Calculate 1s, 2s, and 2p orbital wave functions. And graphically plot them to compare and understand their space distribution.

$$\varphi_{n,l,m}(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

$$= -\sqrt{\left(\frac{2}{na_0}\right)^3 \left(\frac{(n-l-1)!}{2n\{(n+l)!\}^3}\right)} \left(\frac{2r}{na_0}\right)^l \exp\left(-\frac{r}{na_0}\right) L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)$$

$$\times \sqrt{\frac{2l+1}{2}\frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) \times \sqrt{\frac{1}{2\pi}} \exp(im\phi)$$

where $n = 1,2,3,\ldots \geq l+1$ (principal q. n.) q. n. : quantum num.

$l = 0,1,2,3,\ldots \geq |m|$ (azimuthal q. n.)

$m = 0, \pm 1, \pm 2, \ldots$ (magnetic q. n.)

$a_0 = \dfrac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$ (Bohr radius) p.n. : polynomials

$$L_{n+l}^{2l+1}(\rho) = (-1)^{n+l}\frac{(n+l)!}{(n-l-1)!}\left\{\rho^{(n-l-1)} - \frac{(n+l)(n-l-1)}{1!}\rho^{n+l-2} + \frac{(n+l)(n+l-1)(n-l-1)(n-l-2)}{2!}\rho^{n-l-3}\cdots\right\}$$

(assctd. Legendre p.n.)

$$P_l^{|m|}(z) = \frac{(1-z^2)^{\frac{|m|}{2}}}{2^l l!}\frac{d^{l+|m|}}{dz^{l+|m|}}(z^2-1)^l$$

(assctd. Laguerre p.n.)

(1) 1s

$$\varphi_{1,0,0}(r,\theta,\phi) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2}\exp\left(-\frac{r}{a_0}\right)$$

(2) 2s

$$\varphi_{2,0,0}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)\exp\left(-\frac{r}{2a_0}\right)$$

(3) 2p (2p-z, 2p-x, 2p-y)

$$\varphi_{2,1,0}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\exp\left(-\frac{r}{2a_0}\right)\cos\theta \qquad \cos\theta \to \frac{z}{r}$$

$$\varphi_{2,1,1}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\exp\left(-\frac{r}{2a_0}\right)\frac{1}{\sqrt{2}}\sin\theta\exp(i\phi) \qquad \frac{1}{\sqrt{2}}\sin\theta\exp(i\phi) \to \frac{x}{r}$$

$$\varphi_{2,1,-1}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\exp\left(-\frac{r}{2a_0}\right)\frac{1}{\sqrt{2}}\sin\theta\exp(-i\phi) \qquad \frac{1}{\sqrt{2}}\sin\theta\exp(-i\phi) \to \frac{y}{r}$$

(4) 3s

$$= \frac{1}{81\sqrt{3\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left\{27 - 18\left(\frac{r}{a_0}\right) + 2\left(\frac{r}{a_0}\right)^2\right\}\exp\left(-\frac{r}{3a_0}\right)$$