

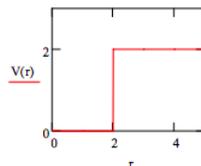
10.16: Variation Method for a Particle in a Finite 3D Spherical Potential Well

This problem deals with a particle of unit mass in a finite spherical potential well of radius $2a_0$ and well height $2E_h$. The trial wave function is given below.

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

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

$$V(r) := \begin{cases} 2 & (r \leq 2) \\ 0 & (r > 2) \end{cases}$$



a. Demonstrate that the wave function is normalized.

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

b. Evaluate the variational integral.

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

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

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

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

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:

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

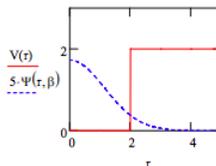
Kinetic energy:

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

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.



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