Numerical solution of the Schrodinger equation with constant source term

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Introduction

The Schrodinger 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 Schrodinger equation with constant source term is given by:

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

Where i is the imaginary number, h a constant, m the particle mass, q the source term, x the spatial coordinate, ψ the dependent variable and t time.

Discretization

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

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

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

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

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

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

Where E specifies the value of ψ at the east boundary.

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 to a high degree of accuracy.