10.15: Variation Method for a 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.

$$\psi(r,\beta) := (\frac{2\beta}{\pi})^{\frac{3}{4}} exp(-\beta r^2)$$

$$T = \frac{1}{2r}\frac{d^2}{dr^2}(r\blacksquare)$$

$$V = r$$

$$\int_0^\infty \blacksquare 4\pi r^2 dr$$

a. Demonstrate the wave function is normalized.

$$\int_0^\infty \psi(r,\beta)^2 4\pi r^2 dr |_{simplify}^{assume,\, \beta>0} \rightarrow 1$$

b. Evaluate the variational integral.

$$E(\beta) := \int_0^\infty \psi(r,\beta[(-\frac{1}{2r})\frac{d^2}{dr^2}(r\psi(r,\beta))]4\pi r^2 dr \ldots |_{simplify}^{assume,\, \beta>0} \rightarrow \frac{1}{2}\frac{3\pi^{\frac{1}{2}}\beta^2 + (2)2^{\frac{1}{2}}\beta^{\frac{1}{2}}}{\pi^{\frac{1}{2}}\beta}$$

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

β := 1 β := Minimize(E, \beta) β = 0.414 E(β) = 1.861

d. Plot the optimized trial wave function.