Computational Physics

Partial Differential Equations:
Time-dependent Schrödinger Equation

Lectures based on course notes by Pablo Laguna and Kostas Kokkotas

revamped by Deirdre Shoemaker

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1-dim Schrödinger Equation

Consider the Schrödinger equation describing the evolution of a quantum state Ψ:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \quad \text{where} \quad H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$$

The wave function Ψ must satisfy the unitary condition

$$\int_{-\infty}^{+\infty} |\Psi|^2 d^3\vec{x} = 1$$

and boundary conditions

$$\Psi(\vec{x} \to \infty, t) = 0$$

For simplicity, we will consider the 1-dim case, where

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

we will also set $\hbar = 1$ and $m = 1/2$

A formal solution to the Schrödinger equation is

$$\Psi(x,t) = e^{-iHt}\Psi(x,0)$$

since

$$i\frac{\partial \Psi}{\partial t} = i(-i\,H)e^{-iHt}\Psi(x,0) = H\,\Psi$$

Therefore

$$\begin{aligned}
\Psi(x,\Delta t) &= e^{-iH\Delta t}\Psi(x,0) = (1 - i\,H\,\Delta t)\Psi(x,0) \\
\Psi(x,2\,\Delta t) &= (1 - i\,H\,\Delta t)\Psi(x,\Delta t) \\
\Psi(x,3\,\Delta t) &= (1 - i\,H\,\Delta t)\Psi(x,2\Delta t) \\
&\vdots \\
\Psi(x,(n+1)\,\Delta t) &= (1 - i\,H\,\Delta t)\Psi(x,n\,\Delta t)
\end{aligned}$$

but $t^n \equiv n\,\Delta t$, so

$$\Psi(x,t^{n+1}) = (1 - i\,H\,\Delta t)\Psi(x,t^n)$$

The approximation $\Psi(x, t^{n+1}) = (1 - i\,H\,\Delta t)\Psi(x, t^n)$ can be rewritten as

$$i\left[\frac{\Psi(x, t^{n+1}) - \Psi(x, t^n)}{\Delta t}\right] = H\,\Psi(x, t^n)$$

which is how we derived the Euler step.

If in addition we approximate the Hamiltonian by

$$H\,\Psi_j^n = -\left[\frac{\Psi_{j+1}^n - 2\,\Psi_j^n + \Psi_{j-1}^n}{\Delta x^2}\right] + V\,\Psi_j^n$$

we get that

$$i\left[\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t}\right] = -\left[\frac{\Psi_{j+1}^n - 2\,\Psi_j^n + \Psi_{j-1}^n}{\Delta x^2}\right] + V\,\Psi_j^n$$

which is a Forward-Time Centered-Space discretization of the Schrdinger equation.

von-Neumann stability analysis. Substitute $\Psi_j^n = \xi^n e^{i\,j\,k\,\Delta t}$ into

$$i\left[\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t}\right] = -\left[\frac{\Psi_{j+1}^n - 2\,\Psi_j^n + \Psi_{j-1}^n}{\Delta x^2}\right] + V\,\Psi_j^n$$

and determine this algorithm's stability criterion.

Consider instead

$$e^{iHt}\Psi(x,t) = \Psi(x,0)$$

Thus,

$$\begin{aligned}
(1 + i\,H\,\Delta t)\Psi(x,\Delta t) &= \Psi(x,0) \\
(1 + i\,H\,\Delta t)\Psi(x,2\,\Delta t) &= \Psi(x,\Delta t) \\
(1 + i\,H\,\Delta t)\Psi(x,3\,\Delta t) &= \Psi(x,2\Delta t) \\
&\vdots \\
(1 + i\,H\,\Delta t)\Psi(x,(n+1)\,\Delta t) &= \Psi(x,n\,\Delta t)
\end{aligned}$$

therefore

$$(1 + i\,H\,\Delta t)\Psi(x,t^{n+1}) = \Psi(x,t^n)$$

or equivalently

$$i\left[\frac{\Psi(x,t^{n+1}) - \Psi(x,t^n)}{\Delta t}\right] = H\,\Psi(x,t^{n+1})$$

implicit evolution

von-Neumann stability analysis. Substitute $\Psi_j^n = \xi^n e^{i\,j\,k\,\Delta t}$ into

$$i\left[\frac{\Psi_j^{n+1}-\Psi_j^n}{\Delta t}\right] = -\left[\frac{\Psi_{j+1}^{n+1}-2\,\Psi_j^{n+1}+\Psi_{j-1}^{n+1}}{\Delta x^2}\right] + V\,\Psi_j^{n+1}$$

and determine this algorithm's stability criterion.

However, the problem with the implicit method $(1 + i\,H\,\Delta t)\Psi_j^{n+1} = \Psi_j^n$ is that $\Psi_j^n \propto \xi^n$, therefore as $n \gg 1$

$$\int_{-\infty}^{+\infty} |\Psi|^2 dx \leq 1$$

also the accuracy in approximating the time derivative is $O(\Delta t)$

Let's consider the following alternative

$$e^{-iH\Delta t} \approx \frac{\left(1 - \frac{1}{2} i\,H\,\Delta t\right)}{\left(1 + \frac{1}{2} i\,H\,\Delta t\right)}$$

Therefore, $\Psi(x, t^{n+1}) = e^{-iHt}\Psi(x, t^n)$ yields

$$\left(1 + \frac{1}{2} i\,H\,\Delta t\right)\Psi(x, t^{n+1}) = \left(1 - \frac{1}{2} i\,H\,\Delta t\right)\Psi(x, t^n)$$

A von-Neumann stability analysis yields

$$\xi = \frac{(1 - i\,A)}{(1 + i\,A)}$$

where

$$A \equiv \left(\frac{4\,\Delta t}{\Delta x^2}\right)\,\sin^2\left(k\,\Delta t/2\right) + \Delta t\,V$$

thus $|\xi|^2 = 1$ marginally stable.

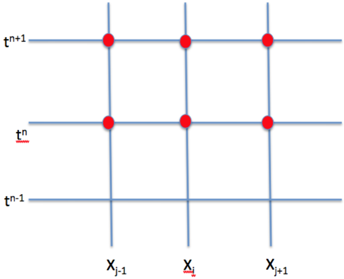
What type of discretization is

$$\Psi_j^{n+1} + \frac{1}{2} i H \Delta t \Psi_j^{n+1} = \Psi_j^n - \frac{1}{2} i H \Delta t \Psi_j^n$$

Re-write is as

$$i \left[\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t} \right] = H \left[\frac{\Psi_j^{n+1} + \Psi_j^n}{2} \right]$$

Crank-Nicolson



Solving

$$\left(I + \frac{1}{2} i\,\Delta t\,H\right)\Psi^{n+1} = \left(I - \frac{1}{2} i\,\Delta t\,H\right)\Psi^{n}$$

implies

$$\Psi^{n+1} = \left(I + \frac{1}{2} i\,\Delta t\,H\right)^{-1}\left(I - \frac{1}{2} i\,\Delta t\,H\right)\Psi^{n}$$

inverting an operator. We accomplish this by re-writing the equation as

$$\begin{aligned} \Psi^{n+1} &= \left(I + \frac{1}{2} i\,\Delta t\,H\right)^{-1}\left[2\,I - \left(I + \frac{1}{2} i\,\Delta t\,H\right)\right]\Psi^{n} \\ &= \left[2\left(I + \frac{1}{2} i\,\Delta t\,H\right)^{-1} - I\right]\Psi^{n} \end{aligned}$$

Given

$$\Psi^{n+1} = \left[2 \left(I + \frac{1}{2} i \, \Delta t \, H \right)^{-1} - I \right] \Psi^n$$

define

$$Q \equiv \frac{1}{2} \left(I + \frac{1}{2} i \, \Delta t \, H \right)$$

so

$$\Psi^{n+1} = Q^{-1} \Psi^n - \Psi^n$$

Therefore, the integration proceeds in two steps.

- First step: Solve the system $Q \, \Phi = \Psi^n$
- Second step: Update the solution with $\Psi^{n+1} = \Phi - \Psi_n$

Depending of the problem, solving the system $Q \, \Phi = \Psi^n$ could be computationally expensive. Is there a way to reduce the cost?

Iterative Crank-Nicolson

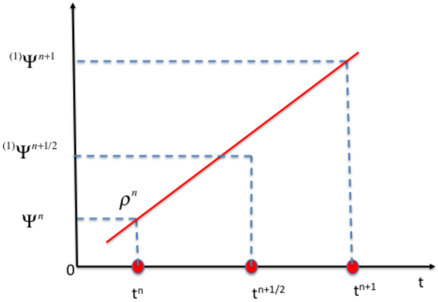
Recall that the approximation to $\partial_t \Psi = \rho[\Psi]$

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \rho \left[\frac{\Psi^{n+1} - \Psi^n}{2} \right]$$

will require a matrix inversion because of Ψ^{n+1} in the r.h.s. of the equation. Is there a way to avoid this?

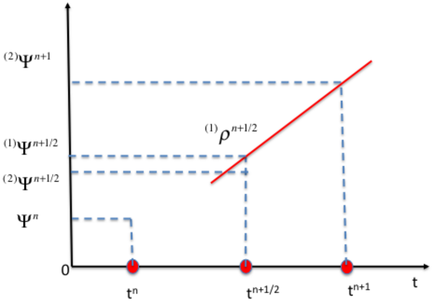
Yes, we will obtain Ψ^{n+1} from a series of intermediate steps similar to the Runge-Kuta method.

ICN - First Step



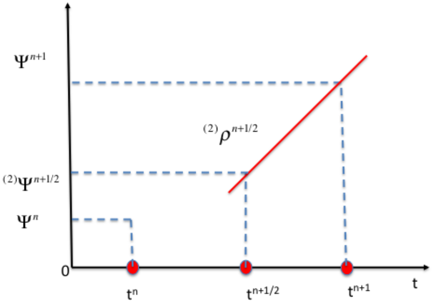
$$
\begin{aligned}
{}^{(1)}\Psi^{n+1} &= \Psi^n + \Delta t\, \rho[\Psi^n] \quad \text{Euler step} \\
{}^{(1)}\Psi^{n+1/2} &= \frac{1}{2}\left[{}^{(1)}\Psi^{n+1} + \Psi^n\right] \quad \text{Average}
\end{aligned}
$$

ICN - Second Step



$$
\begin{aligned}
{}^{(2)}\psi^{n+1} &= \psi^n + \Delta t\, \rho[{}^{(1)}\psi^{n+1/2}] \quad \text{Euler step} \\
{}^{(2)}\psi^{n+1/2} &= \frac{1}{2}\left[{}^{(2)}\psi^{n+1} + \psi^n\right] \quad \text{Average}
\end{aligned}
$$

ICN - Third Step



$$\Psi^{n+1} = \Psi^{n} + \Delta t\, \rho[{}^{(2)}\Psi^{n+1/2})] \quad \text{Euler step}$$

ICN - Summary

$$
\begin{aligned}
{}^{(1)}\Psi^{n+1} &= \Psi^n + \Delta t\,\rho[\Psi^n] \quad \text{Euler step} \\
{}^{(1)}\Psi^{n+1/2} &= \frac{1}{2}\left[{}^{(1)}\Psi^{n+1} + \Psi^n\right] \quad \text{Average} \\
{}^{(2)}\Psi^{n+1} &= \Psi^n + \Delta t\,\rho[{}^{(1)}\Psi^{n+1/2}] \quad \text{Euler step} \\
{}^{(2)}\Psi^{n+1/2} &= \frac{1}{2}\left[{}^{(2)}\Psi^{n+1} + \Psi^n\right] \quad \text{Average} \\
\Psi^{n+1} &= \Psi^n + \Delta t\,\rho[{}^{(2)}\Psi^{n+1/2})] \quad \text{Euler step}
\end{aligned}
$$