**Objectives**

- develop a comprehensive code to solve the diffusion equation (1) with the theta-method, leading to a solution of the semiclassical limit of the nonlinear Schrödinger equation
- implement the Besse relaxation scheme and compare performance with the theta-method for solving the semiclassical limit of the nonlinear Schrödinger equation
- test convergence of each method with known solutions
- develop code to solve systems with several types of boundary conditions, e.g., Dirichlet, Neumann, Robin, and periodic

**Diffusion Equation**

\[
\frac{\partial u(x,t)}{\partial t} = \alpha \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t) \tag{1}
\]

**Theta-Method**

\[
(I - \theta S) \vec{w}^{j+1} = (I + (1 - \theta)S) \vec{w}^j + \vec{F}
\]

\[
\vec{F} = \Delta t \left( (1 - \theta) \vec{f}^j + \theta \vec{f}^{j+1} \right)
\]

\[
\Delta \vec{w}^{j+1} = \vec{b}
\]

- theta-method is a weighted average of the forward-time centered-space (FTCS) and backward-time centered-space (BTCS) schemes.
- \(0 \leq \theta \leq 1\)
- \(\theta < 0.5\) (explicit) conditionally stable: \(\Delta t \leq \frac{\alpha x^2}{2}\)
- \(\theta \geq 0.5\) (implicit) unconditionally stable
- \(\theta = 0.5\) (Crank-Nicolson Scheme): convergence is quadratic.
- \(\theta \neq 0.5\): convergence is linear.

**Convergence**

Numerical approximation of order \(p\) follows:

\[
|u_h - u| \leq Ch^p
\]

\[
\log_2 \left| \frac{u_{h+1} - u}{u_{h/2} - u} \right| = p + O(h)
\]

**Schrödinger Equation**

\[
\frac{i}{\Delta t} \frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} = k|u|^2 u \tag{2}
\]

\[
(I - i\theta S) \vec{w}^{j+1} = (I + (1 - \theta)S) \vec{w}^j + \vec{F}
\]

- fixed point iteration is implemented to solve the nonlinearity

**Besse Relaxation**

\[
\phi = |u|^2
\]

\[
\frac{i}{\Delta t} \frac{\partial u(x,t)}{\partial t} + \frac{\partial^2 u(x,t)}{\partial x^2} = 2\phi u
\]

- Order of convergence may be 2 [1]
- avoids costly computation involved with nonlinearity [1]

\[
\phi_{j+\frac{1}{2}} + \phi_{j-\frac{1}{2}} = |u_{j+1}^i|^2
\]

\[
\left( \frac{i}{\Delta t} u_{j+1}^{i+1} - u_j^i + \Delta \left( u_{j+1}^{i+1} + u_j^i \right) \right) = 2
\]

\[
(u_j^{i+1} + u_j^i) \phi_j^{i+\frac{1}{2}}
\]

**Semiclassical Limit**

\[
\frac{i}{\Delta t} \frac{\partial u}{\partial t} + \epsilon^2 \frac{\partial^2 u}{\partial x^2} = 2|u|^2 u
\]

\[
u(x,0,\epsilon) = A(x)e^{is(x)/\epsilon}
\]

\[
A(x) = \text{sech}(x)
\]

\[
S(x) = -\mu \ln(\cosh(x))
\]

\[-\infty < x < \infty\]

**Solution Profiles**

- Figure 1: The figure shows the convergence of the theta-method for 1-D diffusion with \(\theta = 0.5\). The convergence is 2nd order.
- Figure 2: The figure shows the convergence of the theta-method for 1-D diffusion with \(\theta = 0.75\). The convergence is 1st order.

**References**
