Trigonimetric Trial Wave Function for the 3D Harmonic Oscillator

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

Integral: $\int_0^{\infty} \blacksquare\cdot 4\cdot\pi\cdot r^2\,dr$

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

Potential energy operatory: $V = \frac{1}{2}\cdot k\cdot r^2$

a. Demonstrate the wave function is normalized.

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

b. Evaluate the variational integral.

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

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

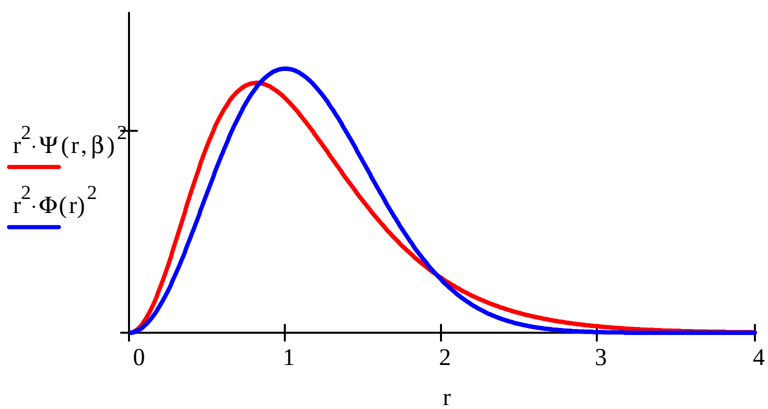
$\beta := 1$ $\quad$ $\beta := \text{Minimize}(E,\beta)$ $\quad$ $\beta = 1.471$ $\quad$ $E(\beta) = 1.597$

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

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



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

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

i. Calculate the probability that tunneling is occuring.

Classical turning point: $1.597 = \frac{1}{2}\cdot r^2 \;\Big|\; \begin{matrix} \text{solve}, r \\ \text{float}, 3 \end{matrix} \rightarrow \begin{pmatrix} -1.79 \\ 1.79 \end{pmatrix}$

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