

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: $\hbar = 2\pi$, $m_e = 1$, $e = -1$.

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

a. Demonstrate the wave function is normalized.

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

b. Evaluate the variational integral.

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

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

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

d. Plot the optimized trial wave function.

