Task 4.3 Solution:

$$V(x) = \infty \qquad x \leq 0$$

$$= -\frac{\hbar^2 V_0}{2ma^2} \qquad 0 < x \leq a$$

$$= 0 \qquad x > a$$

TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V(x)\,\phi = E\phi$$

Solution:

For $0 < x \leq a$:

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} - \frac{\hbar^2 V_0}{2ma^2}\phi = E\phi$$

Let • $x = ay$, where y is a dimensionless constant

• $\lambda = E\,\frac{2ma^2}{\hbar}$

$$\frac{d^2\phi}{dy^2} = -(\lambda + V_0)\,\phi = f\left(\phi, \frac{d\phi}{dy}, y\right)$$

For $x > a$:

Apply as before.

$$\frac{d^2\phi}{dy^2} = -\lambda\phi = f\left(\phi, \frac{d\phi}{dy}, y\right)$$

Apply second-order Runge Kutta:

$$\text{half step}\begin{cases}\phi_h = \phi_i + \dfrac{dy}{2} V_i \\[2ex] V_h = V_i + \dfrac{dy}{2} f\left(\phi, \dfrac{d\phi}{dy}, y\right)\end{cases}$$

N.B. $\dfrac{d^2\phi}{dy^2} = f\left(\overset{\phi}{\cancel{x}}, \dfrac{d\phi}{dy}, y\right)$, $\dfrac{d\phi}{dy} = V$, $\dfrac{dV}{dy} = f(\phi, V, y)$

$$\text{ull step}\begin{cases}\phi_{i+1} = \phi_i + dy\, V_h \\[2ex] V_{i+1} = V_i + dy\, f\left(\phi_h, V_h, y + \dfrac{dy}{2}\right)\end{cases}$$

I have adapted this from the notes, which state for a function $x(t)$:

$$x_h = x(t) + \frac{\Delta t}{2} v(t)$$

$$V_h = v(t) + \frac{\Delta t}{2} f\left(x(t), v(t), t\right)$$

$$x(t + \Delta t) = x(t) + \Delta t\, V_h$$

$$v(t + \Delta t) = v(t) + \Delta t\, f\left(x_h, V_h, t + \frac{\Delta t}{2}\right)$$