Approximate Methods: Particle in an Ice Cream Cone

A Gaussian function is proposed as a trial wavefunction in a variational calculation for a particle experiencing a linear radial potential energy. Determine the optimum value of the parameter β and the optimum ground state energy. Use atomic units: h = 2π, m_e = 1, e = -1.

$$\Psi(r,\beta) := \left(\frac{2\cdot\beta}{\pi}\right)^{\frac{3}{4}}\cdot\exp\left(-\beta\cdot r^2\right) \qquad T = -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\blacksquare) \qquad V = r \qquad \int_0^\infty \blacksquare\cdot 4\cdot\pi\cdot r^2\,dr$$

a. Demonstrate the wave function is normalized.

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

b. Evaluate the variational integral.

$$E(\beta) := \int_0^\infty \Psi(r,\beta)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}\left(r\cdot\Psi(r,\beta)\right)\right]\cdot 4\cdot\pi\cdot r^2\,dr \;... \;+ \int_0^\infty \Psi(r,\beta)\cdot r\cdot\Psi(r,\beta)\cdot 4\cdot\pi\cdot r^2\,dr \;\Bigg|\begin{array}{l}\text{assume}, \beta > 0\\ \text{simplify}\end{array} \rightarrow \frac{1}{2}\cdot\frac{3\cdot\pi^{\frac{1}{2}}\cdot\beta^2 + 2\cdot 2^{\frac{1}{2}}\cdot\beta^{\frac{1}{2}}}{\pi^{\frac{1}{2}}\cdot\beta}$$

c. Minimize the energy with respect to the variational parameter β.

$\beta := 1$ $\qquad \beta := \text{Minimize}(E,\beta)$ $\qquad \beta = 0.414$ $\qquad E(\beta) = 1.861$

d. Plot the optimized trial wave function.