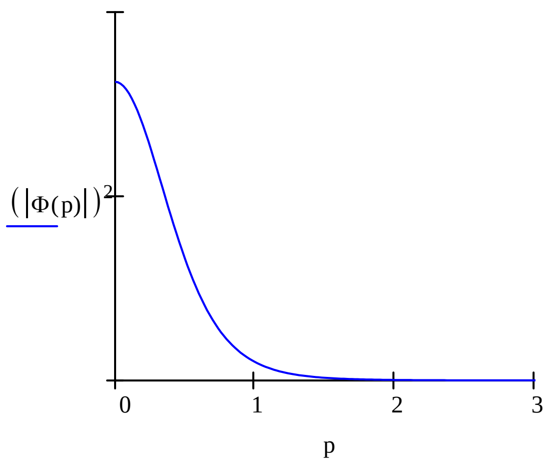
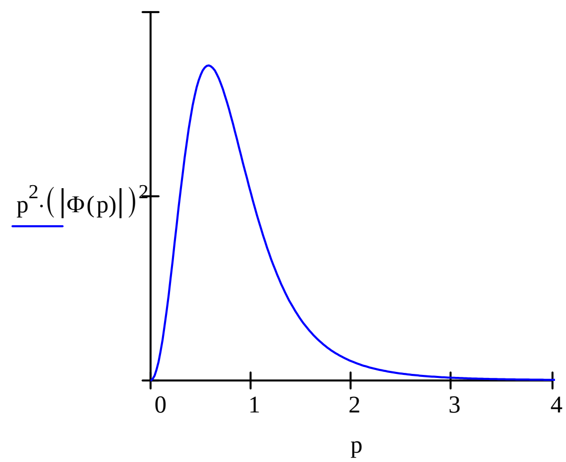
Momentum Distributions for Hydrogen Atomic Orbitals

The Fourier transform for the 1s orbital

$$\Phi(p) := \frac{1}{\sqrt{8\cdot\pi^4}}\cdot\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi}\exp(-r)\cdot\exp(-i\cdot p\cdot r\cdot\cos(\theta))\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr \rightarrow 2\cdot\frac{2^{\frac{1}{2}}}{\pi\cdot[(-1)+i\cdot p]^2\cdot(1+i\cdot p)^2}$$

$p := 0, .02 .. 5$

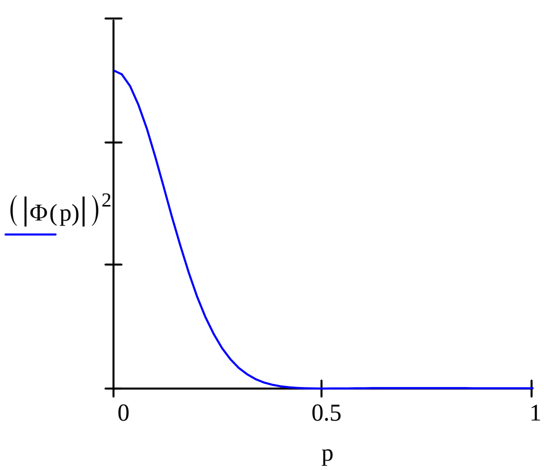


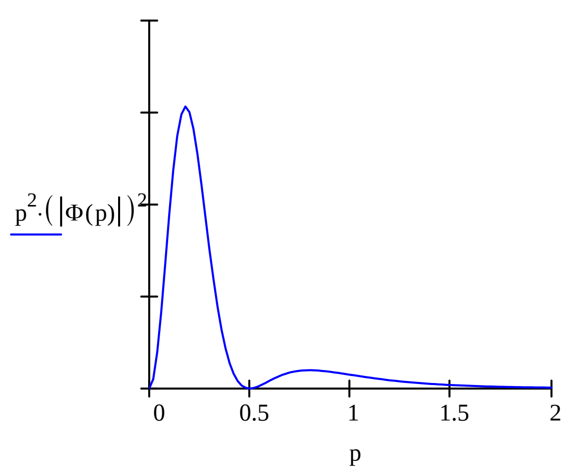


The Fourier transform for the 2s orbital

$$\Phi(p) := \frac{1}{16\cdot\pi^2}\cdot\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi}(2-r)\cdot\exp\left(-\frac{r}{2}\right)\cdot\exp(-i\cdot p\cdot r\cdot\cos(\theta))\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr$$

yields $\Phi(p) := \frac{-16}{\pi}\cdot\frac{(-1)+4\cdot p^2}{[(-1)+2\cdot i\cdot p]^3\cdot(1+2\cdot i\cdot p)^3}$ $\quad$ $p := 0, .02 .. 2$

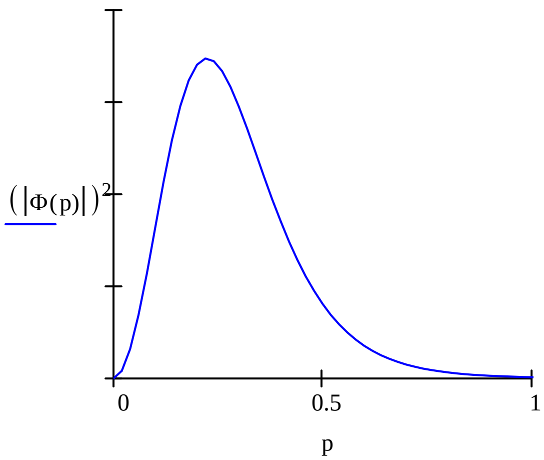


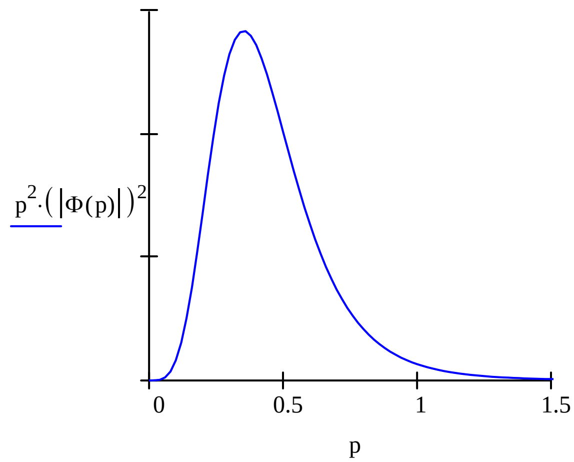


The Fourier transform for the $2p_z$ orbital

$$\Phi(p) := \frac{1}{16\cdot\pi^2}\cdot\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} r\cdot\exp\left(-\frac{r}{2}\right)\cdot\exp(-i\cdot p\cdot r\cdot\cos(\theta))\cdot\cos(\theta)\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr$$

yields $\Phi(p) := 64\cdot\frac{i}{\pi}\cdot\frac{p}{[(-1)+2\cdot i\cdot p]^3\cdot(1+2\cdot i\cdot p)^3}$

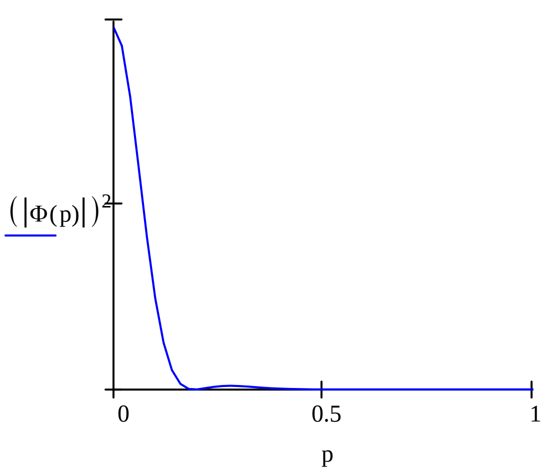


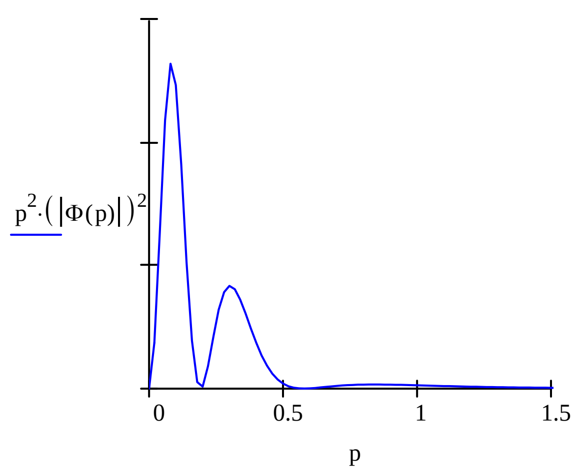


The Fourier transform for the 3s orbital

$$\Phi(p) := \frac{1}{162\cdot\sqrt{6}\cdot\pi^2}\cdot\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi}\left(27-18\cdot r+2\cdot r^2\right)\cdot\exp\left(-\frac{r}{3}\right)\cdot\exp(-i\cdot p\cdot r\cdot\cos(\theta))\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr$$

yields $\Phi(p) := 18\cdot\frac{6^{\frac{1}{2}}}{\pi}\cdot\frac{(-30)\cdot p^2+1+81\cdot p^4}{[(-1)+3\cdot i\cdot p]^4\cdot(1+3\cdot i\cdot p)^4}$





The Fourier transform for the $3p_z$ orbital

$$\Phi(p) := \frac{1}{162\cdot\pi^2}\cdot\int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi}\left(6\cdot r - r^2\right)\cdot\exp\left(-\frac{r}{3}\right)\cdot\exp\left(-i\cdot p\cdot r\cdot\cos(\theta)\right)\cdot\cos(\theta)\cdot r^2\cdot\sin(\theta)\,d\phi\,d\theta\,dr$$

yields $\Phi(p) := (-432)\cdot\frac{i}{\pi}\cdot p\cdot\frac{9\cdot p^2 - 1}{[(-1) + 3\cdot i\cdot p]^4\cdot(1 + 3\cdot i\cdot p)^4}$