Schrödinger Equation

$$i\psi_t + \frac{\partial^2\psi}{\partial x^2} - V(x)\psi = 0 \qquad (\hbar = 1,\ m = \tfrac{1}{2})$$

Implicit first order in time approximation:

$$j\,\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = -\frac{\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}}{\Delta x^2} + V_i\,\psi_i^{n+1}$$

Stability: $$\xi_i = \frac{1}{1 + j\left[\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_i\,\Delta t\right]}$$

Unconditionally stable, but not unitary, ie.

$$\int_{-\infty}^{\infty} |\psi|^2\,dx = 1$$

is not fulfilled.

To obtain a unitary solution, we consider

$$i\,\frac{\partial\psi}{\partial t} = H\psi \quad , \quad H \doteq -\frac{\partial^2}{\partial x^2} + V(x)$$

Formal solution $\psi(x,t) = \psi(x_0)\,e^{-iHt}$ defined by power series of the Operator.

(unstable) FTCS approx: $$j\,\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = H\psi_i^n$$

$$\Rightarrow \quad \psi_i^{n+1} = (1 - jH\Delta t)\,\psi_i^n$$

(stable) implicit approx: $$\psi_i^{n+1} = \frac{1}{1 + jH\Delta t}\,\psi_j^n$$

In fact $\quad 1 - j\Delta t H \approx e^{-j\Delta t H} \quad$ and $\quad \dfrac{1}{1+jH\Delta t} \approx 1 - jH\Delta t + O(\Delta t^2)$

are just two approximations which are first order.

A second order unitary approximation is

$$e^{-j\Delta t H} \simeq \frac{1 - \frac{1}{2} j H \Delta t}{1 + \frac{1}{2} j H \Delta t}$$

which gives (starting from $\psi(x, \Delta t) = \psi(x, 0)\, e^{-jH\Delta t}$)

$$\left(1 + \tfrac{1}{2} j H \Delta t\right) \psi_i^{n+1} = \left(1 - \tfrac{1}{2} j H \Delta t\right) \psi_j^n .$$

Replacing H by its finite-difference form we obtain a complex tri-diagonal system.

$$\psi_i^{n+1} - \frac{j\Delta t}{4\Delta x^2}\left[\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}\right] + j\Delta t V_i \psi_i^{n+1}$$

$$= \psi_j^n + \frac{j\Delta t}{4\Delta x^2}\left[\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n\right] - j\Delta t V_i \psi_i^n$$

$$\Rightarrow \qquad A\, \vec{\psi}^{\,n+1} = A^* \vec{\psi}^{\,n},$$

$$a = -j\Delta t / 4\Delta x^2$$

$$d_j = 1 + j\left(\frac{\Delta t}{2\Delta x^2} + \Delta t V_i\right)$$

$$A = \begin{pmatrix} d_0 & a & 0 & 0 & & \\ a & d_1 & a & 0 & & \\ 0 & a & d_2 & a & & \\ & & & \ddots & \ddots & a \\ 0 & \cdots & \cdots & 0 & a & d_{N-1} \end{pmatrix}$$

Splitting methods

Consider the linear ODE system

$$\frac{d\vec{y}}{dt} = A\vec{y}(t) \qquad \text{with} \quad A = A_1 + A_2 .$$

The formal solution is $\vec{y}(\Delta t) = e^{A\Delta t}\,\vec{y}(0)$.

If we can solve $\dfrac{d\vec{y}}{dt} = A_1\vec{y}(t)$ and $\dfrac{d\vec{y}}{dt} = A_2\vec{y}(t)$

we can approximate

$$\vec{y}(\Delta t) = e^{A\Delta t}\,\vec{y}(0) \approx e^{A_2\Delta t}\, e^{A_1\Delta t}\,\vec{y}(0).$$

This is of first order in Δt since

$$e^{A\Delta t} = \mathbf{I} + \Delta t\,(A_1 + A_2) + \tfrac{1}{2}\,\Delta t^2 \left(A_1 + A_2 \right)^2 + \ldots$$

$$e^{A_2\Delta t}\, e^{A_1\Delta t} = I + \Delta t\,(A_1 + A_2) + \tfrac{1}{2}\,\Delta t^2 \left(A_1^2 + 2A_2A_1 + A_2^2 \right) + \ldots$$

$$\underbrace{\frac{1}{\Delta t}\left(e^{A\Delta t} - e^{A_2\Delta t}\, e^{A_1\Delta t} \right)\vec{y}(0)}_{\text{local error}} = \frac{1}{2}\,\Delta t\,\underbrace{\left(A_1A_2 - A_2A_1 \right)}_{[A_1, A_2]}\,\vec{y}(0) + \mathcal{O}(\Delta t^2)$$

Thus, the method is first order in time if A_1 and A_2 do not commute.

Up to here we always start with a full step with operator A_1, then carry out one step with operator A_2.

Better accuracy can be obtained by alternating the first operator ~~and to~~ in every half-step:

$$\vec{y}(\Delta t) = \left(e^{\frac{1}{2}\Delta t A_2} e^{\frac{1}{2}\Delta t A_1}\right)\left(e^{\frac{1}{2}\Delta t A_1} e^{\frac{1}{2}\Delta t A_2}\right) \vec{y}(0)$$

$$= e^{\frac{1}{2}\Delta t A_2} e^{\Delta t A_1} e^{\frac{1}{2}\Delta t A_2} \vec{y}(0) \quad \text{(Strang splitting).}$$

Strang splitting is second order in time.

These results hold for non-linear systems as well.

Split-step Fourier method for the nonlinear Schrödinger eq.

$$i\psi_t + P\psi_{xx} + Q|\psi|^2\psi = 0$$

$$i\psi_t + \mathcal{L}\psi + \mathcal{N}\psi = 0$$

$$\Rightarrow \quad \begin{aligned} i\psi_t + \mathcal{L}\psi &= 0 \qquad & \psi_t &= i\mathcal{L}\psi \quad & \Rightarrow \quad \psi(t) &= \psi(0)e^{i\mathcal{L}t} \\ i\psi_t + \mathcal{N}\psi &= 0 \qquad & \psi_t &= i\mathcal{N}\psi \quad & \Rightarrow \quad \psi(t) &= \psi(0)e^{i\mathcal{N}t} \end{aligned}$$

Strang-Splitting:

$$\psi(\Delta t) = e^{i\mathcal{L}\frac{\Delta t}{2}} e^{i\mathcal{N}\Delta t} e^{i\mathcal{L}\frac{\Delta t}{2}} \psi(0)$$

$$\psi(n\Delta t) = e^{i\mathcal{L}\frac{\Delta t}{2}} \left(e^{i\mathcal{N}\Delta t} e^{i\mathcal{L}\Delta t} \right)^n e^{i\mathcal{N}\Delta t} e^{i\mathcal{L}\frac{\Delta t}{2}} \psi(0)$$

How to compute $e^{i\mathcal{L}\Delta t}\psi$ and $e^{i\mathcal{N}\Delta t}\psi$?

For $\mathcal{N} = Q|\psi|^2$:

$$i\psi_t = -Q|\psi|^2\psi$$

$$\Rightarrow \psi_t = iQ|\psi|^2\psi$$

$$\frac{d}{dt}|\psi|^2 = \frac{d}{dt}(\psi\psi^*) = \psi\frac{d\psi^*}{dt} + \psi^*\frac{d\psi}{dt}$$

$$= \psi(-iQ|\psi|^2\psi^*) + \psi^*(iQ|\psi|^2\psi) = 0$$

$$\Rightarrow |\psi(t)|^2 = |\psi(0)|^2$$

$$\Rightarrow \psi(\Delta t) = \psi(0)\, e^{iQ|\psi(t)|^2\Delta t}$$

$$= \psi(0)\, e^{iQ|\psi(0)|^2\Delta t}$$

For $\mathcal{L} = \partial_{xx}$:

$$i\psi_t = -P\partial_{xx}\psi$$

$$\psi_t = +iP\frac{\partial^2\psi}{\partial x^2}$$

Forward-Fourier transf.:

$$\hat{\psi}_t = iP(-k^2)\hat{\psi}$$

$$\hat{\psi}(\Delta t) = e^{-iPk^2\Delta t}\hat{\psi}(0) \xrightarrow[\text{Fourier-transf.}]{\text{Backward}} \psi(\Delta t)$$