Introduction to Computational Physics – Exercise 4

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The Numerov algorithm is an efficient approach to numerically solve the time-independet 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

$$\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + mgz \right\} \Psi(z) = E\Psi(z) \quad, \tag{1}$$

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

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

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

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

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

$$\frac{1}{z_0} := \left(\frac{2m^2 g}{\hbar^2}\right)^{1/3} \tag{4}$$

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

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

The differential equation then becomes:

$$\frac{1}{z_0^{5/2}}\frac{\partial^2}{\partial x^2}\psi(x) - \frac{1}{z_0^3}\frac{1}{\sqrt{z_0}}\left(\frac{E}{mg} - z\right)\psi(x) = 0 \qquad \Longleftrightarrow \qquad \frac{\partial^2}{\partial x^2}\psi(x) - \frac{1}{z_0}\left(\frac{E}{mg} - z\right)\psi(x) = 0 \tag{6}$$

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

$$[E_0] = [mgz_0] = \text{kg}\,\text{m}\,\text{s}^{-2}\,\text{m} = \text{kg}\,\text{m}^2\,\text{s}^{-2} = \text{J} \tag{7}$$

After this proper choice of length and energy units

$$x := \frac{z}{z_0} = z\left(\frac{2m^2 g}{\hbar^2}\right)^{1/3} \qquad \text{and} \qquad \epsilon := \frac{E}{E_0} = \frac{E}{mgz_0} = \frac{E}{mg}\left(\frac{2m^2 g}{\hbar^2}\right)^{1/3} \tag{8}$$

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

$$\frac{\partial^2}{\partial x^2}\psi(x) + (\epsilon - x)\psi(x) \qquad \Longleftrightarrow \qquad \psi''(x) + (\epsilon - x)\psi(x) = 0 \tag{9}$$