The Wigner Function for the 3p State of the 1D Hydrogen Atom

Frank Rioux

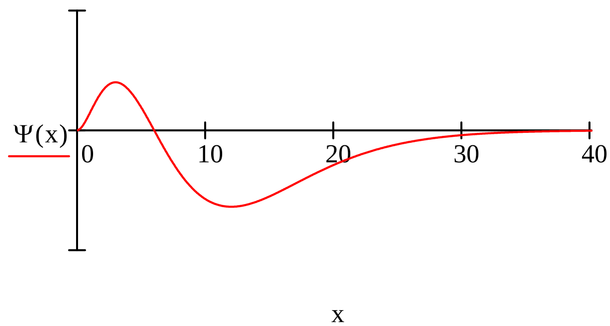
This tutorial presents three pictures of the 3p state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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

$$\frac{-1}{2}\cdot\frac{d^2}{dx^2}\blacksquare + \frac{L\cdot(L+1)}{2\cdot x^2}\cdot\blacksquare - \frac{1}{x}\cdot\blacksquare$$

The 3p wave function is:

$$\Psi(x) := \frac{8}{27\cdot\sqrt{6}}\cdot\left(1-\frac{x}{6}\right)\cdot x^2\cdot\exp\left(\frac{-x}{3}\right) \qquad \int_0^{\infty}\Psi(x)^2\,dx = 1$$

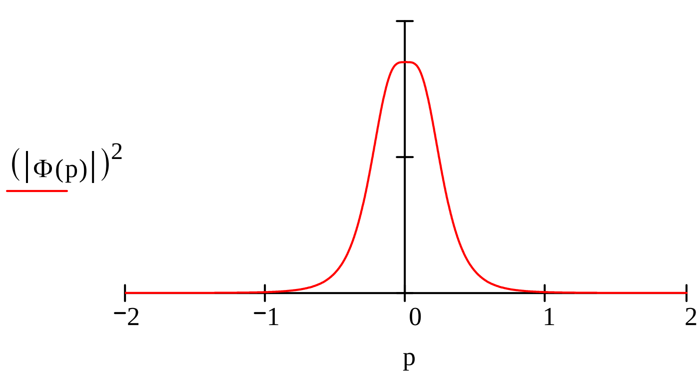


The 3p state energy is -0.0556 E_h.

$$\frac{-1}{2}\cdot\frac{d^2}{dx^2}\Psi(x) + \frac{1}{x^2}\cdot\Psi(x) - \frac{1}{x}\cdot\Psi(x) = E\cdot\Psi(x) \text{ solve}, E \rightarrow \frac{-1}{18} = -0.0556$$

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

$$\Phi(p) := \frac{1}{\sqrt{2\cdot\pi}}\cdot\int_0^{\infty}\exp(-i\cdot p\cdot x)\cdot\Psi(x)\,dx \rightarrow \frac{2}{3}\cdot2^{\frac{1}{2}}\cdot6^{\frac{1}{2}}\cdot\frac{(-1)+6\cdot i\cdot p}{(3\cdot i\cdot p+1)^4\cdot\pi^{\frac{1}{2}}}$$

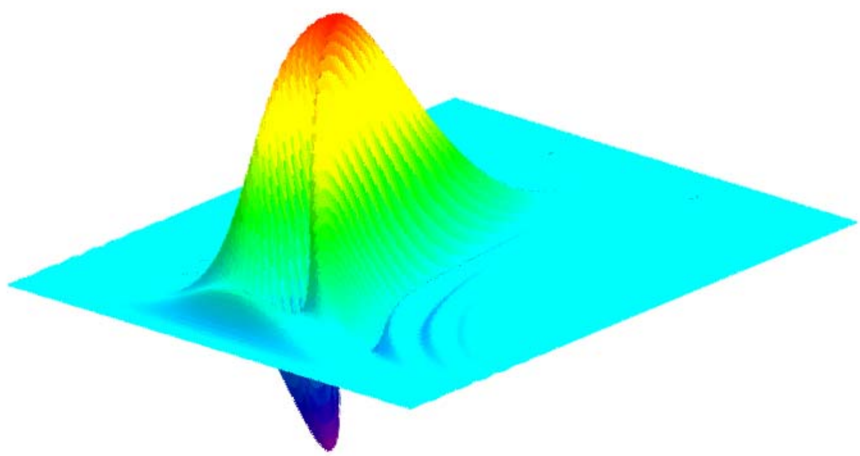


The Wigner function (phase-space representation) for the 3p state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$N := 150 \qquad i := 0..N \qquad x_i := \frac{35\cdot i}{N} \qquad j := 0..N \qquad p_j := -2+\frac{4\cdot j}{N} \qquad Wigner_{i,j} := W\left(x_i, p_j\right)$



Wigner