

1.82: The Position-Momentum Uncertainty Relation in the Hydrogen Atom

The hydrogen atom coordinate and momentum wave functions can be used to illustrate the uncertainty relation involving position and momentum.

The 1s wave function is used to calculate the average distance of the electron from the nucleus.

$$\Psi_{1s}(r) := \frac{1}{\sqrt{\pi}} \cdot \exp(-r) \quad r_{1s} := \int_0^\infty r \cdot \Psi_{1s}(r)^2 \cdot 4 \cdot \pi \cdot r^2 dr \quad r_{1s} = 1.500$$

The Fourier transform of the 1s wave function yields the momentum wave function. The momentum wave function is used to calculate the average magnitude of the electron momentum.

$$\begin{aligned} \Phi_{1s}(p) &:= \frac{1}{\sqrt{8 \cdot \pi^3}} \cdot \int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi_{1s}(r) \cdot \exp(-i \cdot p \cdot r \cdot \cos(\theta)) \cdot r^2 \cdot \sin(\theta) d\phi d\theta dr \rightarrow 2 \\ &\quad \cdot \frac{2^{\frac{1}{2}}}{\pi \cdot [(-1) + i \cdot p]^2 \cdot (1 + i \cdot p)^2} \\ p_{1s} &:= \int_0^\infty p \cdot (|\Phi_{1s}(p)|)^2 \cdot 4 \cdot \pi \cdot p^2 dp \quad p_{1s} = 0.849 \end{aligned}$$

The 2s wave function is used to calculate the average distance of the electron from the nucleus.

$$\Psi_{2s}(r) := \frac{1}{\sqrt{32 \cdot \pi}} \cdot (2 - r) \cdot \exp\left(-\frac{r}{2}\right) \quad r_{2s} := \int_0^\infty r \cdot \Psi_{2s}(r)^2 \cdot 4 \cdot \pi \cdot r^2 dr \quad r_{2s} = 6.000$$

The Fourier transform of the 2s wave function yields the momentum wave function. The momentum wave function is used to calculate the average magnitude of the electron momentum.

$$\begin{aligned} \Phi_{2s}(p) &:= \frac{1}{\sqrt{8 \cdot \pi^3}} \cdot \int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi_{2s}(r) \cdot \exp(-i \cdot p \cdot r \cdot \cos(\theta)) \cdot r^2 \cdot \sin(\theta) d\phi d\theta dr \rightarrow \frac{-16}{\pi} \\ &\quad \cdot \frac{(-1) + 4 \cdot p^2}{[(-1) + 2 \cdot i \cdot p]^3 \cdot (1 + 2 \cdot i \cdot p)^3} \\ p_{2s} &:= \int_0^\infty p \cdot (|\Phi_{2s}(p)|)^2 \cdot 4 \cdot \pi \cdot p^2 dp \quad p_{2s} = 0.340 \end{aligned}$$

The 3s wave function is used to calculate the average distance of the electron from the nucleus

$$\Psi_{3s}(r) := \frac{1}{81 \cdot \sqrt{3 \cdot \pi}} \cdot (27 - 18 \cdot r + 2 \cdot r^2) \exp\left(-\frac{r}{3}\right) \quad r_{3s} := \int_0^\infty r \cdot \Psi_{3s}(r)^2 \cdot 4 \cdot \pi \cdot r^2 dr \quad r_{3s} = 13.500$$

The Fourier transform of the 3s wave function yields the momentum wave function. The momentum wave function is used to calculate the average magnitude of the electron momentum.

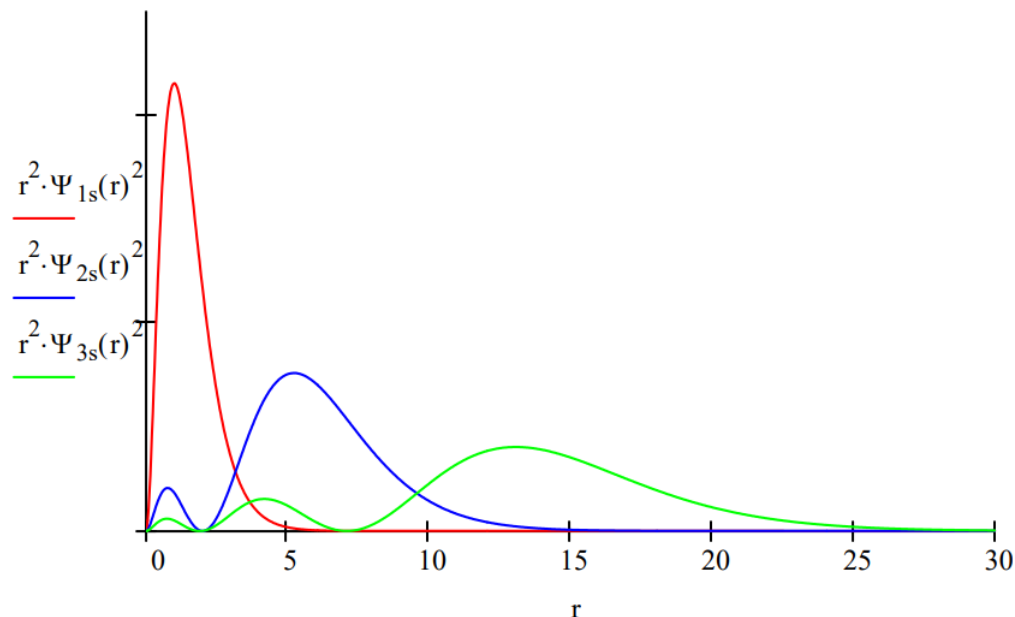
$$\begin{aligned} \Phi_{3s}(p) &:= \frac{1}{\sqrt{8 \cdot \pi^3}} \cdot \int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi_{3s}(r) \cdot \exp(-i \cdot p \cdot r \cdot \cos(\theta)) \cdot r^2 \cdot \sin(\theta) d\phi d\theta dr \rightarrow 18 \cdot \frac{2^2}{\pi} \cdot 3^{\frac{1}{2}} \\ &\quad \cdot \frac{1 - 30 \cdot p^2 + 81 \cdot p^4}{[(-1) + 3 \cdot i \cdot p]^4 \cdot (1 + 3 \cdot i \cdot p)^4} \\ p_{3s} &:= \int_0^\infty p \cdot (|\Phi_{3s}(p)|)^2 \cdot 4 \cdot \pi \cdot p^2 dp \quad p_{3s} = 0.218 \end{aligned}$$

These results can be summarize in both tabular and graphical form.

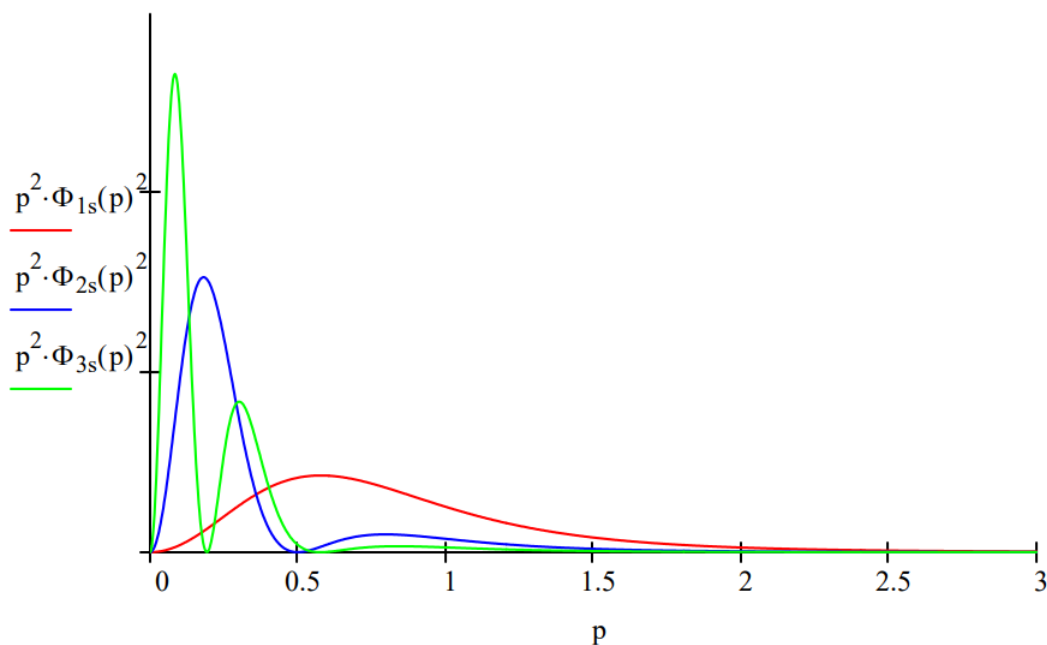
Orbital	AveragePosition	AverageMomentum
1s	1.5	0.849
2s	6.0	0.340
3s	13.5	0.218

The table shows that the average distance of the electron from the nucleus increases from 1s to 3s, indicating an increase in the uncertainty in the location of the electron. At the same time the average magnitude of electron momentum decreases from 1s to 3s, indicating a decrease in momentum uncertainty. The spatial and momentum distribution functions shown below illustrate this effect graphically.

Spatial Distribution Functions



Momentum Distribution Functions



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