Approximate Methods: Particle in a Gravitational Field

Frank Rioux
Chemistry Department
CSB|SJU

The particle of unit mass in a gravitational field for which g = 1 has the energy operator shown below.

$$-\frac{1}{2}\cdot\frac{d^2}{dz^2}\blacksquare + z\cdot\blacksquare \qquad\qquad \int_0^{\infty}\blacksquare\, dz$$

The following trial wave function for this problem is:

$$\Psi(\alpha,z) := 2\cdot\left(\frac{2\cdot\alpha}{\pi^{\frac{1}{3}}}\right)^{\frac{3}{4}}\cdot z\cdot\exp\left(-\alpha\cdot z^2\right)$$

Determine whether or not the wave function is normalized.

$$\int_0^{\infty}\Psi(\alpha,z)^2\, dz \ \begin{vmatrix} \text{assume}, \alpha > 0 \\ \text{simplify} \end{vmatrix} \rightarrow 1$$

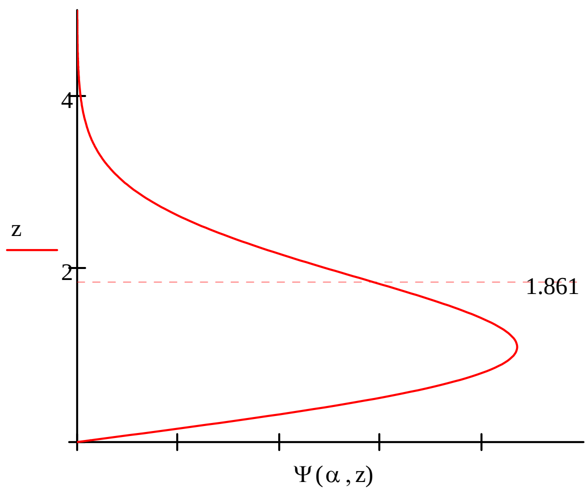
Evaluate the variational energy integral.

$$E(\alpha) := \int_0^{\infty}\Psi(\alpha,z)\cdot-\frac{1}{2}\cdot\frac{d^2}{dz^2}\Psi(\alpha,z)\, dz \ldots + \int_0^{\infty} z\cdot\Psi(\alpha,z)^2\, dz \ \begin{vmatrix} \text{assume}, \alpha > 0 \\ \text{simplify} \end{vmatrix} \rightarrow \frac{1}{2\cdot\pi^{\frac{1}{2}}}\cdot\frac{3\cdot\pi^{\frac{1}{2}}\cdot\alpha^2 + 2\cdot 2^{\frac{1}{2}}\cdot\alpha^{\frac{1}{2}}}{\alpha}$$

Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

$\alpha := 1$ $\qquad$ $\alpha := \text{Minimize}(E,\alpha)$ $\qquad$ $\alpha = 0.4136$ $\qquad$ $E(\alpha) = 1.8611$ $\qquad$ $E_{exact} := 1.8558$

Plot the wave function with the distance of the particle from the surface on the vertical axis.



Tunneling threshold.

$$E(0.4136) = z \;\Big|\begin{array}{l}\text{solve}, z\\ \text{float}, 4\end{array} \rightarrow 1.861$$

Find that distance below which there is a 90% probability of finding the particle.

$a := 1$ Given $\int_0^a \Psi(\alpha, z)^2\, dz = .90$ $\text{Find}(a) = 1.9440$

Find the most probable value of the position of the particle from the surface.

$$\frac{d}{dz}\Psi(0.4136, z) = 0 \;\Big|\begin{array}{l}\text{solve}, z\\ \text{float}, 3\end{array} \rightarrow \begin{pmatrix} -1.10 \\ 1.10 \end{pmatrix}$$

Calculate the probability that the particle will be found below the most probable distance from the surface.

$$\int_0^{1.10} \Psi(\alpha, z)^2\, dz = 0.4279$$

Calculate the probability that tunneling is occuring: $\int_{1.861}^{\infty} \Psi(\alpha, z)^2\, dz = 0.1256$

Kinetic energy: $\int_0^{\infty} \Psi(\alpha, z) \cdot -\frac{1}{2} \cdot \frac{d^2}{dz^2}\Psi(\alpha, z)\, dz = 0.6204$ Potential energy: $\int_0^{\infty} z \cdot \Psi(\alpha, z)^2\, dz = 1.2407$

What is the apparent virial theorem for this system: $E = 3 \cdot T = \frac{3}{2} \cdot V$