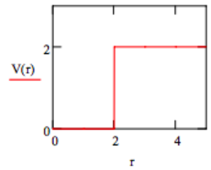
10.16: Variation Method for a Particle in a Finite 3D Spherical Potential Well

This problem deals with a particle of unit mass in a finite spherical potential well of radius 2 a_o and well height 2 E_h. The trial wave function is given below.

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

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

$$V(r) := if[(r \leq 2), 0, 2]$$



a. Demonstrate that 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.

$$E(\beta) := \int_0^\infty \psi(r,\beta)[-\frac{1}{2r}\frac{d^2}{dr^2}(r\psi(r,\beta))]4\pi r^2 dr\ldots|_{simplify}^{assume,\,\beta>0} + \int_2^\infty 2\psi(r,\beta)^2 4\pi r^2 dr$$

$$E(\beta) := \frac{1}{2}\frac{3\pi^{\frac{1}{2}}\beta + 4\pi^{\frac{1}{2}} + 16exp(-8\beta)2^{\frac{1}{2}}\beta^{\frac{1}{2}} - 4\pi^{\frac{1}{2}}erf((2)2^{\frac{1}{2}}\beta^{\frac{1}{2}})}{\pi^{\frac{1}{2}}}$$

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

β := 5 β := Minimize (E, \beta) β = 0.381 $E(\beta) = 0.786$

d. Calculate the average value of r.

$$\int_0^\infty r\psi(r,\beta)^2 4\pi r^2 dr = 1.293$$

e. Calculate the kinetic and potential energy.

Potential energy:

$$\int_2^\infty r\psi(r,\beta)^2 4\pi r^2 dr = 0.215$$

Kinetic energy:

$$E(\beta) - 0.215 = 0.571$$

f. Calculate the probability that the particle is in the barrier.

$$1 - \int_0^2 \psi(r,\beta)^2 4\pi r^2 dr = 0.107$$

g. Plot the wavefunction on the same graph as the potential energy.