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.

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

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

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

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

The return to coordinate space is carried out in the numeric mode, integrating over the range of momentum values shown above (+/-10 is effectively +/- \(\infty\)).
\[ \langle x | \Psi_2 \rangle = \int_{-\infty}^{\infty} \langle x | p \rangle \langle p | \Psi_2 \rangle \, dp \quad \text{where} \quad \langle x | p \rangle = \frac{1}{\sqrt{2\pi}} \exp \left( \frac{ipx}{\hbar} \right) \]

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

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