The Wigner Function for the 4s State of the 1D Hydrogen Atom
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This tutorial presents three pictures of the 4s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

The energy operator for the one-dimensional hydrogen atom in atomic units is:

$$\frac{-1}{2} \frac{d^2}{dx^2} \Psi(x) - \frac{1}{x} \Psi(x)$$

The position 4s wave function is:

$$\Psi(x) := \frac{x}{4} \left( 1 - \frac{3}{4}x + \frac{1}{8}x^2 - \frac{1}{192}x^3 \right) \exp\left(\frac{-x}{4}\right)$$

$$\int_0^\infty \Psi(x)^2 \, dx = 1$$

The 4s energy is -0.03125 $E_h$:

$$\frac{-1}{2} \frac{d^2}{dx^2} \Psi(x) - \frac{1}{x} \Psi(x) = E \Psi(x)$$

solve $E \rightarrow \frac{-1}{32} = -0.03125$

The momentum wave function is generated by the following Fourier transform of the coordinate wave function.

$$\Phi(p) := \frac{1}{\sqrt{2\pi}} \int_0^\infty \exp(-ip \cdot x) \Psi(x) \, dx \rightarrow (-2)^\frac{1}{2} \frac{1}{2} \frac{64 \cdot i \cdot p^3 - 48 \cdot p^2 - 12 \cdot i \cdot p + 1}{(4 \cdot i \cdot p + 1)^5 \cdot \pi^2}$$

$$\left( \left| \Phi(p) \right| \right)^2$$
The Wigner function (phase-space representation) for the hydrogen atom 4s state is generated using the momentum wave function.

\[
W(x,p) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi(p + \frac{s}{2}) \cdot \exp(-i \cdot s \cdot x) \cdot \Phi(p - \frac{s}{2}) \, ds
\]

The Wigner distribution is displayed graphically.

\[
\begin{align*}
N &:= 100 & i &:= 0..N & x_i &:= \frac{50 \cdot i}{N} & j &:= 0..N & p_j &:= -2 + \frac{4 \cdot j}{N} & Wigner_{i,j} &:= W(x_i, p_j)
\end{align*}
\]

Just as for the 2s and 3s states, the Wigner distribution for the 4s state takes on negative values.