The Wigner Function for the 4s State of the 1D Hydrogen Atom

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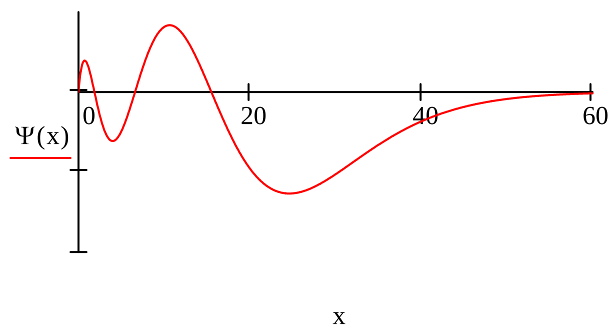
This tutorial presents three pictures of the 4s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

The energy operator for the one-dimensional hydrogen atom in atomic units is: $\frac{-1}{2}\cdot\frac{d^2}{dx^2}\blacksquare - \frac{1}{x}\cdot\blacksquare$

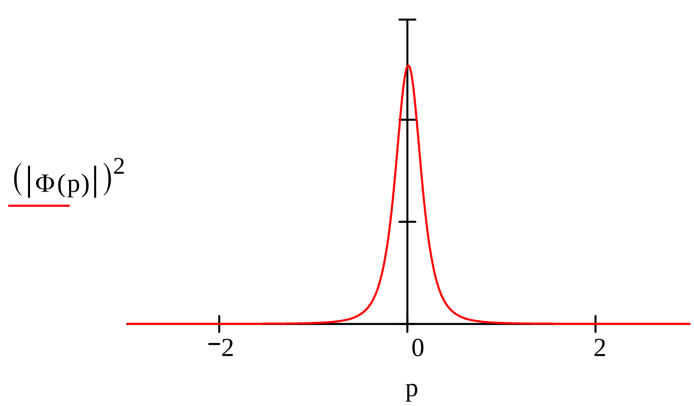
The position 4s wave function is: $\Psi(x) := \frac{x}{4}\cdot\left(1-\frac{3}{4}\cdot x+\frac{1}{8}\cdot x^2-\frac{1}{192}\cdot x^3\right)\cdot\exp\left(\frac{-x}{4}\right)$ $\quad\int_0^\infty \Psi(x)^2\,dx = 1$



The 4s energy is -0.03125 E_h. $\frac{-1}{2}\cdot\frac{d^2}{dx^2}\Psi(x) - \frac{1}{x}\cdot\Psi(x) = E\cdot\Psi(x)$ solve, E $\rightarrow \frac{-1}{32} = -0.03125$

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

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

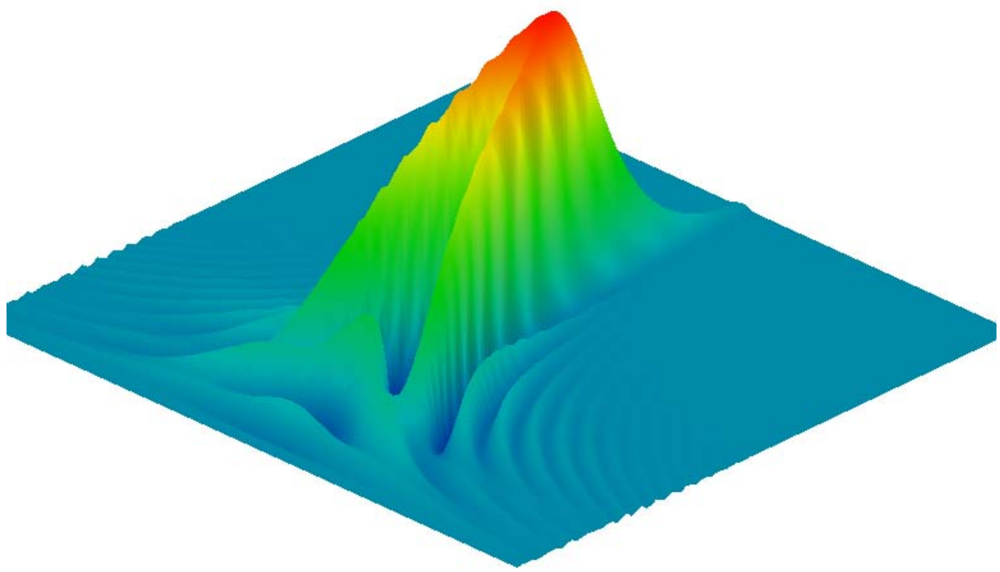


The Wigner function (phase-space representation) for the hydrogen atom 4s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$N := 100 \qquad i := 0..N \qquad x_i := \frac{50\cdot i}{N} \qquad j := 0..N \qquad p_j := -2+\frac{4\cdot j}{N} \qquad Wigner_{i,j} := W\left(x_i, p_j\right)$



Wigner

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