Numerical Solution to the 1-D Non-linear Schrödinger Equation

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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

$$\frac{\partial u(x,t)}{\partial t} = \alpha \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t) \qquad (1)$$

$$\frac{\partial u(i,j+1)}{\partial t} \approx \frac{u_i^{j+1} - u_i^j}{\Delta t}$$

$$\frac{\partial^2 u(i,j)}{\partial x^2} \approx \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2}$$

$$\frac{\partial^2 u(i,j+1)}{\partial x^2} \approx \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{(\Delta x)^2}$$

$$\mathbf{S} = \lambda \begin{bmatrix} -2 & 1 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & \dots \\ 0 & 1 & -2 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & -2 & 1 \\ \dots & 0 & 0 & 1 & -2 \end{bmatrix}$$

Theta-Method

$$(\mathbf{I} - \theta \mathbf{S})\vec{u}^{j+1} = (\mathbf{I} + (1-\theta)\mathbf{S})\vec{u}^j + \vec{F}$$

$$\vec{F} = \Delta t((1-\theta)\vec{f}^j + \theta \vec{f}^{j+1})$$

$$\mathbf{A}\vec{u}^{j+1} = \mathbf{b}$$

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

Convergence

Numerical approximation of order p follows:

$$|u_h - u| \le Ch^p$$

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

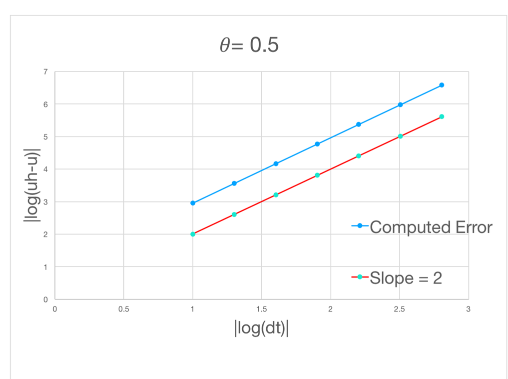


Figure 1: The figure shows the convergence of the theta-method for 1-D diffusion with $\theta = 0.5$. The convergence is 2nd order.

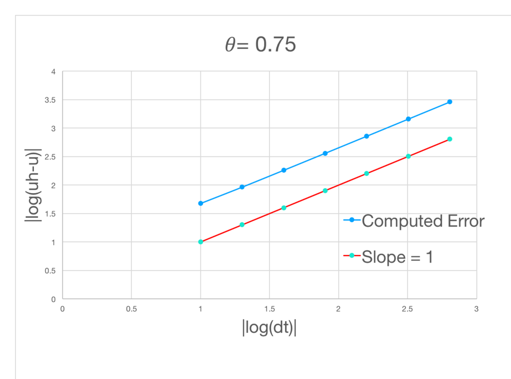


Figure 2: The figure shows the convergence of the theta-method for 1-D diffusion with $\theta = 0.75$. The convergence is 1st order.

Schrödinger Equation

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} = k|u|^2 u \qquad (2)$$

$$(\mathbf{I} - i\theta\mathbf{S})\vec{u}^{j+1} = (\mathbf{I} + i(1-\theta)\mathbf{S})\vec{u}^j + \vec{F}$$

- fixed point iteration is implemented to solve the nonlinearity

Besse Relaxation

$$\phi = |u|^2$$

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

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

$$\frac{\phi_i^{j+\frac{1}{2}} + \phi_i^{j-\frac{1}{2}}}{2} = |u_i^j|^2$$

$$i\frac{u_i^{j+1} - u_i^j}{\Delta t} + \Delta\left(\frac{u_i^{j+1} + u_i^j}{2}\right) = (u_i^{j+1} + u_i^j)\phi_i^{j+\frac{1}{2}}$$

Semiclassical Limit

$$i\epsilon\frac{\partial u}{\partial t} + \epsilon^2\frac{\partial^2 u}{\partial x^2} = 2|u|^2 u$$

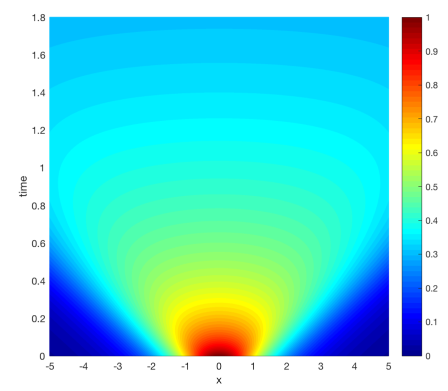
$$u(x,0,\epsilon) = A(x)e^{iS(x)/\epsilon}$$

$$A(x) = \operatorname{sech}(x) \qquad (3)$$

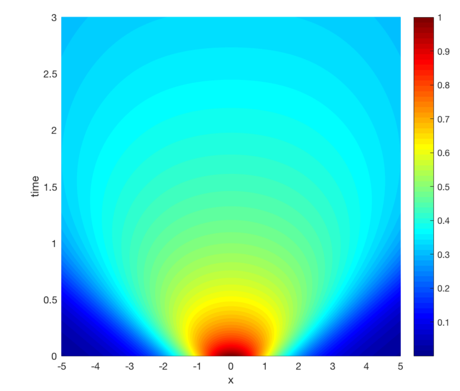
$$S(x) = -\mu \ln(\cosh(x))$$

$$-\infty < x < \infty$$

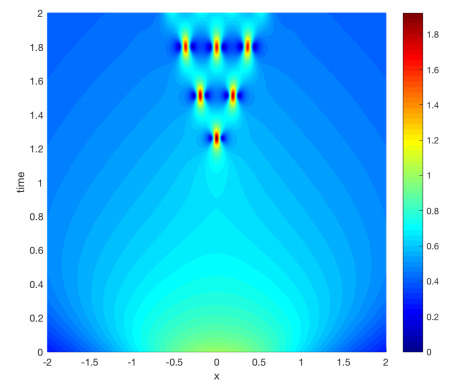
Solution Profiles



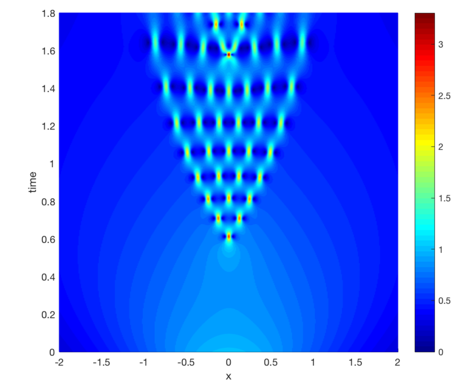
$\mu = -3$



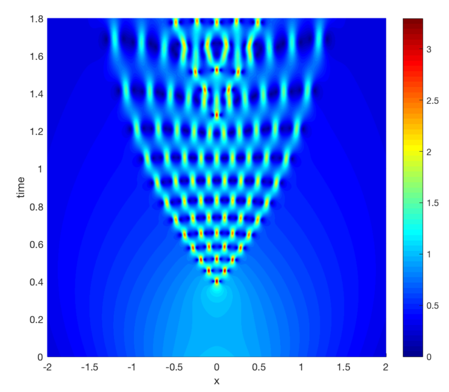
$\mu = -2$



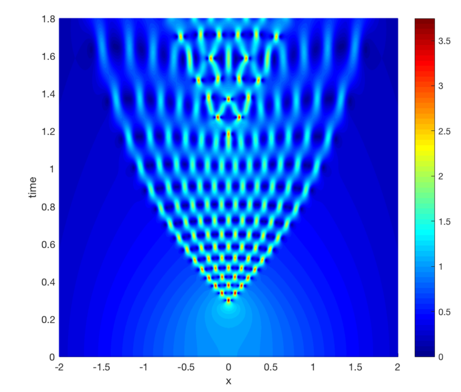
$\mu = -1.5$



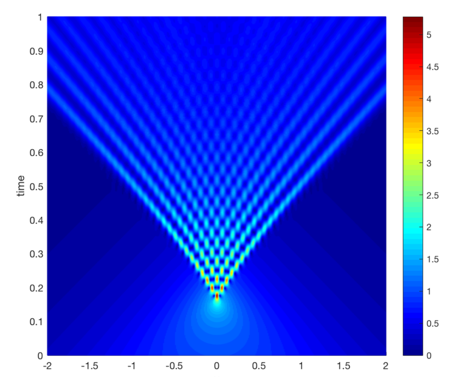
$\mu = -1$



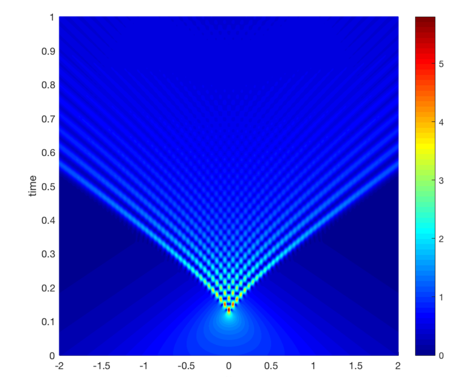
$\mu = -0.5$



$\mu = 0$



$\mu = 2$



$\mu = 3$

References

[1] Christophe Besse. A relaxation scheme for the nonlinear schrodinger equation. *SIAM Journal on Numerical Analysis*, 42(3):934–952, 2004.

[2] Alexander Tovbis, Stephanos Venakides, and Xin Zhou. On semiclassical (zero dispersion limit) solutions of the focusing nonlinear schrödinger equation. *Communications on Pure and Applied Mathematics*, 57(7):877–985, 2004.