

Schrodinger Equation:  $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi$

Radius wave function:  $R(r)^{(2)} + \left(\frac{2\mu}{\hbar^2} (E + \frac{e^2}{r}) - \frac{l(l+1)}{r^2}\right)R(r) = 0$

$R_{nl}(r) = N_{nl} e^{-\frac{\zeta}{2} r} \zeta^l F(-n+l+1, 2l+2, \zeta)$ , 其中  $\zeta = \frac{2Zr}{na}$ ,  $N_{nl} = \left(\frac{2Z}{a}\right)^{\frac{3}{2}} \frac{1}{n^2(2l+1)!} \sqrt{\frac{(n+1)!}{(n-l-1)!}}$

Spherical harmonic function:  $\sin\theta \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{\partial^2 Y}{\partial \varphi^2} = -l(l+1)\sin^2\theta Y$

$Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \cdot P_l^m(\cos\theta) e^{im\varphi}$ , 其中  $\theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right)$

Wave function of Hydrogen:  $\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)^3}} e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l (L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)) Y_l^m(\theta, \phi)$

Space Density Distribution Probability function:  $W_{nlm}(r, \theta, \varphi) = |R_{nl}(r)Y_{lm}(\theta, \varphi)|^2$

薛定谔方程:  $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi$

径向波函数的方程:  $R(r)^{(2)} + \left(\frac{2\mu}{\hbar^2} \left(E + \frac{e^2}{r}\right) - \frac{l(l+1)}{r^2}\right)R(r) = 0$

径向波函数的解:

$$R_{nl}(r) = N_{nl} e^{-\frac{\zeta}{2} r} \zeta^l F(-n+l+1, 2l+2, \zeta), \text{ 其中 } \zeta = \frac{2Zr}{na}, N_{nl} = \left(\frac{2Z}{a}\right)^{\frac{3}{2}} \frac{1}{n^2(2l+1)!} \sqrt{\frac{(n+1)!}{(n-l-1)!}}$$

球谐函数的方程:  $\sin\theta \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{\partial^2 Y}{\partial \varphi^2} = -l(l+1)\sin^2\theta Y$

球谐函数的解:  $Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \cdot P_l^m(\cos\theta) e^{im\varphi}$ , 其中  $\theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right)$

氢原子波函数:  $\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)^3}} e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l (L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)) Y_l^m(\theta, \varphi)$

核外电子空间概率密度分布函数:  $W_{nlm}(r, \theta, \varphi) = |R_{nl}(r)Y_{lm}(\theta, \varphi)|^2$

$$1,0,0: W_{100} = \frac{1}{\pi} * \frac{1}{a^3} e^{-\frac{2r}{a}}$$

$$2,0,0: W_{200} = \frac{1}{8\pi} * \frac{1}{a^3} (1 - \frac{r}{2a})^2 e^{-\frac{r}{a}}$$

$$2,1,0: W_{210} = \frac{1}{32\pi} * \frac{1}{a^5} * r^2 * e^{-\frac{r}{a}} * \cos^2\theta$$

$$2,1,\pm 1: W_{211} = \frac{1}{64\pi} * \frac{1}{a^5} * r^2 e^{-\frac{r}{a}} * \sin^2\theta$$

$$3,0,0: W_{300} = \frac{1}{27\pi} * \frac{1}{a^3} * (1 - \frac{2}{3} * \frac{r}{a} + \frac{2}{27} (\frac{r}{a})^2)^2 e^{-\frac{2r}{3a}}$$

$$3,1,0: W_{310} = \frac{8}{729\pi} * \frac{1}{a^5} * r^2 (1 - \frac{1}{6} * \frac{r}{a})^2 e^{-\frac{2r}{3a}} * \cos^2\theta$$

$$3,1,\pm 1: W_{311} = \frac{4}{729\pi} * \frac{1}{a^5} * r^2 (1 - \frac{1}{6} * \frac{r}{a})^2 * e^{-\frac{2r}{3a}} * \sin^2\theta$$

$$3,2,0: W_{320} = \frac{1}{39366\pi} * \frac{1}{a^7} * r^4 e^{-\frac{2r}{3a}} * (3\cos^2\theta - 1)^2$$

$$3,2,\pm 1: W_{321} = \frac{1}{6561\pi} * \frac{1}{a^7} * r^4 e^{-\frac{2r}{3a}} * \sin^2\theta \cos^2\theta$$

$$3,2,\pm 2: W_{322} = \frac{1}{26244\pi} * \frac{1}{a^7} * r^4 e^{-\frac{2r}{3a}} * \sin^4\theta$$

$$4,0,0: W_{400} = \frac{1}{64\pi} * \frac{1}{a^3} * (1 - \frac{3}{4} * \frac{r}{a} + \frac{1}{8} (\frac{r}{a})^2 - \frac{1}{192} (\frac{r}{a})^3)^2 e^{-\frac{r}{2a}}$$

$$4,1,0: W_{410} = \frac{5}{1024\pi} * \frac{1}{a^5} (1 - \frac{1}{4} * \frac{r}{a} + \frac{1}{80} (\frac{r}{a})^2)^2 e^{-\frac{r}{2a}} * \cos^2\theta$$

$$4,1,\pm 1: W_{411} = \frac{5}{2048\pi} * \frac{1}{a^5} * r^2 (1 - \frac{1}{4} * \frac{r}{a} + \frac{1}{80} (\frac{r}{a})^2)^2 e^{-\frac{r}{2a}} * \sin^2\theta$$

$$4,2,0: W_{420} = \frac{1}{65536\pi} * \frac{1}{a^7} * r^4 (1 - \frac{1}{12} * \frac{r}{a})^2 e^{-\frac{r}{2a}} * (3\cos^2\theta - 1)^2$$

$$4,2,\pm 1: W_{421} = \frac{3}{32768\pi} * \frac{1}{a^7} * r^4 (1 - \frac{1}{12} * \frac{r}{a})^2 e^{-\frac{r}{2a}} \sin^2\theta \cos^2\theta$$

$$4,2,\pm 2: W_{422} = \frac{3}{131072\pi} * \frac{1}{a^7} * r^4 (1 - \frac{1}{12} * \frac{r}{a})^2 e^{-\frac{r}{2a}} * \sin^4\theta$$

$$4,3,0: W_{430} = \frac{1}{47185920\pi} * \frac{1}{a^9} * r^6 e^{-\frac{r}{2a}} * (5\cos^3\theta - 3\cos\theta)^2$$

$$4,3,\pm 1: W_{431} = \frac{1}{62914560\pi} * \frac{1}{a^9} * r^6 e^{-\frac{r}{2a}} * \sin^2\theta (5\cos^2\theta - 1)^2$$

$$4,3,\pm 2: W_{432} = \frac{1}{6291456\pi} * \frac{1}{a^9} * r^6 e^{-\frac{r}{2a}} * \sin^4\theta \cos^2\theta$$

$$4,3,\pm 3: W_{433} = \frac{1}{37748736\pi} * \frac{1}{a^9} * r^6 e^{-\frac{r}{2a}} * \sin^6\theta$$