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

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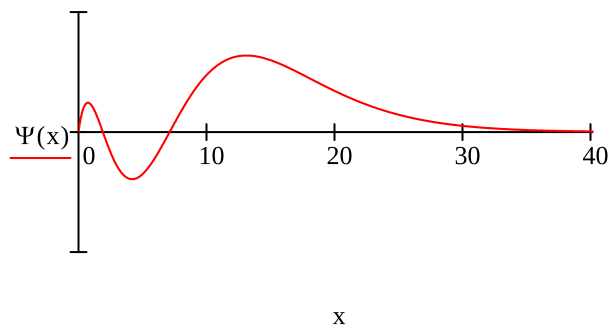
This tutorial presents three pictures of the 3s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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 3s wave function is: $\Psi(x) := \frac{2}{243}\cdot\sqrt{3}\cdot x\cdot\left(27 - 18\cdot x + 2\cdot x^2\right)\cdot\exp\left(-\frac{x}{3}\right)$ $\quad \int_0^\infty \Psi(x)^2\,dx = 1$

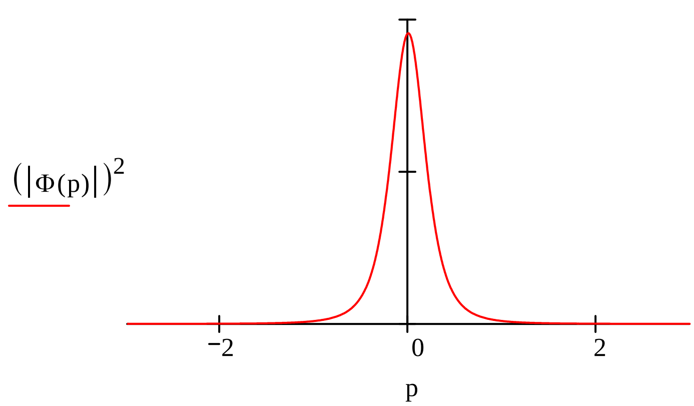


The 3s energy is -0.0556 E_h.

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

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

$$\Phi(p) := \frac{1}{\sqrt{2\cdot\pi}}\cdot\int_0^\infty \exp(-i\cdot p\cdot x)\cdot\Psi(x)\,dx \rightarrow \left(-2^{\frac{1}{2}}\right)\cdot 3^{\frac{1}{2}}\cdot\frac{9\cdot p^2 + 6\cdot i\cdot p - 1}{(3\cdot i\cdot p + 1)^4\cdot\pi^{\frac{1}{2}}}$$

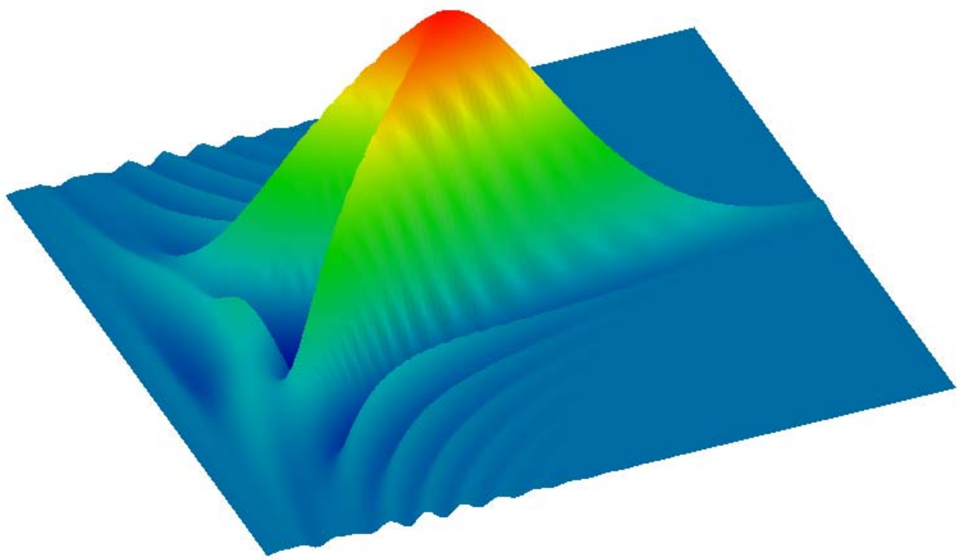


The Wigner function (phase-space representation) for the hydrogen atom 3s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$N := 100 \quad i := 0..N \quad x_i := \frac{30\cdot i}{N} \quad j := 0..N \quad p_j := -2+\frac{4\cdot j}{N} \quad Wigner_{i,j} := W(x_i, p_j)$



Wigner

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