10.19: Trigonometric Trial Wave Function for the 3D Harmonic Potential Well

Trial wave function: $\Psi(r,\beta) := \sqrt{\frac{3\beta^3}{\pi^3}}\, sech(\beta r)$

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

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

Potential energy operatory: $V = \frac{1}{2}kr^2$

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.

$$E(\beta) := \int_0^\infty \Psi(r,\beta)[\frac{-1}{2r}\frac{d^2}{dr^2}(r\Psi(r,\beta))]4\pi r^2 dr + \int_0^\infty \Psi(r,\beta)\frac{1}{2}r^2\Psi(r,\beta)4\pi r^2 dr$$

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

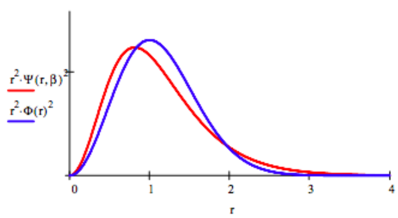
β := 1 β := Minimize (E, β) β = 1.471 E(β) = 1.597

d. The exact ground state energy for the 3D harmonic oscillator is 1.5 E_h. Calculate the percent error.

$$\frac{E(\beta)-1.5}{1.5} = 6.488\%$$

e. Compare the optimized trial wave function with the exact solution by plotting the radial distribution functions.

$$\Phi(r) := (\frac{1}{\pi})^{\frac{3}{4}} exp(\frac{r^2}{2})$$



h. Calculate the overlap integral between the trial wave function and the exact wave function.

$$\int_0^\infty \Psi(r,\beta)\Phi(r)4\pi r^2 dr = 0.989$$

i. Calculate the probability that tunneling is occurring.

Classical turning point:

$$1.597 = \frac{1}{2}r^2|_{float,\,3}^{solve,\,r} \rightarrow \begin{pmatrix} -1.79 \\ 1.79 \end{pmatrix}$$

Tunneling probability:

$$\int_{1.79}^\infty \Psi(r,\beta)^2 4\pi r^2 dr = 12.598\%$$