

The Numerov algorithm is an efficient approach to numerically solve the time-independent Schrödinger equation. We want to use the Numerov algorithm to calculate the stationary states $\Psi(z)$ of neutrons in the gravitational field of the Earth. For small changes in the vertical amplitude z the potential can be expressed as $V(z) = mgz$ for $z \geq 0$. By placing a perfectly reflecting horizontal mirror at $z = 0$ the potential becomes $V(z) = \infty$ for $z < 0$. Neutrons that fall onto the mirror are reflected upwards, and so we only seek solutions for $z \geq 0$. The stationary Schrödinger equation for this problem is given by

$$\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + mgz \right\} \Psi(z) = E \Psi(z) \quad , \quad (0.1)$$

with E being the energy eigenvalue of the Hamilton operator. We can rewrite this equation to:

$$\frac{\partial^2}{\partial z^2} \Psi(z) - \frac{2m}{\hbar^2} (E - mgz) \Psi(z) = 0 \quad \Longleftrightarrow \quad \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{2m^2 g}{\hbar^2} \left(\frac{E}{mg} - z \right) \Psi(z) = 0 \quad (0.2)$$

By looking at the units of the factor in front of the bracket

$$\left[\frac{2m^2 g}{\hbar^2} \right] = \frac{\text{kg}^2 \text{ m s}^{-2}}{(\text{J s})^2} = \frac{\text{kg}^2 \text{ m}}{\text{s}^4} \left(\frac{\text{kg m}^2}{\text{s}^2} \right)^{-2} = \frac{\text{kg}^2 \text{ m}}{\text{s}^4} \frac{\text{s}^4}{\text{kg}^2 \text{ m}^4} = \text{m}^{-3} \quad , \quad (0.3)$$

we find a suitable definition for the characteristic length scale z_0 :

$$\frac{1}{z_0} := \left(\frac{2m^2 g}{\hbar^2} \right)^{1/3} \quad (0.4)$$

If we use the notation $x := z/z_0$ and $\Psi(z) := \psi(x)/\sqrt{z_0}$, the second order partial derivative becomes:

$$\frac{\partial^2}{\partial z^2} \Psi(z) = \frac{1}{\sqrt{z_0}} \frac{1}{z_0^2} \frac{\partial^2}{\partial x^2} \psi(x) = \frac{1}{z_0^{5/2}} \frac{\partial^2}{\partial x^2} \psi(x) \quad (0.5)$$

The differential equation then becomes:

$$\frac{1}{z_0^{5/2}} \frac{\partial^2}{\partial x^2} \psi(x) - \frac{1}{z_0^3} \frac{1}{\sqrt{z_0}} \left(\frac{E}{mg} - z \right) \psi(x) = 0 \quad \Longleftrightarrow \quad \frac{\partial^2}{\partial x^2} \psi(x) - \frac{1}{z_0} \left(\frac{E}{mg} - z \right) \psi(x) = 0 \quad (0.6)$$

We now define the characteristic energy scale as $E_0 := mgz_0$. The unit of E_0 is then given by:

$$[E_0] = [mgz_0] = \text{kg m s}^{-2} \text{ m} = \text{kg m}^2 \text{ s}^{-2} = \text{J} \quad (0.7)$$

After this proper choice of length and energy units

$$x := \frac{z}{z_0} = z \left(\frac{2m^2 g}{\hbar^2} \right)^{1/3} \quad \text{and} \quad \epsilon := \frac{E}{E_0} = \frac{E}{mgz_0} = \frac{E}{mg} \left(\frac{2m^2 g}{\hbar^2} \right)^{1/3} \quad (0.8)$$

the Schrödinger equation for neutrons in the gravitational field of the Earth can be rewritten as:

$$\frac{\partial^2}{\partial x^2} \psi(x) + (\epsilon - x) \psi(x) \quad \Longleftrightarrow \quad \psi''(x) + (\epsilon - x) \psi(x) = 0 \quad (0.9)$$