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

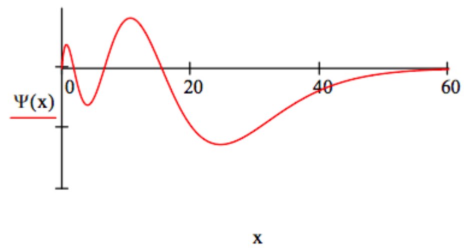
This tutorial presents three pictures of the 4s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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

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

The position 4s wave function is:

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

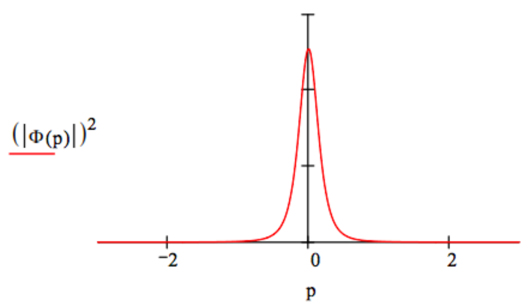


The 4s energy is -0.03125 E_h.

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

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

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

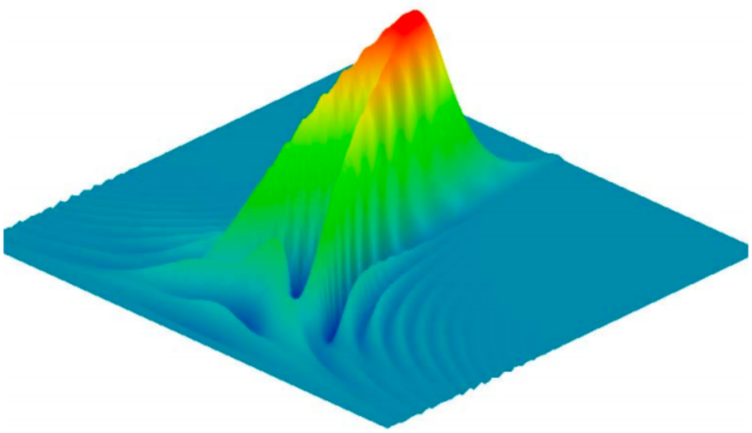


The Wigner function (phase-space representation) for the hydrogen atom 4s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

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



Wigner

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