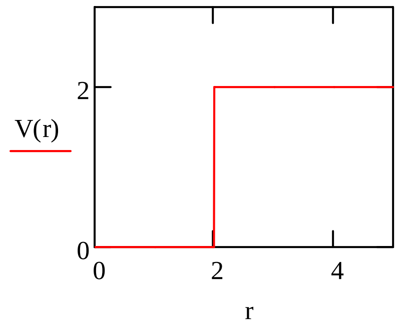
Variation Method for a Particle in a Finite Spherical Potential

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.

$$\Psi(r,\beta) := \left(\frac{2\cdot\beta}{\pi}\right)^{\frac{3}{4}}\cdot\exp(-\beta\cdot r^2) \qquad T = -\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\blacksquare) \qquad V(r) := \text{if}[(r \le 2), 0, 2]$$



a. Demonstrate that the wave function is normalized.

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

b. Evaluate the variational integral.

$$E(\beta) := \int_0^{\infty} \Psi(r,\beta)\cdot\left[-\frac{1}{2\cdot r}\cdot\frac{d^2}{dr^2}(r\cdot\Psi(r,\beta))\right]\cdot 4\cdot\pi\cdot r^2\, dr \ldots \;\Bigg|\; \begin{matrix}\text{assume}, \beta > 0\\ \text{simplify}\end{matrix}$$
$$+ \int_2^{\infty} 2\cdot\Psi(r,\beta)^2\cdot 4\cdot\pi\cdot r^2\, dr$$

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

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

$$\beta := .5 \qquad \beta := \text{Minimize}(E,\beta) \qquad \beta = 0.381 \qquad E(\beta) = 0.786$$

d. Calculate the average value of r.

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

e. Calculate the kinetic and potential energy.

Potential energy: $\int_2^\infty 2\cdot\Psi(r,\beta)^2\cdot 4\cdot\pi\cdot r^2\,dr = 0.215$ Kinetic energy: $E(\beta) - 0.215 = 0.571$

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

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

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