

Neutral Atom Solver

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1 Units

This code uses Hartree units where $\frac{\hbar^2}{m_e} = e = 4\pi\epsilon_0 = 1$. m_e is the mass of the electron

2 Grids

2.1 Uniform Grid

2.2 Exponential Grid

3 Second Order Differential Equation Solver

This section focus on solving two differential equations: Schrödinger's equation, and Poisson's equation, which for our special case of the neutral atom and after some manipulation can be written as:

$$\frac{d^2y}{dx^2} = f(x)y + g(x) \tag{1}$$

3.1 Schrödinger's equation

$$\frac{-1}{2} \tag{2}$$