Numerical solution of the Schrödinger equation with constant source term

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Introduction

The nonrelativistic Schrödinger equation is solved numerically using the finite volume method. Central differencing is applied to the diffusion terms. Time discretization is fully implicit.

Model equations

The one-dimensional Schrödinger equation is:

$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \tag{1}$$

Where i is the imaginary number, h a constant, m the particle mass, V the potential, x the spatial coordinate, ψ the dependent variable and t time. The potential V is a function of x and t.

Discretization

The discrete form of equation (1) for the first node is:

$$ih\Delta x\frac{\psi_0^p - \psi_0^{p-1}}{\Delta t} = \frac{h^2}{2m}\frac{\psi_0^p - \psi_W}{1/2\Delta x} - \frac{h^2}{2m}\frac{\psi_1^p - \psi_0^p}{\Delta x} + V\Delta x\psi_0^p \tag{2}$$

Where the subscript 0 indicates the first, or left-most, node, the subscript W indicates the value of ψ at the west boundary and p indicates the timestep. The discrete form of equation (1) for central nodes is:

$$ih\Delta x\frac{\psi_j^p - \psi_j^{p-1}}{\Delta t} = \frac{h^2}{2m}\frac{\psi_j^p - \psi_{j-1}^p}{\Delta x} - \frac{h^2}{2m}\frac{\psi_{j+1}^p - \psi_j^p}{\Delta x} + V\Delta x\psi_j^p \tag{3}$$

Where j denotes node j. The discrete form of (1) for the last node is:

$$ih\Delta x\frac{\psi_{n-1}^p - \psi_{n-1}^{p-1}}{\Delta t} = \frac{h^2}{2m}\frac{\psi_{n-1}^p - \psi_{n-2}^p}{\Delta x} - \frac{h^2}{2m}\frac{\psi_E - \psi_{n-1}^p}{1/2\Delta x} + V\Delta x\psi_{n-1}^p \tag{4}$$

Where E indicates the value of ψ at the east boundary and n is the number of nodes.

Verification

In order to verify that the computations proceed correctly it is verified that the linear system represented by (2) to (4) is satisfied. Analysis of results show that the linear system is satisfied with an error in the order of 1e-14.