Computer Lab 6.1: Hydrogen Atom Calcualtions

Full kinetic energy operator in spherical coordinaties:

Kinetic energy operator for s states:

$$-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\blacksquare$$

Kinetic energy operator for p states:

$$-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\blacksquare\ \ldots$$
$$+\frac{-1}{2\cdot r^2\cdot\sin(\theta)}\cdot\left[\frac{d}{d\theta}\left(\sin(\theta)\cdot\frac{d}{d\theta}\blacksquare\right)\right]\ \ldots$$
$$+\frac{-1}{2\cdot r^2\cdot\sin(\theta)^2}\cdot\frac{d^2}{d\phi^2}\blacksquare$$

Position operator: r

Potential energy operator: $-\frac{1}{r}$

Triple integral with volume element:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi}\blacksquare\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr$$

Orbitals:

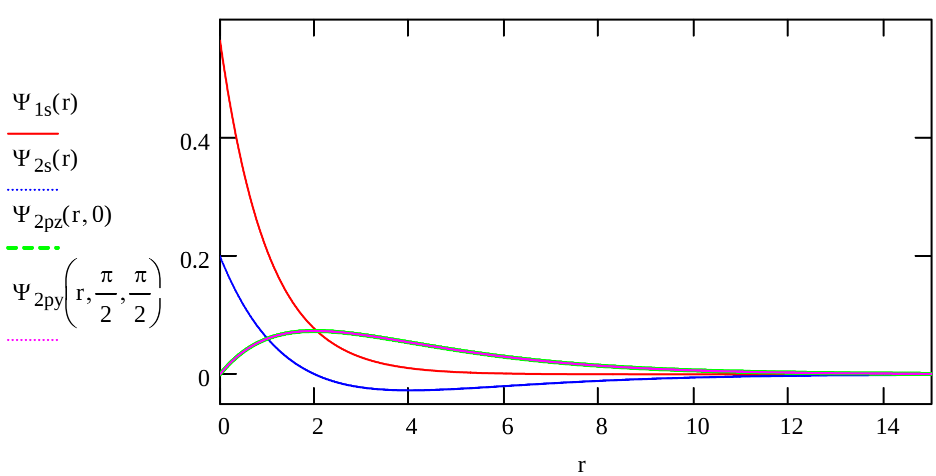
$$\Psi_{1s}(r) := \frac{1}{\sqrt{\pi}}\cdot\exp(-r)$$

$$\Psi_{2s}(r) := \frac{1}{\sqrt{32\cdot\pi}}\cdot(2-r)\cdot\exp\left(-\frac{r}{2}\right)$$

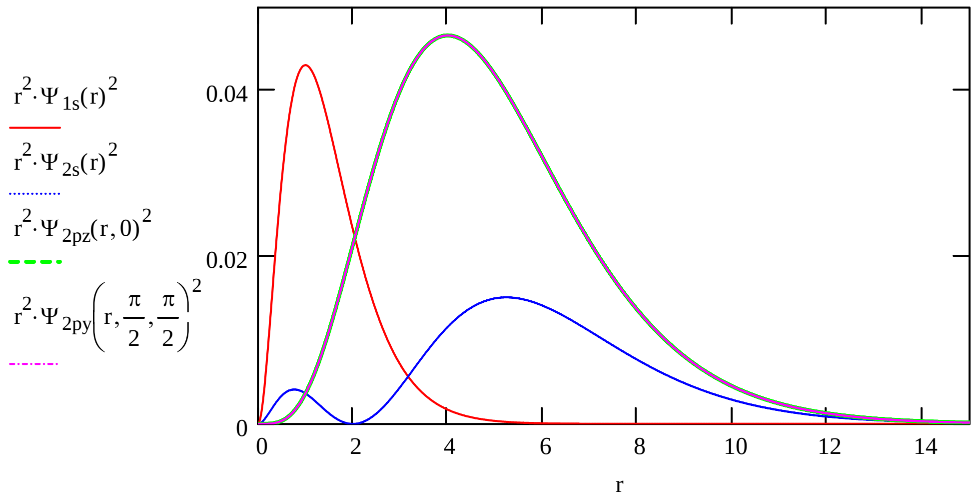
$$\Psi_{2pz}(r,\theta) := \frac{1}{\sqrt{32\cdot\pi}}\cdot r\cdot\exp\left(-\frac{r}{2}\right)\cdot\cos(\theta)$$

$$\Psi_{2py}(r,\theta,\phi) := \frac{1}{\sqrt{32\cdot\pi}}\cdot r\cdot\exp\left(-\frac{r}{2}\right)\cdot\sin(\theta)\cdot\sin(\phi)$$

Plot the wave functions on the same graph:



Plot the radial distribution functions for each orbital on the same graph:



Demonstrate that the 1s orbital is normalized:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)^2\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 1$$

Demonstrate that the 2s orbital is normalized:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2s}(r)^2\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 1$$

Demonstrate that the $2p_z$ orbital is normalized:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2pz}(r,\theta)^2\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 1$$

Demonstrate that the 1s and the $2p_z$ orbitals are orthogonal:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)\cdot\Psi_{2pz}(r,\theta)\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 0$$

Demonstrate that 1s and 2s orbitals are orthogonal:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)\cdot\Psi_{2s}(r)\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 0$$

Demonstrate that the $2p_y$ and the $2p_z$ orbitals are orthogonal:

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2py}(r,\theta,\phi)\cdot\Psi_{2pz}(r,\theta)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow 0$$

Determine the most probable value for r using the Trace function and calculus:

$$\frac{d}{dr}r^2\cdot\Psi_{1s}(r)^2 = 0 \text{ solve}, r \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Calculate the probability that an electron in the 1s orbital will be found within one Bohr radius of the nucleus.

$$\int_0^{1}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)^2\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \text{ float}, 3 \rightarrow .325$$

Find the distance from the nucleus for which the probability of finding a 1s electron is 0.75.

$a := 2$ Given $\int_0^{a} \Psi_{1s}(r)^2\cdot 4\cdot\pi\cdot r^2\, dr = .75$ $\text{Find}(a) = 1.96$

Calculate <T>, <V>, and <r> for the 1s orbital. Is the virial theorem obeyed? Explain.

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)\cdot -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\left(\Psi_{1s}(r)\right)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{1}{2}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)\cdot -\frac{1}{r}\cdot\Psi_{1s}(r)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow -1$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{1s}(r)\cdot r\cdot\Psi_{1s}(r)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{3}{2}$$

Calculate <T>, <V>, and <r> for the 2s orbital. Is the virial theorem obeyed? Explain.

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2s}(r)\cdot -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{2s}(r)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{1}{8}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2s}(r)\cdot -\frac{1}{r}\cdot\Psi_{2s}(r)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{-1}{4}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2s}(r)\cdot r\cdot\Psi_{2s}(r)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow 6$$

Calculate <T>, <V>, and <r> for the $2p_y$ orbital. Is the virial theorem obeyed? Explain.

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2py}(r,\theta,\phi)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{2py}(r,\theta,\phi)\ \ldots\right. \\ + \frac{-1}{2\cdot r^2\cdot\sin(\theta)}\cdot\left[\frac{d}{d\theta}\left(\sin(\theta)\cdot\frac{d}{d\theta}\Psi_{2py}(r,\theta,\phi)\right)\right]\ \ldots \\ \left. + \frac{-1}{2\cdot r^2\cdot\sin(\theta)^2}\cdot\frac{d^2}{d\phi^2}\Psi_{2py}(r,\theta,\phi)\right]\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{1}{8}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2py}(r,\theta,\phi)\cdot-\frac{1}{r}\cdot\Psi_{2py}(r,\theta,\phi)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{-1}{4}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2py}(r,\theta,\phi)\cdot r\cdot\Psi_{2py}(r,\theta,\phi)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow 5$$

Calculate <T>, <V>, and <r> for the $2p_z$ orbital. Is the virial theorem obeyed? Explain.

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2pz}(r,\theta)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{2pz}(r,\theta)\ \ldots\right. \\ + \frac{-1}{2\cdot r^2\cdot\sin(\theta)}\cdot\left[\frac{d}{d\theta}\left(\sin(\theta)\cdot\frac{d}{d\theta}\Psi_{2pz}(r,\theta)\right)\right]\ \ldots \\ \left. + \frac{-1}{2\cdot r^2\cdot\sin(\theta)^2}\cdot\frac{d^2}{d\phi^2}\Psi_{2pz}(r,\theta)\right]\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{1}{8}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2pz}(r,\theta)\cdot-\frac{1}{r}\cdot\Psi_{2pz}(r,\theta)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow \frac{-1}{4}$$

$$\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi_{2pz}(r,\theta)\cdot r\cdot\Psi_{2pz}(r,\theta)\cdot r^2\cdot\sin(\theta)\, d\phi\, d\theta\, dr \rightarrow 5$$

Summarize your results in the following table:

Ψ	T	V	E	r
1s	0.5	−1	−0.5	1.5
2s	0.125	−0.25	−0.125	6
2pz	0.125	−0.25	−0.125	5
2py	0.125	−0.25	−0.125	5

Demonstrate that the 1s orbital is an eigenfunction of the energy operator. What is the eigenvalue?

$$T = -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\blacksquare \qquad V = -\frac{1}{r} \qquad H = T + V \qquad \Psi(r) = \frac{1}{\sqrt{\pi}}\cdot\exp(-r)$$

$$\frac{-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{1s}(r) - \frac{1}{r}\cdot\Psi_{1s}(r)}{\Psi_{1s}(r)} \text{ simplify } \rightarrow \frac{-1}{2}$$

Demonstrate that the 2s orbital is an eigenfunction of the energy operator. What is the eigenvalue?

$$\frac{-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{2s}(r) - \frac{1}{r}\cdot\Psi_{2s}(r)}{\Psi_{2s}(r)} \text{ simplify } \rightarrow \frac{-1}{8}$$

Demonstrate that the $2p_y$ orbital is an eigenfunction of the energy operator. What is the eigenvalue?

$$\frac{\left[\begin{array}{l}-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}r\cdot\Psi_{2py}(r,\theta,\phi)\ \ldots \\ +\frac{-1}{2\cdot r^2\cdot\sin(\theta)}\cdot\left[\frac{d}{d\theta}\left(\sin(\theta)\cdot\frac{d}{d\theta}\Psi_{2py}(r,\theta,\phi)\right)\right]\ \ldots \\ +\frac{-1}{2\cdot r^2\cdot\sin(\theta)^2}\cdot\frac{d^2}{d\phi^2}\Psi_{2py}(r,\theta,\phi)\end{array}\right] - \frac{1}{r}\cdot\Psi_{2py}(r,\theta,\phi)}{\Psi_{2py}(r,\theta,\phi)} \text{ simplify } \rightarrow \frac{-1}{8}$$