スピン量子数（電子）　$s=\frac{1}{2}$

スピン磁気〜　　$m_s=\frac{1}{2}, -\frac{1}{2}$
$\uparrow \quad \downarrow$

l, m との類比

与えられた $l \longrightarrow m = l, \cdots, 0, \cdots -l$

$\longleftrightarrow \quad s=\frac{1}{2} \longrightarrow m_s = \frac{1}{2}, -\frac{1}{2}$

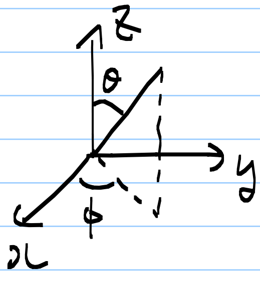
$l \leftrightarrow$（角度運動）角運動量

朝永振一郎「スピンはめぐる」

$(x, y, z) \longrightarrow (r, \theta, \phi)$

$$\frac{\partial}{\partial x} = \underline{\underline{\frac{\partial r}{\partial x}}}\frac{\partial}{\partial r} + \underline{\underline{\frac{\partial \theta}{\partial x}}}\frac{\partial}{\partial \theta} + \underline{\underline{\frac{\partial \phi}{\partial x}}}\frac{\partial}{\partial \phi} \quad \cdots ①$$

$$\begin{cases} r^2 = x^2 + y^2 + z^2 & \cdots ② \\ \cos\theta = \dfrac{z}{r} & \cdots ③ \\ \tan\phi = \dfrac{y}{x} & \cdots ④ \end{cases}$$



$\frac{\partial}{\partial x}② \Rightarrow \quad 2r\frac{\partial r}{\partial x} = 2x$

$$\underline{\underline{\frac{\partial r}{\partial x}}} = \frac{x}{r} = \sin\theta\cos\phi$$

$\frac{\partial}{\partial x}③ \Rightarrow \quad -\sin\theta\,\underline{\underline{\frac{\partial \theta}{\partial x}}} = z\frac{\partial}{\partial x}\left(\frac{1}{r}\right) = z\cdot\left(-\frac{1}{r^2}\right)\underline{\underline{\frac{\partial r}{\partial x}}}$

$$\rightarrow \quad \frac{\partial \theta}{\partial x} = \frac{r\cos\theta}{r^2 \cancel{\sin\theta}} \cdot \cancel{\sin\theta}\cos\phi = \frac{\cos\theta\cos\phi}{r}$$

$$\frac{\partial}{\partial x}④ \Longrightarrow \frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}$$

①は $\dfrac{\partial f}{\partial x} = \underbrace{\sin\theta\cos\phi\dfrac{\partial f}{\partial r} + \dfrac{\cos\theta\cos\phi}{r}\dfrac{\partial f}{\partial \theta} - \dfrac{\sin\phi}{r\sin\theta}\dfrac{\partial}{\partial \phi}}$

$$\frac{\partial^2}{\partial x^2} = \left(\sim\sim\sim\right)\left(\sim\sim\sim\right) f$$

$$= \cdots\cdot \ 9項$$

同様にして $\dfrac{\partial}{\partial y} \rightarrow \dfrac{\partial^2}{\partial y^2}$, $\dfrac{\partial}{\partial z} \rightarrow \dfrac{\partial^2}{\partial z^2}$

$$\rightarrow \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

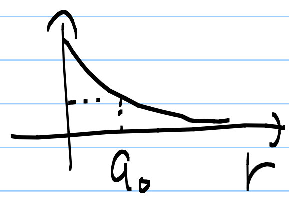
$\cos^2\theta + \sin^2\theta = 1$

$$=$$

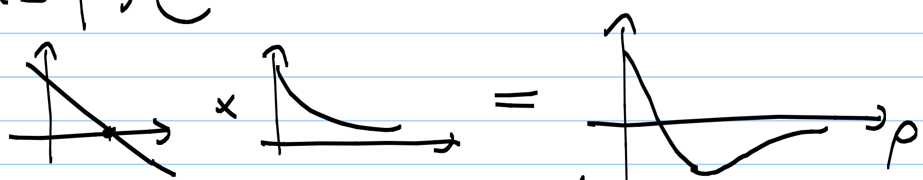
$$a_0 = \frac{\hbar^2}{m_e e^2} \cong 0.529\ \text{Å} \quad (ボーア半径)$$

H の 1s AO (Atomic Orbital)

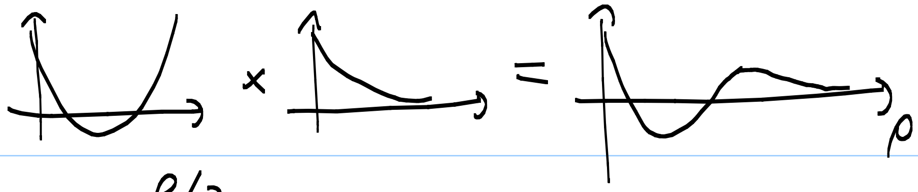
$$\psi = \underbrace{\sqrt{\frac{1}{\pi a_0^3}}}_{規格化定数} \underline{\underline{e^{-r/a_0}}}$$



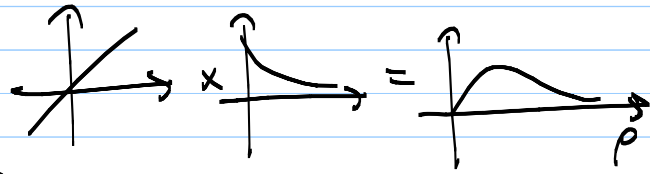
2s $\quad (2-\rho)e^{-\rho/2}$



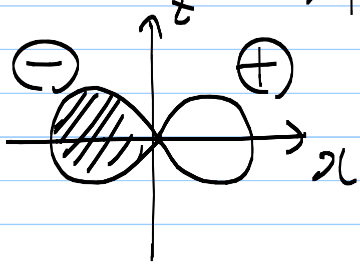
3s $\quad (27-18\rho+2\rho^2)e^{-\rho/3}$



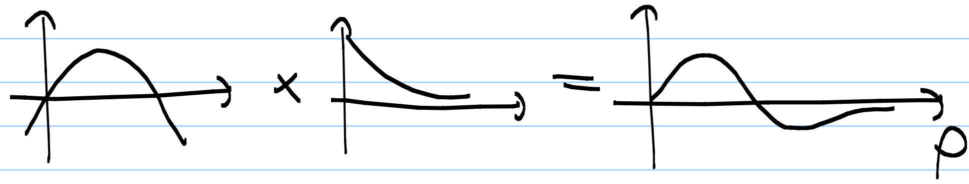
2p $\rho e^{-\rho/2}$ →



$2p_x$



3p $(6\rho-\rho^2)e^{-\rho/2}$



レポート課題(6月末まで)

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\hat{\Lambda}$$

を導きなさい。

$$\psi_{1s} \propto e^{-\rho}, \quad \psi_{2s} \propto (2-\rho)e^{-\rho/2}$$

$$\psi_{2p_z} \propto \rho e^{-\rho/2}\cos\theta$$

が $\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi$

を満たすことを確かめよ。

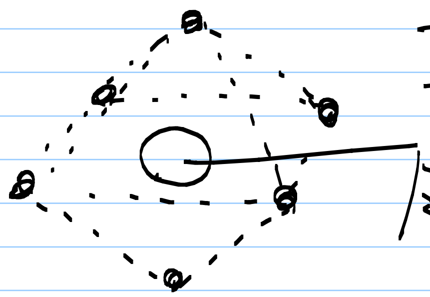
$$V(r) = -\frac{Ze^2}{r}$$

ψ_{2p_x}, ψ_{2p_y} はどうか？

$\psi_{2p_{\pm1}} \propto \psi_{2p_x} \pm i\,\psi_{2p_y}$ はどうか？

$l = 1 \rightarrow m = -1, 0, 1$

$\psi_{2p_0} = \psi_{2p_z}$



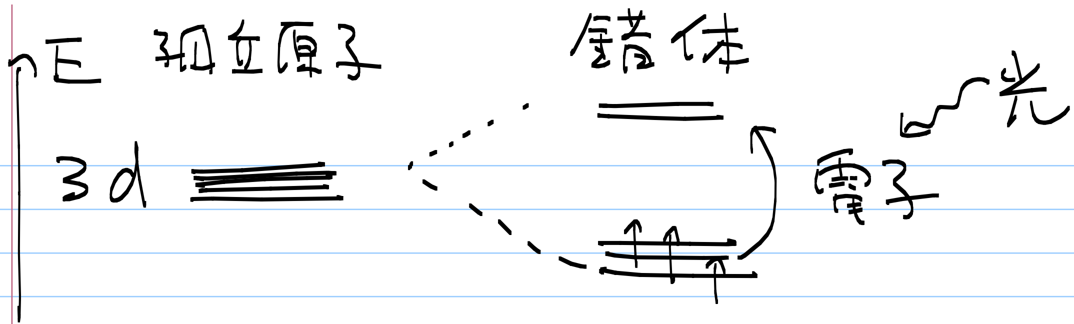
正八面体

イオン

遷移金属

Fe, Cr …

3d 電子



藤永「入門分子軌道法」

$$(fg)' = f'g + fg'$$

$$\sin\theta\cos\phi \frac{\partial}{\partial r} \cdot \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta}$$

$$= \sin\theta\cos\theta\cos^2\phi \frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial\theta}\right)$$

$$= \sim \left(-\frac{1}{r^2}\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\partial^2}{\partial r\,\partial\theta}\right)$$