

2.60: The Wigner Distribution for the 4s State of the 1D Hydrogen Atom

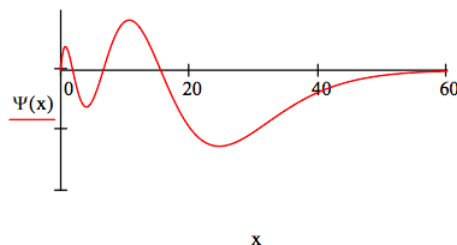
This tutorial presents three pictures of the 4s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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

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

The position 4s wave function is:

$$\Psi(x) = \frac{x}{4} \left(1 - \frac{3}{4}x + \frac{1}{8}x^2 - \frac{1}{192}x^3 \right) \exp\left(-\frac{x}{4}\right) \quad \int_0^\infty \Psi(x)^2 dx = 1$$

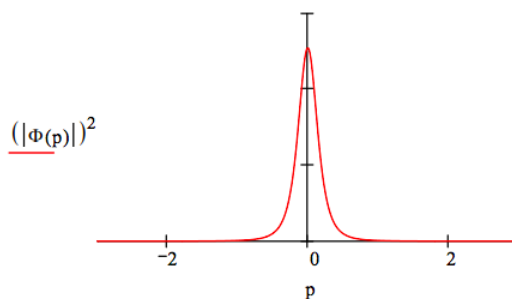


The 4s energy is $-0.03125 E_h$.

$$\frac{-1}{2} \frac{d^2}{dx^2} \Psi(x) - \frac{1}{x} \Psi(x) = E \Psi(x) \text{ solve, } E \rightarrow \frac{-1}{32} = -0.03125$$

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

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

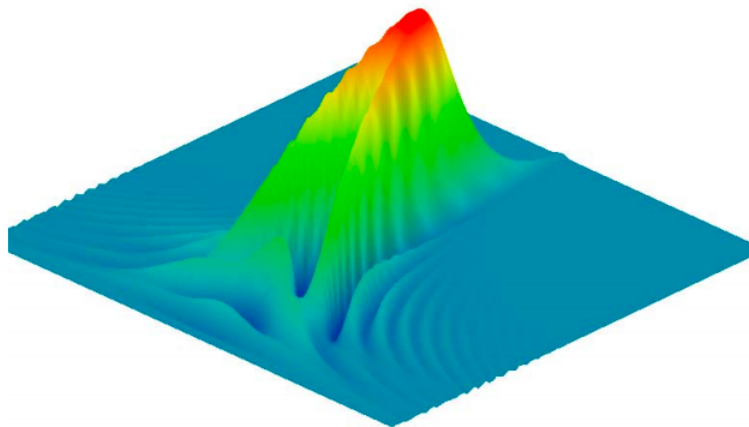


The Wigner function (phase-space representation) for the hydrogen atom 4s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$$N = 100 \quad i = 0 \dots N \quad x_i = \frac{50i}{N} \quad j = 0 \dots N \quad p_j = -2 + \frac{4j}{N} \quad \text{Wigner}_{i,j} = W(x_i, p_j)$$



Wigner

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

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