Numerical Solution of Diffusion Eqn

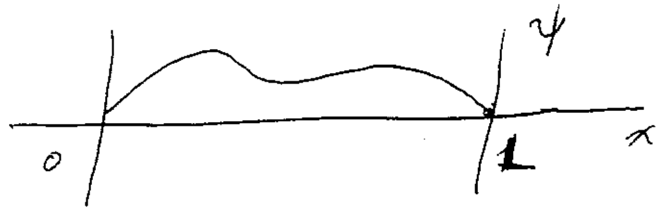
System

$$\frac{\partial \psi}{\partial t} = D \frac{\partial^2 \psi}{\partial x^2}, \qquad \psi(x,t)$$

$$\psi(x,0) = \sum_{m=0}^{M} \sin\left(m\pi \frac{x}{L}\right) A_m$$

$$\psi(0,t) = 0, \quad \psi(L,t) = 0$$

Dirichlet problem



Discretize

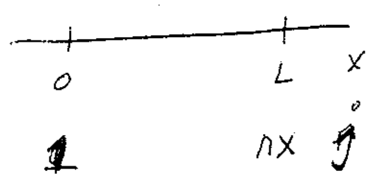
$$\psi(x,t) \rightarrow \psi_j^n$$

$$\partial_t \psi \rightarrow \frac{\psi_j^{n+1} - \psi_j^n}{\tau}$$

$$\partial_x \psi \rightarrow \frac{\psi_{j+1} - \psi_{j-1}}{2\Delta}$$

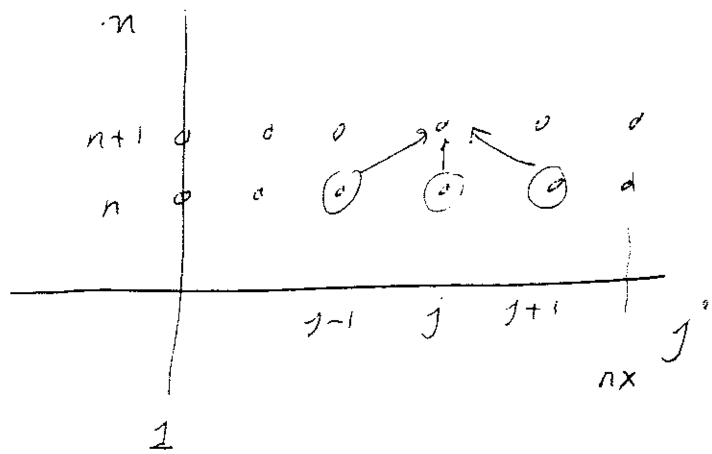
$$\partial_x^2 \psi \rightarrow \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta^2}$$

$$x = L \frac{(j-1)}{(nx-1)}$$



$$\boxed{\psi_j^{n+1} = \psi_j^n + \frac{\tau D}{\Delta^2}\left[\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n\right]}$$

Explicit
time-stepping



$$\boxed{\begin{array}{lll} \text{Dirichlet} & \psi_1^n = 0, \quad \psi_{nx}^n = 0, & j = 2, nx-1 \\ \text{zero-derivative} & \psi_0^n = \psi_2^n, \quad \psi_{nx+1}^n = \psi_{nx-1}^n, & j = 1, nx \\ \text{periodic} & \psi_0 = \psi_{nx-1}, \quad \psi_{nx+1} = \psi_2, & j = 1, nx \end{array}}$$

Boundary conditions

Stability analysis – explicit scheme

Let $\psi_j^n \rightarrow \psi^n e^{ikx} \rightarrow \psi^n e^{ikj\Delta}$, $\Delta = \frac{L}{n_x}$

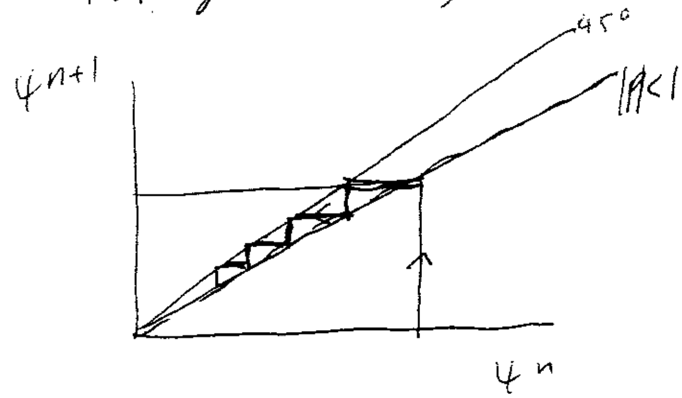
$$\Rightarrow \psi_j^{n+1} = \psi_j^n + \frac{\tau D}{\Delta^2}\left[\psi_j^n e^{ik\Delta} - 2\psi_j^n \cancel{e} + \psi_j^n e^{-ik\Delta}\right]$$

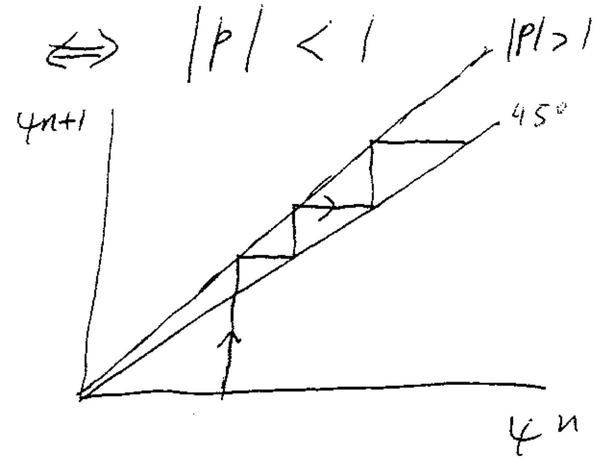
$$\Rightarrow \psi_j^{n+1} = \psi_j^n + \frac{\tau D}{\Delta^2}\psi_j^n \, 2(\cos k\Delta - 1)$$

let $\psi_j^{n+1} = p\,\psi_j^n$

$$\Rightarrow \boxed{p(k) = 1 - \frac{2\tau D}{\Delta^2}(1 - \cos k\Delta)}$$

For given k, stable $\Leftrightarrow |p| < 1$





$-1 \leqslant \cos k\Delta \leqslant 1$, $\boxed{1 - \frac{4\tau D}{\Delta^2} \leqslant p \leqslant 1}$

$$\therefore \boxed{\text{stable if } \tau < \Delta^2/2D}$$

stability analysis - Implicit

$$\boxed{\psi_j^{n+1} = \psi_j^{n} + \frac{\tau D}{\Delta^2}\left[\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}\right]}$$

implicit
time stepping

$$\Rightarrow \begin{pmatrix} & & \\ & M & \\ & & \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \psi_{j-1} \\ \psi_j \\ \psi_{j+1} \\ 0 \\ \vdots \end{pmatrix}^{n+1} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \psi \\ \psi \\ \psi \\ 0 \\ 0 \end{pmatrix}^{n}$$

$$M = \begin{pmatrix} \ddots & \ddots & & 0 \\ \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{pmatrix} \qquad \text{tridiagonal}$$

$$\Rightarrow \rho(k)\left[1 + \frac{2\tau D}{\Delta^2}\left(1 - \cos k\Delta\right)\right] = 1$$

$$\Rightarrow |\rho| < 1, \quad \boxed{\text{unconditionally stable}}$$