Time-dependent Schroedinger Equation

Example of a parabolic PDE, like the diffusion equation, (but with complex numbers). Here restrict to 1 spatial dimension.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Typical problem: Given an initial wave-function, $\psi(x, t = 0)$, see how it propagates forward in time.

Formal solution is known, namely

$$\psi(x,t) = \exp\,(\frac{-it\mathcal{H}}{\hbar})\psi(x,0)$$

where the Hamilitonian operator is

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

Numerical evolution in time of the wave-function depends on a suitable approximation for the exponential factor.

This needs to both be stable numerically, and preserve the normalization of the wave-function.

For this particular problem, the standard method is to use Cayley's form for approximating the exponential factor,

$$\exp\left(\frac{-i\Delta t\mathcal{H}}{\hbar}\right) \approx \frac{1-\frac{i\Delta t\mathcal{H}}{2\hbar}}{1+\frac{i\Delta t\mathcal{H}}{2\hbar}}$$

leading to the following equation for evolving the wave-function from time t to time $t+\Delta t$.

$$\left[1+\frac{i\Delta t\mathcal{H}}{2\hbar}\right]\psi(x,t+\Delta t) = \left[1-\frac{i\Delta t\mathcal{H}}{2\hbar}\right]\psi(x,t) \tag{1}$$

Now discretizing in x and t, so that $\psi(m,n) \equiv \psi(m\Delta x, n\Delta t)$, and using the finite difference form of the $\mathcal{H}$ operator.

LHS of equation 1

$$\text{LHS} = \psi(m,n+1) + \frac{i\Delta t}{2\hbar}V(m)\psi(m,n+1) + \tag{2}$$

$$\frac{i\Delta t}{2\hbar}\left(-\frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\left(\psi(m+1,n+1) - 2\psi(m,n+1) + \psi(m-1,n+1)\right)\right.$$

Similarly RHS.

$$\text{RHS} = \psi(m,n) - \frac{i\Delta t}{2\hbar}V(m)\psi(m,n) - \tag{3}$$

$$\frac{i\Delta t}{2\hbar}\left(-\frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\left(\psi(m+1,n) - 2\psi(m,n) + \psi(m-1,n)\right)\right.$$

So this is an example of an **implicit** method. We don't have an explicit formula for $\psi(m,n+1)$ in terms of known quantities at time-step n. But we do have a tri-diagonal system of equations relating a triplet of time-advanced points with a RHS consisting of known quantities at the current time.

The method is stable, conserves the normalization and has second-order accuracy in both space and time. This kind of method is advocated in general for diffusion type equations and is called the Crank-Nicolson method.

Simplifying this, by setting $\hbar = 1$ and $m = 1$ (the mass not the index ...), multiplying each element by

$$\frac{4i(\Delta x)^2}{\Delta t}$$

We then find:

$$\psi(m-1, n+1) - 2c_1\psi(m, n+1) + \psi(m+1, n+1) = -\psi(m-1, n) + 2c_2\psi(m, n) - \psi(m+1, n)$$

with

$$c_1 = 1 + (\Delta x)^2 V(m) - 2i\frac{(\Delta x)^2}{\Delta t}$$

and

$$c_2 = 1 + (\Delta x)^2 V(m) + 2i\frac{(\Delta x)^2}{\Delta t}$$

So we can then use this to set up a matrix solution, preferably in a way which is consistent with the use of complex numbers.

Movies show example with a Gaussian wave-packet with initial wave-function

$$\psi(x, 0) = \exp\left(-(x - x_0)^2/\sigma^2\right) \exp\left(ik_0 x\right)$$

with $x_0 = 0.4$, $k_0 = 250$, $\sigma^2 = 0.001$.