

2.56: The Wigner Distribution for the 2s State of the 1D Hydrogen Atom

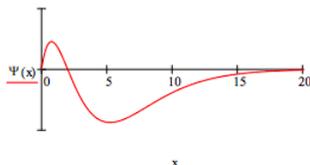
This tutorial presents three pictures of the 2s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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

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

The 2s wave function is:

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

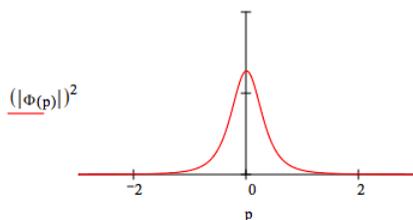


The 2s state energy is $-0.125 E_h$.

$$\frac{\frac{-1}{2} \frac{d^2}{dx^2} \Psi(x) - \frac{1}{x} \Psi(x)}{\Psi(x)} \text{ simplify } \rightarrow \frac{-1}{8}$$

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

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

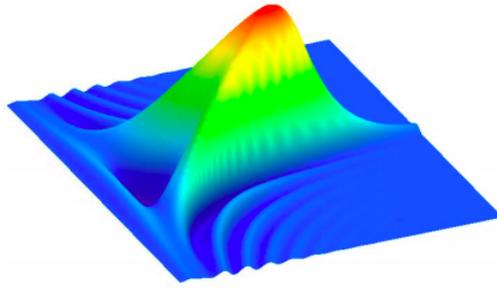


The Wigner function (phase-space representation) for the 2s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

$$N = 100 \quad i = 0 \dots N \quad x_i = \frac{15i}{N} \quad j = 0 \dots N \quad p_j = -3 \frac{6j}{N} \quad \text{Wigner}_{i,j} = W(x_i, p_j)$$



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.

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