# Trigonimetric Trial Wave Function for the Hydrogen Atom

Trial wave function: $\Psi(r,\beta) := \sqrt{\frac{3\cdot\beta^3}{\pi^3}}\cdot \mathrm{sech}(\beta\cdot r)$

Integral: $\int_0^{\infty} \blacksquare \cdot 4\cdot\pi\cdot r^2\, dr$

Kinetic energy operator: $T = -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\blacksquare)$

Potential energy operatory: $V = -\frac{1}{r}$

**a**. Demonstrate the wave function is normalized.

$$\int_0^{\infty} \Psi(r,\beta)^2\cdot 4\cdot\pi\cdot r^2\, dr \;\Big|\; \begin{array}{l}\text{assume}, \beta > 0\\ \text{simplify}\end{array} \rightarrow 1$$

**b**. Evaluate the variational integral.

$$E(\beta) := \int_0^{\infty} \Psi(r,\beta)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\Psi(r,\beta))\right]\cdot 4\cdot\pi\cdot r^2\, dr \ldots \;\Big|\; \begin{array}{l}\text{assume}, \beta > 0\\ \text{simplify}\end{array} \rightarrow \frac{1}{6}\cdot\beta\cdot\frac{12\cdot\beta + \beta\cdot\pi^2 - 72\cdot\ln(2)}{\pi^2}$$
$$+ \int_0^{\infty} \Psi(r,\beta)\cdot -\frac{1}{r}\cdot\Psi(r,\beta)\cdot 4\cdot\pi\cdot r^2\, dr$$

**c**. Minimize the energy with respect to the variational parameter $\beta$.

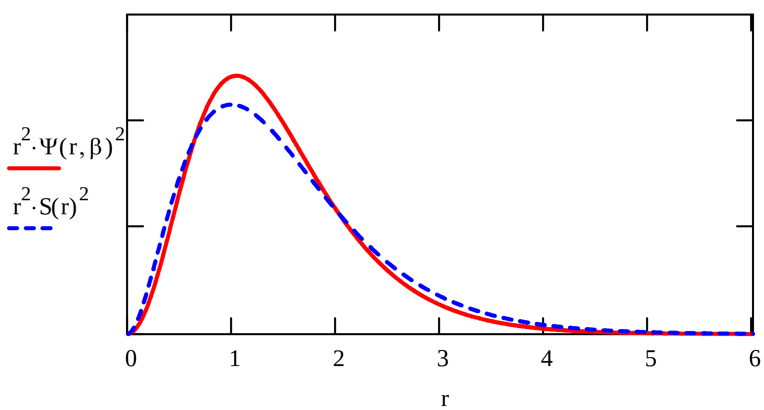
$\beta := 1$ $\quad \beta := \text{Minimize}(E,\beta)$ $\quad \beta = 1.141$ $\quad E(\beta) = -0.481$

**d**. The exact ground state energy for the hydrogen atom is -.5 $E_h$.
Calculate the percent error.

$$\frac{-.5 - E(\beta)}{-.5}\cdot 100 = 3.84$$

**e.** Compare optimized trial wave function with the exact solution by plotting the radial distribution functions.

$$S(r) := \frac{1}{\sqrt{\pi}}\cdot\exp(-r)$$



**f.** Calculate the kinetic and potential energy contributions for the trial wave function. Is the virial theorem satisfied?

kinetic energy

$$\int_0^{\infty} \Psi(r,\beta)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\Psi(r,\beta))\right]\cdot 4\cdot\pi\cdot r^2\,dr = 0.481$$

potential energy

$$\int_0^{\infty} \Psi(r,\beta)\cdot-\frac{1}{r}\cdot\Psi(r,\beta)\cdot 4\cdot\pi\cdot r^2\,dr = -0.962$$

Yes, the virial theorem is satisfied: T = -E = -V/2.

g. Given that the virial theorem is (of course) satisfied for the exact solution, explain the difficiency of the trigonometric trial wave function.

For the exact solution T = 0.500 and V = -1.00. Thus, while the kinetic energy is lower by 0.019 for the trial wave function, its potential energy is higher by twice that amount. As can be seen in the graph above, an electron in the trial wave function spends less time close to the nucleus.