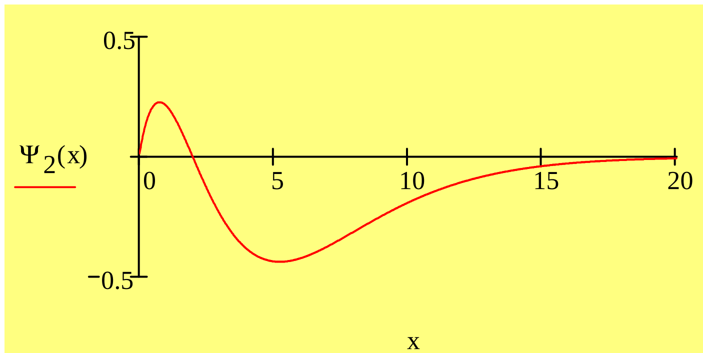
From Coordinate Space to Momentum Space and Back

Frank Rioux
Chemistry Department
CSB|SJU

The 2s state of the one-dimensional hydrogen atom is used to illustrate transformations back and forth between the coordinate and momentum representations.

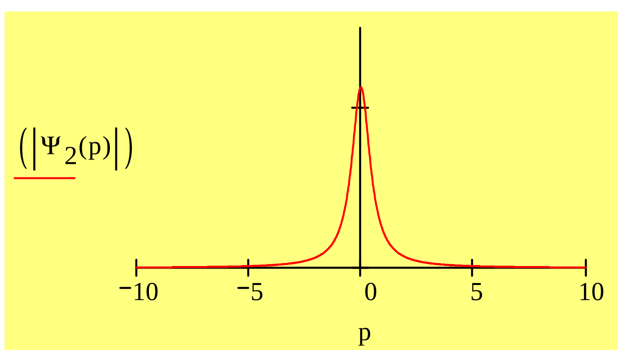
$$\Psi_2(x) := \frac{1}{\sqrt{8}} \cdot x \cdot (2 - x) \cdot \exp\left(-\frac{x}{2}\right)$$



The 2s state is Fourier transformed into momentum space (using atomic units) and the magnitude of the momentum wave function is displayed.

$$\langle p|\Psi_2\rangle = \int_0^\infty \langle p|x\rangle\langle x|\Psi_2\rangle dx \quad \text{where} \quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-ipx}{\hbar}\right)$$

$$\Psi_2(p) := \frac{1}{\sqrt{2 \cdot \pi}} \cdot \int_0^\infty \exp(-i \cdot p \cdot x) \cdot \Psi_2(x)\, dx \text{ simplify } \rightarrow \frac{2}{\pi^{\frac{1}{2}}} \cdot \frac{2 \cdot i \cdot p - 1}{(2 \cdot i \cdot p + 1)^3}$$



The return to coordinate space is carried out in the numeric mode, integrating over the range of momentum values shown above (+/-10 is effectively +/- ∞).

$$\langle x|\Psi_2\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\Psi_2\rangle dp \quad \text{where} \quad \langle x|p\rangle = \frac{1}{\sqrt{2\pi}}\exp\left(\frac{ipx}{\hbar}\right)$$

$$\Psi_2(x) := \int_{-10}^{10} \frac{1}{\sqrt{2\cdot\pi}}\cdot\exp(i\cdot p\cdot x)\cdot\Psi_2(p)\, dp$$

The graphical display below shows that we have successfully returned to coordinate space.