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

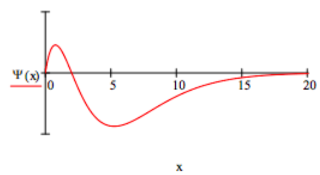
This tutorial presents three pictures of the 2s state of the one-dimensional hydrogen atom using its position, momentum and phase-space representations.

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

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

The 2s wave function is:

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

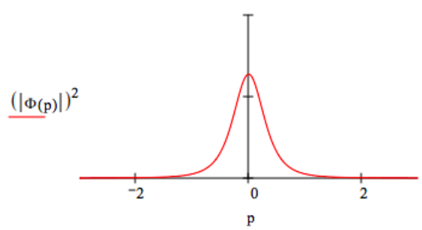


The 2s state energy is -0.125 E_h.

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

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

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

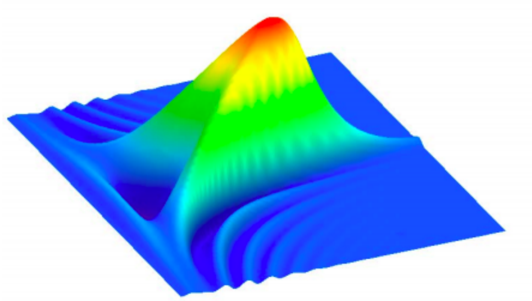


The Wigner function (phase-space representation) for the 2s state is generated using the momentum wave function.

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

The Wigner distribution is displayed graphically.

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



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.
