Solving the time dependent Schrodinger equation

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

This has the formal solution

$$\Psi(\vec{x},t) = \mathrm{e}^{-itH/\hbar}\Psi(\vec{x},0)$$

For an eigenstate the time dependence is just a phase

$$\Psi_n(\vec{x},t) = \mathrm{e}^{-itE_n/\hbar}\Psi_n(\vec{x})$$

We can expand an arbitrary state in eigenstates, and thus

$$\Psi(\vec{x},t) = \sum_n C_n \mathrm{e}^{-itE_n/\hbar}\Psi_n(\vec{x})$$

But to use this we need to know all the eigenstates.
What to do if this is not possible?

Split-operator (Trotter approximation) method

Time evolution operator

$$U(t) = \mathrm{e}^{-iHt/\hbar} = \mathrm{e}^{-i(K+V)t/\hbar} \neq \mathrm{e}^{-iKt/\hbar}\mathrm{e}^{-iVt/\hbar}$$

For any operators A, B:

$$\mathrm{e}^{A+B} = \lim_{n\to\infty}\left(\mathrm{e}^{A/n}\mathrm{e}^{B/n}\right)^n$$

If we use this formula for large but finite n, there is a small error

$$\mathrm{e}^{A+B} = \left(\mathrm{e}^{A/n}\mathrm{e}^{B/n}\right)^n + [A,B]O(\Delta_t)^2$$

Introduce time-step in time evolution

$$U(t) \approx \left(\mathrm{e}^{-iK\Delta_t/\hbar}\mathrm{e}^{-iV\Delta_t/\hbar}\right)^n + O(\Delta_t)^2$$

Why is this useful?

Only diagonal operations (multiplications) if we switch back and forth between real space and momentum space wave functions

The potential energy is diagonal in real space:

$$e^{-iV\Delta_t/\hbar}|\Psi\rangle = \int d\vec{x} e^{-iV(\vec{x})\Delta_t/\hbar}\Psi(\vec{x})|\vec{x}\rangle$$

The kinetic energy is diagonal in momentum space

$$e^{-iK\Delta_t/\hbar}|\Psi\rangle = \int d\vec{p} e^{-i(p^2/2m)\Delta_t/\hbar}\Psi(\vec{p})|\vec{p}\rangle$$

If we go back and forth between real and momentum space wave functions, the time evolution is obtained just by multiplications

Fourier transforms:

$$\Psi(\vec{p}) = \int d\vec{x} e^{-i\vec{p}\cdot\vec{x}}\Psi(\vec{x})$$

$$\Psi(\vec{x}) = \int d\vec{p} e^{i\vec{p}\cdot\vec{x}}\Psi(\vec{p})$$

We need to calculate a series of many Fourier integrals

How can the FT be carried out efficiently?

One dimension: discrete Fourier transform in periodic box

$$x = n\Delta_x, \quad \Delta_x = L/N, \quad n = -N/2+1, \ldots, N/2$$

$$k = m\Delta_k, \quad \Delta_k = 2\pi/L, \quad m = -N/2+1, \ldots, N/2$$

$$f(n\Delta_x) = \frac{1}{\sqrt{N}} \sum_m \mathrm{e}^{-in\Delta_x m\Delta_k} g(m\Delta_k)$$

$$g(m\Delta_k) = \frac{1}{\sqrt{N}} \sum_n \mathrm{e}^{in\Delta_x m\Delta_k} f(n\Delta_x)$$

It looks like these transforms each require N^2 operations

Fast Fourier transform (FFT): only Nlog(N) operations

Read about how the FFT works (e.g., Numerical Recipes)
Subroutines available from many sources (e.g. gams.nist.gov)

FFT subroutines available on course web site

`DCFFTF(size,f,wsave)`

$$f(m) = \sum_n e^{-inm2\pi/N} f(n)$$

`DCFFTB(size,f,wsave)`

$$f(m) = \sum_n e^{inm2\pi/N} f(n)$$

Before using these, an initialization must be called

`DCFFTI(size,wsave)`

`wsave` is a work-space vector of size at least `4*n+15`

Note that the summation over n is for n=1,...,size.
The function is periodic:
n=size/2+1,...,size correspond to negative function arguments.

Propagation of a Gaussian wave packet

Momentum space wave function corresponding to a Gaussian wave packet centered at x=0 with average momentum $\mathbf{k_0}$, width $\mathbf{a}$

$$\Psi(k) \propto \mathrm{e}^{-a^2(k-k_0)^2/2} \;\rightarrow\; \Psi(x) \propto \mathrm{e}^{-x^2/a^2-ik_0x}$$

Start in momentum space

$$\Psi(k_m) \propto \mathrm{e}^{-a^2(k_m-k_0)^2/2}, \quad k_m = m\Delta_k, \quad \Delta_k = 2\pi/L, \quad m = -N/2+1,\ldots,N/2$$

```
dk=2.d0*pi/len
do i=-n/2+1,n/2
    k=dble(i)*dk
    if (i>0) then
       j=i
    else
       j=i+n
    endif
    psi(j)=exp(-(a*(k-k0)/2.d0)**2)
 enddo
```

Prepare time evolution operators:

- time-step `dt` has been read in
- here a square potential barrier between `vbeg,vend`

```
do i=-n/2+1,n/2
   x=dble(i)*dx
   k=dble(i)*dk
   if (i>0) then
      j=i
   else
      j=i+n
   endif
   if (x>=vbeg.and.x<=vend) then
      pot(j)=exp(-dt*(0,1)*vmax)
   else
      pot(j)=1.d0
   endif
   kin(j)=exp(-dt*0.5d0*(0,1)*k**2)
enddo
```

Fourier transform to real space: `DCFFTB(n,psi,wsave)`

Evolve with potential factor: `psi=psi*pot`

Fourier transform to momentum space: `DCFFTF(n,psi,wsave)`

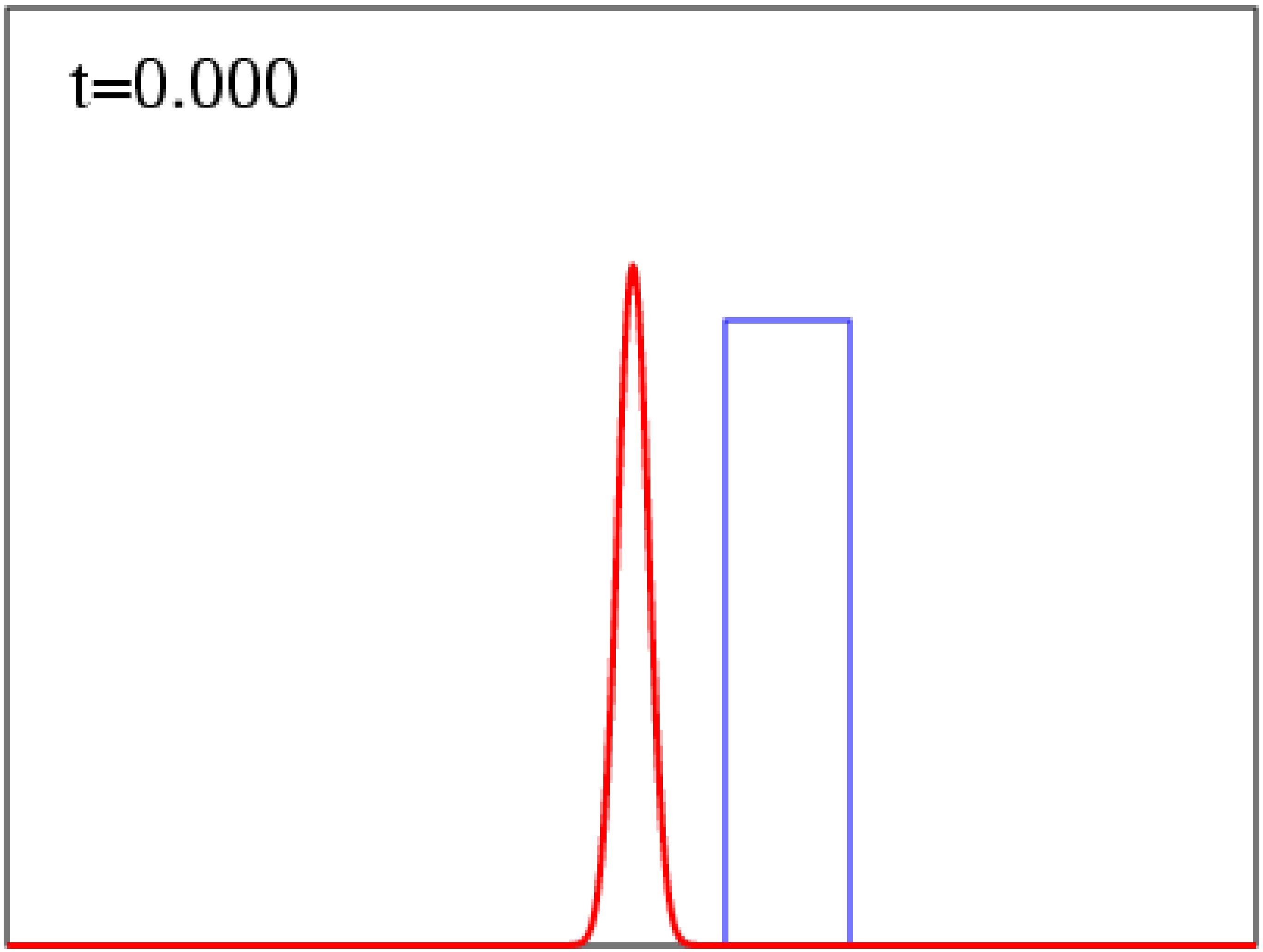
Evolve with kinetic factor: `psi=psi*kin`

Repeat as many times as desired

Convergence checks
- as a function of space/momentum discretization
- as a function of time-step

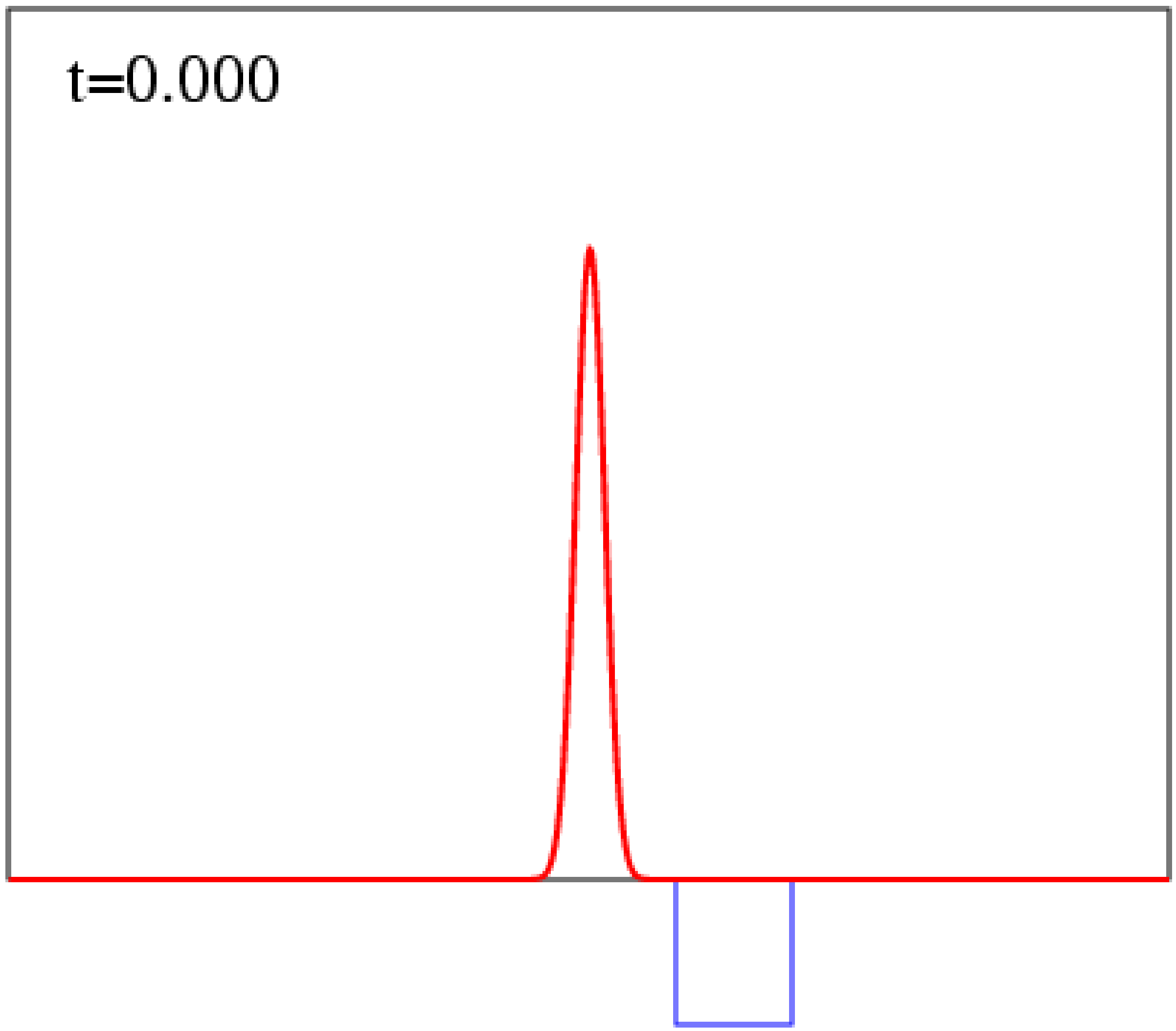
Wave packet incident on repulsive square potential barrier

$L=40$, $N=1024$, $V=50$ for $3 < x<7$, $a=1$, $k_0=10$, $\Delta_t=0.001$



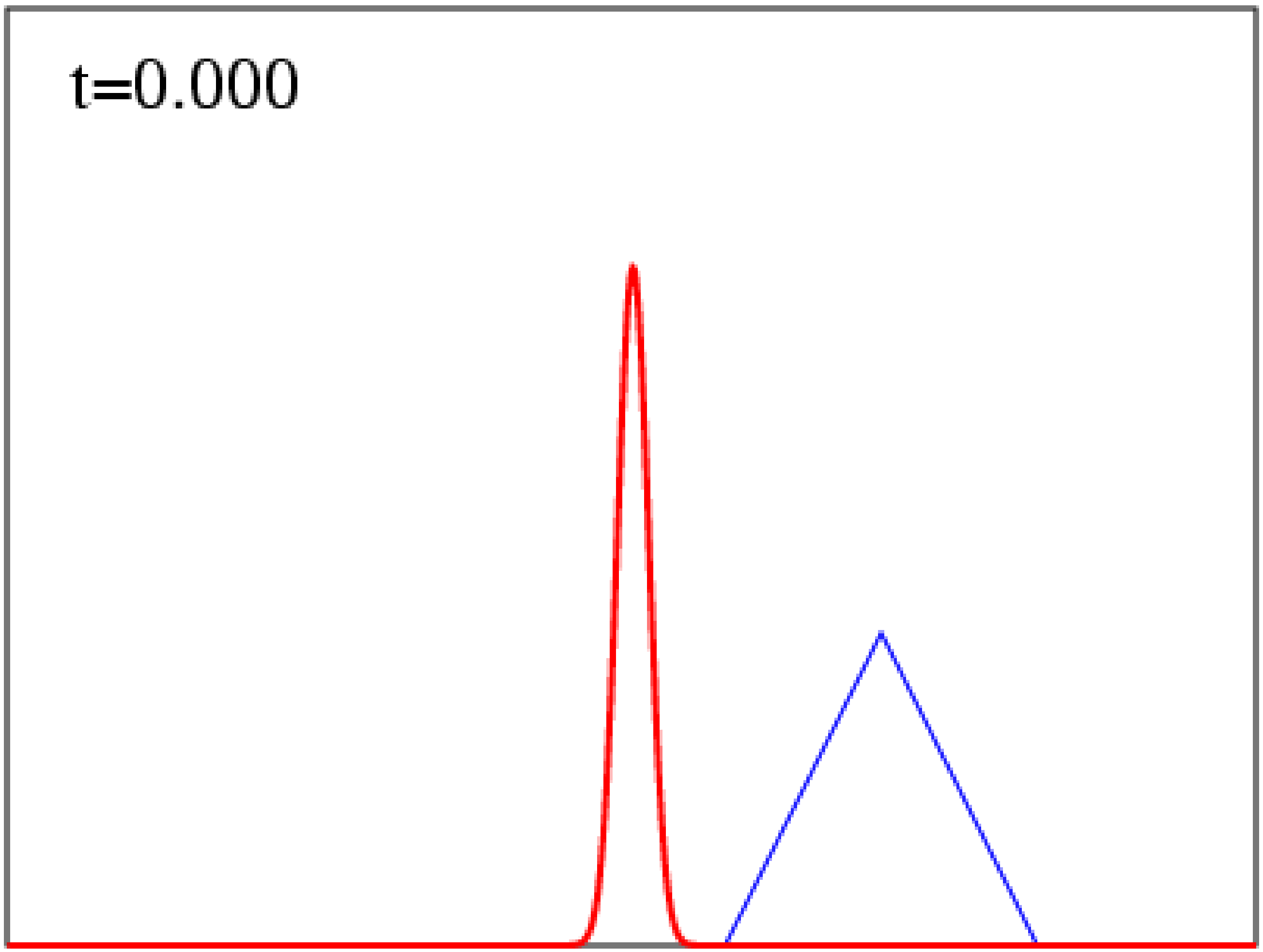
Wave packet incident on attractive square potential barrier

L=40, N=1024, V=-50 for 3 < x<7, a=1, k_0=10, Δ_t=0.001



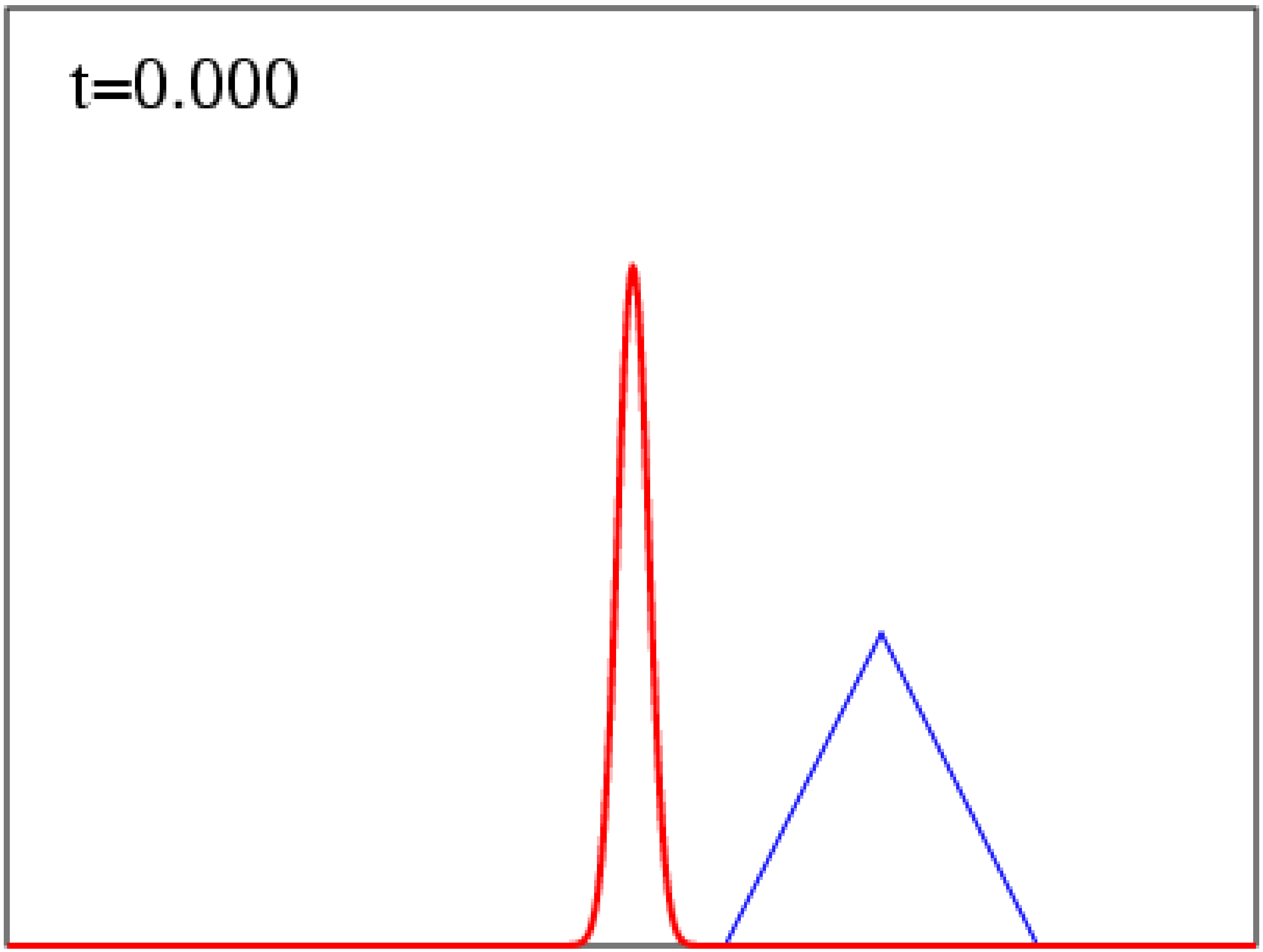
Wave packet incident on a repulsive triangular potential barrier

L=40, N=1024, a=1, k_0=10, Δ_t=0.001
potential between x=3 and x=13, Vmax=10



Wave packet incident on a repulsive triangular potential barrier

$L=40$, $N=1024$, $k_0=10$, $\Delta_t=0.001$
potential between $x=3$ and $x=13$, $V_{max}=5$



Wave packet incident on a repulsive triangular potential barrier

L=40, N=1024, V=-50 for 3 < x<7, a=1, k_0=10, Δ_t=0.001
potential between x=3 and x=13, Vmax=7.5