

## Physics 452: Numerically Solving the Schrödinger Equation (1-D)

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We seek to solve

$$i \frac{\partial \Psi(x,t)}{\partial t} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \Psi(x,t), \quad (1)$$

where the equation has been scaled to atomic units. If we pretend that the Hamiltonian on the right-hand-side is constant, we may approximate a solution as follows:

$$\Psi(x,t + \Delta t) \cong \exp \left\{ -i\Delta t \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \right\} \Psi(x,t). \quad (2)$$

We might get away with this if the time step  $\Delta t$  is sufficiently short. We could then repeatedly use this to evolve the solution a later time.

The strange occurrence of an operator in the exponent only makes sense in terms of an exponential expansion:

$$e^\alpha = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}. \quad (3)$$

The potential  $V(x,t)$  need not participate in the expansion since it can be factored out from the exponent containing  $\partial^2/\partial x^2$ . It is natural to wonder, however, whether  $V(x,t)$  should be written to the right or the left of  $\partial^2/\partial x^2$ . We'll split the difference and place  $V(x,t)/2$  both before and after.

With the above clarifications, Eq. (2) takes the form

$$\Psi(x,t + \Delta t) \cong e^{-i\frac{\Delta t}{2}V(x,t)} \sum_{n=0}^{\infty} \frac{1}{n!} \left[ i \frac{\Delta t}{2} \frac{\partial^2}{\partial x^2} \right]^n e^{-i\frac{\Delta t}{2}V(x,t)} \Psi(x,t). \quad (4)$$

Thus, we need to deal with an object of the form

$$\sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{\partial^{2n} f(x)}{\partial x^{2n}}, \quad \text{where } a = i \frac{\Delta t}{2} \text{ and } f(x) \equiv e^{-i\frac{\Delta t}{2}V(x,t)} \Psi(x,t). \quad (5)$$

Here, we have suppressed the dependence on  $t$ , although it is understood to be there still.

We apply the Fourier integral theorem:

$$\begin{aligned}
\sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{\partial^{2n} f(x)}{\partial x^{2n}} &= F^{-1} \left\{ F \left\{ \sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{\partial^{2n} f(x)}{\partial x^{2n}} \right\} \right\} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-ikx} \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{a^n}{n!} \int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n} f(x')}{\partial x'^{2n}} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-ikx} \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{a^n}{n!} \int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n} f(x')}{\partial x'^{2n}}
\end{aligned} \tag{6}$$

With integration by parts, the final integral becomes

$$\int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n} f(x')}{\partial x'^{2n}} = e^{ikx'} \frac{\partial^{2n-1} f(x')}{\partial x'^{2n-1}} \Big|_{-\infty}^{\infty} - ik \int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n-1} f(x')}{\partial x'^{2n-1}} \tag{7}$$

A normalizable function must go to zero at infinity, so we can drop the first term on the right. We integrate by parts again and get

$$\int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n} f(x')}{\partial x'^{2n}} = (ik)^2 \int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n-2} f(x')}{\partial x'^{2n-2}}. \tag{8}$$

We can do this repeatedly until we exhaust the available even number of derivatives:

$$\int_{-\infty}^{\infty} dx' e^{ikx'} \frac{\partial^{2n} f(x')}{\partial x'^{2n}} = (ik)^{2n} \int_{-\infty}^{\infty} dx' e^{ikx'} f(x') \tag{9}$$

Then

$$\begin{aligned}
\sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{\partial^{2n} f(x)}{\partial x^{2n}} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-ikx} \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{(-ak^2)^n}{n!} \int_{-\infty}^{\infty} dx' e^{ikx'} f(x') \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-ikx} e^{-ak^2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx' e^{ikx'} f(x')
\end{aligned} \tag{10}$$

Finally, we place this result back into Eqs. (4) and (5):

$$\Psi(x, t + \Delta t) \cong e^{-\frac{\Delta t}{2} V(x, t)} F^{-1} \left\{ e^{-\frac{\Delta t}{2} k^2} F \left\{ e^{-\frac{\Delta t}{2} V(x, t)} \Psi(x, t) \right\} \right\} \tag{11}$$

We thus have a numerically straightforward strategy for updating the Schrödinger equation. Given an initial  $\Psi(x, t)$ , we first multiply by  $\exp\{-iV(x, t)\Delta t/2\}$ . Second, we take a Fourier transform. Third, we append the factor  $\exp\{-ik^2 \Delta t/2\}$  in Fourier space. Fourth, we take the inverse Fourier transform. Finally, we multiply by

$\exp\{-iV(x,t)\Delta t/2\}$  to arrive at  $\Psi(x,t + \Delta t)$ , ready to begin again. Since we only multiply by phases and perform Fourier transforms,  $\Psi(x,t)$  is guaranteed to remain normalized.

## Matlab Code

```
% This program integrates the 1-D Schrodinger equation for
a
% specified intial wave function and static potential.
%
% J. Peatross
%
close all;
% Number of spatial points on grid
nmax=2048;
% Width of grid in units of Bohr radii
xWidth=10;
dx=xWidth/nmax;
x=-dx*(nmax/2):dx:dx*(nmax/2-1);
% Potential in units of hBar^2/(mass*(Bohr radius)^2)
V=x.^2/2;
psi=exp(-x.^2/2);
% Number of time steps
nsteps=1000;
% Integration time in units of mass*(Bohr radius)^2/hBar
tmax=2;
dt=tmax/nsteps;
% Number of movie frames displayed
frames=100;
nframe=round(nsteps/frames);
% Integrate Schrodinger equation using FFT method
dnu=1/(dx*nmax);
nu=-dnu*(nmax/2):dnu:dnu*(nmax/2-1);
nu=fftshift(nu);
for n=0:nsteps;
    if rem(n,nframe)==0
        plot(x,real(psi),'g',
x,imag(psi),'y',x,(abs(psi)).^2,'b',x,V,'r')
        ylim([-1 1])
        xlabel('x')
        ylabel('|psi|^2 (blue), Re{psi} (green), Im{Psi}
(yellow), V (red)')
        text(-.8*xWidth/2,.75, strcat('t =',num2str(n*dt)))
        drawnow
    end
    psi=psi.*exp(-i*dt*V);
    psi2=fft(psi);
    psi2=psi2.*exp(-i*dt/2*(2*pi*nu).^2);
    psi=ifft(psi2);
end
```