_{pp\pi} \sin^2\theta .$



$V_{pp\sigma} \cos^2\theta - V_{pp\pi} \sin^2\theta$

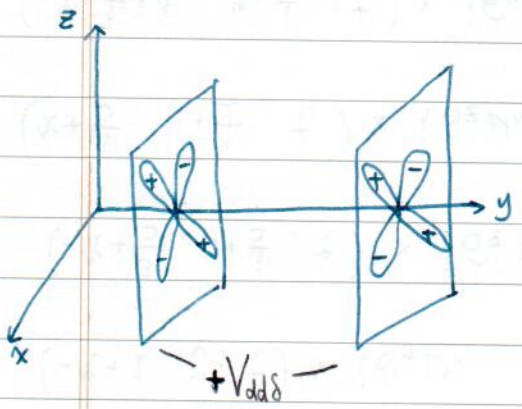
2016 / 9 / 23 (~~2~~) (3)

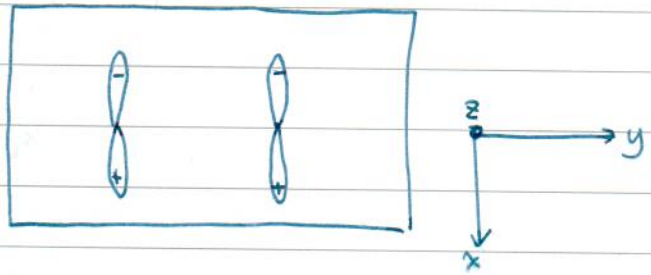


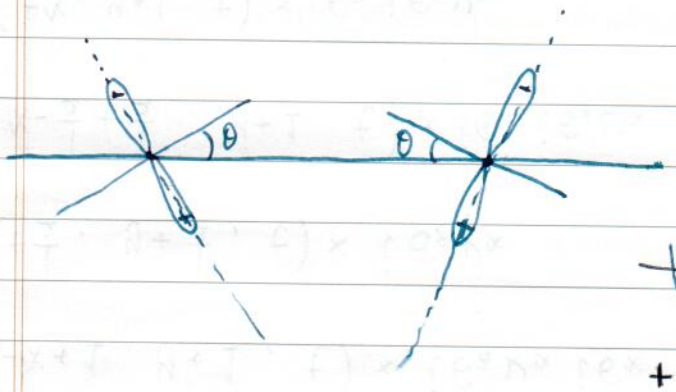

$= V_{pp\sigma}\cos(\theta-\phi)\cos(\theta+\phi) - V_{pp\pi}\sin(\theta-\phi)\sin(\theta+\phi)$

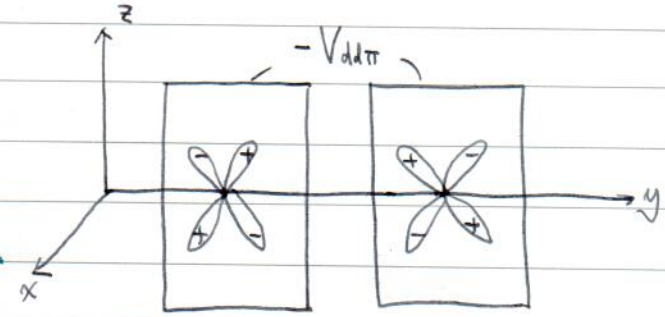
check! $\theta=0$, $\phi=\frac{\pi}{2}$ should be $V_{pp\pi}$

$\therefore V_{pp\sigma}\cos\left(-\frac{\pi}{2}\right)\cos\frac{\pi}{2} - V_{pp\pi}\sin\left(-\frac{\pi}{2}\right)\sin\frac{\pi}{2} = V_{pp\pi}$




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

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