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

径向波函数的解：

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

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

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

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

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