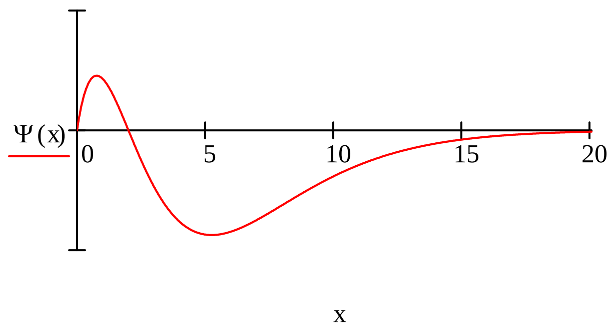
The Wigner Function for the 2s State of the 1D Hydrogen Atom

Frank Rioux

This tutorial presents three pictures of the 2s 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: $\frac{-1}{2}\cdot\frac{d^2}{dx^2}\blacksquare - \frac{1}{x}\cdot\blacksquare$

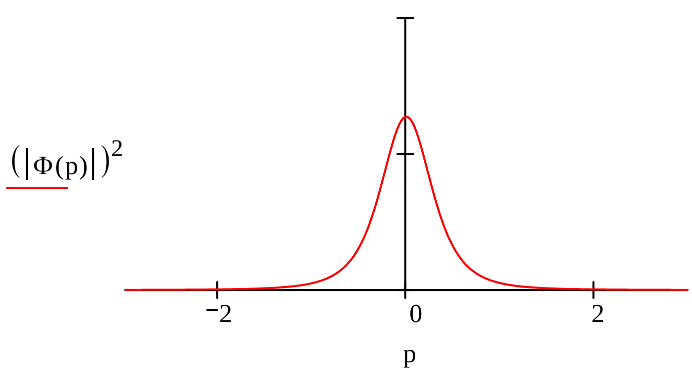
The 2s wave function is: $\Psi(x) := \frac{1}{\sqrt{8}}\cdot x\cdot(2-x)\cdot\exp\left(-\frac{x}{2}\right)$ $\int_0^\infty \Psi(x)^2\,dx = 1$



The 2s state energy is -0.125 E_h. $\frac{\frac{-1}{2}\cdot\frac{d^2}{dx^2}\Psi(x) - \frac{1}{x}\cdot\Psi(x)}{\Psi(x)}$ simplify $\rightarrow \frac{-1}{8}$

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

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

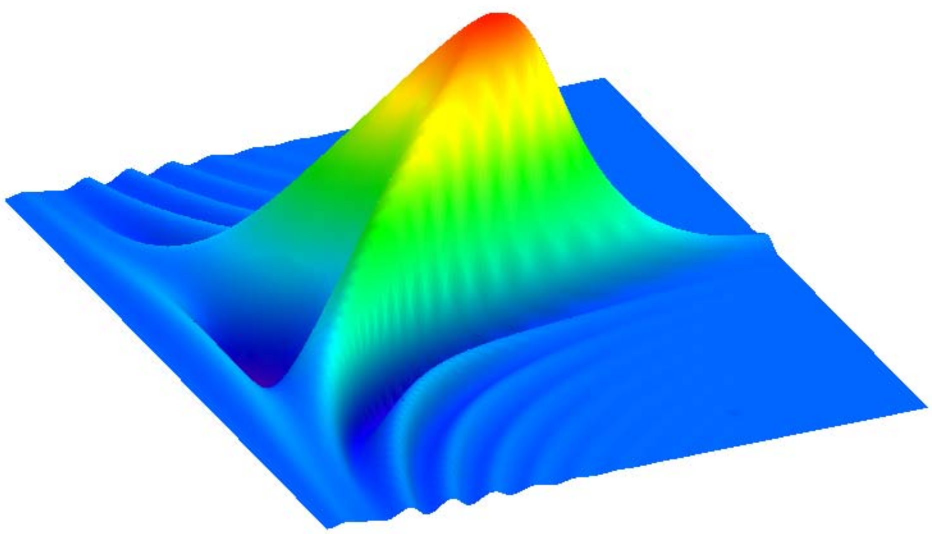


The Wigner function (phase-space representation) for the 2s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$N := 100 \quad i := 0..N \quad x_i := \frac{15\cdot i}{N} \quad j := 0..N \quad p_j := -3+\frac{6\cdot j}{N} \quad Wigner_{i,j} := W(x_i, p_j)$



Wigner

If we rotate this figure to look below the plane, we see that for the 2s state of the 1D hydrogen atom the Wigner distribution takes on negative values.