

# 03-Cprogramming

February 8, 2018

## 1 3. C programming

The following code is needed only if you are using the notebook, because make command treats spaces and TAB characters differently. We need to be able to reconfigure Jupyter to treat TABS as characters, not replace them with 4 spaces, as it does by default.

```
In [1]: %%javascript
        IPython.tab_as_tab_everywhere = function(use_tabs) {
            if (use_tabs === undefined) {
                use_tabs = true;
            }
            // apply setting to all current CodeMirror instances
            IPython.notebook.get_cells().map(
                function(c) { return c.code_mirror.options.indentWithTabs=use_tabs; }
            );
            // make sure new CodeMirror instances created in the future also use this setting
            CodeMirror.defaults.indentWithTabs=use_tabs;
        };

        IPython.tab_as_tab_everywhere()

<IPython.core.display.Javascript object>
```

### 1.1 Gaussian packet evolution: a C project

More homework! This is the second part of the homework, which is to try to reproduce the functionality of an old Fortran program. We do not know Fortran and little of C syntax, but hopefully the computational content, i.e. the algorithmic core, will be self-explanatory. The task is to "port", or convert this old code to C, and learn some basic C programming in the process.

```
In [2]: %%bash

        ## first, a refresher: what does this bash script do?? Add a few comment lines as appropriate

        if [ ! -d ~/5P10 ]; then
            mkdir ~/5P10
```

```

fi
cd ~/5P10
rm -rf packet
mkdir packet

```

```

In [3]: %cd ~/5P10/packet

/home/esternin/5P10/packet

```

```

In [4]: %%bash
        pwd
        ls -l

/home/esternin/5P10/packet
total 0

```

First, let's review the old Fortran code to see how it works and what its output looks like.

```

In [5]: %%file packet.f
C packet.f -- propagation of a Gaussian wave packet through a barrier in 1D
C      x = coordinate (in units of a, the barrier is from -a to +a)
C      P = wavefunction (not normalized)
C      E = energy of the wavefunction (in units of V, the barrier height)
C
C      Written by:      E.Sternin
C      Completed:      30.03.93
C=====
      real*4           x(601),x0,p0,sp,p_now,p_step,Pi,A0,t
      complex*8       P(601),I,A
      integer         j,Nargs,Nwaves
      character*80    buffer

      Nwaves = 20      ! add up (2*Nwaves+1) eigenwaves to form a packet
      x0 = -30.        ! start the packet far away from the barrier
      p0 = 0.5         ! keep incident energy low, E=0.5**2 < 1 (units of V)
      sp = 0.1         ! p0 +/- 4 sigma_p > 0,          all eigenwaves move to the right

      Nargs = iargc()  ! arguments supplied on the command line ?
      if (Nargs .lt. 1) then
        write(*,'(A,$)') ' Error: need time t: '
        read(*,*) t
      else
        call getarg(1,buffer)
        read(buffer,*) t
      end if

      I = cmplx(0.,1.)          !complex i

```

```

Pi = 2.*acos(0.)
A0 = 1./sqrt( sqrt(2.*Pi) * sp ) /float (2*Nwaves+1)

do j = 1,601
  x(j) = -75 + (j-1)*0.25
  P(j) = cmplx(0.,0.)
end do

p_step = 4.*sp/float(Nwaves)      ! calculate over +/- 4*sigma_p
do j = -Nwaves,Nwaves            ! in Nwaves steps
  p_now = p0 + j * p_step
  E = p_now**2
  A = A0*exp( - ( (p_now-p0)/(2*sp) )**2 - I*(p_now*x0 + E*t) )
  call add_wave(x,P,A,E)
end do

C..output the saved values as is, without normalization
10   do j=1,      601
      write(*,*) x(j),abs(P(j))**2,real(P(j)),aimag(P(j))
end do
end

C=====
      subroutine add_wave(x,P,A,E)
C..adds the specified wave to the the supplied complex storage array P
C the values of Psi are only calculated at points given in real array x
      real*4          x(601),E
      complex*8      P(601),I,A,k1,K2,C1,b,c,d,f

      I = cmplx(0.,1.)      !complex i

      k1 = sqrt(cmplx(E,0.))
      K2 = sqrt(cmplx(E-1.,0.))

      C1 = -2*k1*K2-k1**2-2*k1*K2*exp(4*I*K2)+exp(4*I*K2)*k1**2
*      -K2**2+K2**2*exp(4*I*K2)

      b = (k1**2-K2**2)/ C1 *(exp(2*I*(2*K2-k1))-exp(-2*I*k1))
      c = -2*k1*(K2+k1)/ C1 *exp(I*(K2-k1))
      d = (-2*K2+2*k1)*k1/ C1 *exp(I*(-k1+3*K2))
      f = -4*k1*K2/ C1 *exp(2*I*(K2-k1))

      do j = 1,296          ! left of the barrier, x < -1
        P(j) = P(j) + A * ( exp(I*k1*x(j)) + b*exp(-I*k1*x(j)) )
      end do
      do j=297,304        ! inside the barrier, -1 < x < 1
        P(j) = P(j) + A * ( c*exp(I*K2*x(j)) + d*exp(-I*K2*x(j)) )
      end do

```

```

do j=305,601                                ! to the right of the barrier, x > 1
  P(j) = P(j) + A * f*exp(I*k1*x(j))
end do

return
end

```

Writing packet.f

```

In [18]: %%bash
gfortran -o packet packet.f
./packet 40

```

-75.0000000	1.96023257E-06	8.77547078E-04	1.09093706E-03
-74.7500000	1.82045062E-06	1.01503159E-03	8.88910319E-04
-74.5000000	1.73418891E-06	1.13934174E-03	6.60370453E-04
-74.2500000	1.72351565E-06	1.24439807E-03	4.18317009E-04
-74.0000000	1.78586924E-06	1.32473465E-03	1.75918191E-04
-73.7500000	1.89733987E-06	1.37641025E-03	-5.32418489E-05
-73.5000000	2.01731950E-06	1.39714230E-03	-2.55563966E-04
-73.2500000	2.09439304E-06	1.38478726E-03	-4.20425145E-04
-73.0000000	2.08815527E-06	1.34157971E-03	-5.36953798E-04
-72.7500000	1.96922588E-06	1.26916065E-03	-5.98713057E-04
-72.5000000	1.73377737E-06	1.17202860E-03	-6.00105326E-04
-72.2500000	1.40628003E-06	1.05583435E-03	-5.39901666E-04
-72.0000000	1.03724994E-06	9.27589601E-04	-4.20508557E-04
-71.7500000	6.92532581E-07	7.95061758E-04	-2.45783187E-04
-71.5000000	4.43797006E-07	6.65725674E-04	-2.46243435E-05
-71.2500000	3.53931824E-07	5.47598756E-04	2.32524064E-04
-71.0000000	4.64492956E-07	4.48164472E-04	5.13460371E-04
-70.7500000	7.85790803E-07	3.73223447E-04	8.04049196E-04
-70.5000000	1.29298166E-06	3.28127062E-04	1.08872144E-03
-70.2500000	1.93195683E-06	3.15745245E-04	1.35361066E-03
-70.0000000	2.62589083E-06	3.38269514E-04	1.58476015E-03
-69.7500000	3.28651595E-06	3.95180687E-04	1.76927901E-03
-69.5000000	3.83478164E-06	4.83024662E-04	1.89775368E-03
-69.2500000	4.21086088E-06	5.98888146E-04	1.96270063E-03
-69.0000000	4.38410598E-06	7.35657639E-04	1.96033507E-03
-68.7500000	4.35984521E-06	8.86410533E-04	1.89053488E-03
-68.5000000	4.17116462E-06	1.04239804E-03	1.75629475E-03
-68.2500000	3.87792215E-06	1.19528465E-03	1.56499748E-03
-68.0000000	3.54403505E-06	1.33645989E-03	1.32586202E-03
-67.7500000	3.23056088E-06	1.45724276E-03	1.05214270E-03
-67.5000000	2.97883844E-06	1.55024452E-03	7.58670038E-04
-67.2500000	2.80352128E-06	1.60967337E-03	4.60947951E-04
-67.0000000	2.69476050E-06	1.63207762E-03	1.76304573E-04
-66.7500000	2.61299533E-06	1.61450752E-03	-7.97556131E-05

-66.5000000	2.51203733E-06	1.55792257E-03	-2.91400909E-04
-66.2500000	2.34614959E-06	1.46510801E-03	-4.46775230E-04
-66.0000000	2.08429469E-06	1.34065363E-03	-5.35670319E-04
-65.7500000	1.72119576E-06	1.19045167E-03	-5.51380508E-04
-65.5000000	1.28981821E-06	1.02388021E-03	-4.91413812E-04
-65.2500000	8.50275796E-07	8.49914155E-04	-3.57661454E-04
-65.0000000	4.84994189E-07	6.79052668E-04	-1.54537032E-04
-64.7500000	2.82709209E-07	5.20876376E-04	1.06756575E-04
-64.5000000	3.20579090E-07	3.85980820E-04	4.14243783E-04
-64.2500000	6.45942976E-07	2.82163615E-04	7.52546766E-04
-64.0000000	1.26368809E-06	2.17078952E-04	1.10297999E-03
-63.7500000	2.13198837E-06	1.95043162E-04	1.44704757E-03
-63.5000000	3.16631758E-06	2.17700610E-04	1.76604756E-03
-63.2500000	4.24724749E-06	2.85472372E-04	2.04101764E-03
-63.0000000	5.24817187E-06	3.94371396E-04	2.25668866E-03
-62.7500000	6.04795923E-06	5.39795437E-04	2.39928742E-03
-62.5000000	6.55504118E-06	7.12396111E-04	2.45917309E-03
-62.2500000	6.72689112E-06	9.02541215E-04	2.43152422E-03
-62.0000000	6.56544489E-06	1.09797518E-03	2.31514475E-03
-61.7500000	6.12861822E-06	1.28629222E-03	2.11520004E-03
-61.5000000	5.50341974E-06	1.45479967E-03	1.84037443E-03
-61.2500000	4.79634036E-06	1.59180793E-03	1.50415674E-03
-61.0000000	4.10773055E-06	1.68611656E-03	1.12460728E-03
-60.7500000	3.51199446E-06	1.72967336E-03	7.21265911E-04
-60.5000000	3.04656032E-06	1.71629013E-03	3.17660917E-04
-60.2500000	2.70658597E-06	1.64393231E-03	-6.38172496E-05
-60.0000000	2.44762691E-06	1.51251513E-03	-3.99906014E-04
-59.7500000	2.21115170E-06	1.32758426E-03	-6.69829722E-04
-59.5000000	1.93523533E-06	1.09681441E-03	-8.55706516E-04
-59.2500000	1.58132946E-06	8.31471640E-04	-9.43389896E-04
-59.0000000	1.15117166E-06	5.46015042E-04	-9.23601212E-04
-58.7500000	6.96210464E-07	2.55807769E-04	-7.94212101E-04
-58.5000000	3.10616684E-07	-2.11259467E-05	-5.56929444E-04
-58.2500000	1.20390737E-07	-2.67395400E-04	-2.21111812E-04
-58.0000000	2.56541142E-07	-4.66421829E-04	1.97463436E-04
-57.7500000	8.25106667E-07	-6.03376422E-04	6.79001911E-04
-57.5000000	1.87918408E-06	-6.65937783E-04	1.19821157E-03
-57.2500000	3.39837993E-06	-6.45499444E-04	1.72676297E-03
-57.0000000	5.28219744E-06	-5.38554392E-04	2.23431340E-03
-56.7500000	7.35717913E-06	-3.46145709E-04	2.69023469E-03
-56.5000000	9.40185237E-06	-7.51864864E-05	3.06532206E-03
-56.2500000	1.11809504E-05	2.63452530E-04	3.33339814E-03
-56.0000000	1.24820490E-05	6.52841758E-04	3.47215310E-03
-55.7500000	1.31673269E-05	1.07204251E-03	3.46670626E-03
-55.5000000	1.31818224E-05	1.49678183E-03	3.30778863E-03
-55.2500000	1.25843872E-05	1.90045475E-03	2.99543981E-03
-55.0000000	1.15273106E-05	2.25543324E-03	2.53778091E-03
-54.7500000	1.02349368E-05	2.53525679E-03	1.95125840E-03

-54.5000000	8.96054371E-06	2.71489052E-03	1.26091787E-03
-54.2500000	7.94261359E-06	2.77374568E-03	4.98947629E-04
-54.0000000	7.35255207E-06	2.69523030E-03	-2.97128689E-04
-53.7500000	7.28275381E-06	2.47116061E-03	-1.08449056E-03
-53.5000000	7.71300893E-06	2.09917175E-03	-1.81837473E-03
-53.2500000	8.53753500E-06	1.58579578E-03	-2.45413673E-03
-53.0000000	9.59492263E-06	9.45997075E-04	-2.94957822E-03
-52.7500000	1.07135056E-05	2.03106902E-04	-3.26684164E-03
-52.5000000	1.17637628E-05	-6.11433934E-04	-3.37489438E-03
-52.2500000	1.27123058E-05	-1.46040926E-03	-3.25261592E-03
-52.0000000	1.36412191E-05	-2.30117701E-03	-2.88891047E-03
-51.7500000	1.47498858E-05	-3.08695436E-03	-2.28486280E-03
-51.5000000	1.63353143E-05	-3.77088925E-03	-1.45454728E-03
-51.2500000	1.87299502E-05	-4.30688309E-03	-4.25099803E-04
-51.0000000	2.22337785E-05	-4.65292996E-03	7.64213735E-04
-50.7500000	2.70391229E-05	-4.77324473E-03	2.06282735E-03
-50.5000000	3.31695010E-05	-4.64084372E-03	3.41058243E-03
-50.2500000	4.04509083E-05	-4.23978781E-03	4.74079186E-03
-50.0000000	4.84937918E-05	-3.56642436E-03	5.98117150E-03
-49.7500000	5.67711140E-05	-2.63119512E-03	7.06030661E-03
-49.5000000	6.46740809E-05	-1.45877257E-03	7.90860690E-03
-49.2500000	7.16222858E-05	-8.82214517E-05	8.46253522E-03
-49.0000000	7.71898267E-05	1.42793136E-03	8.66895821E-03
-48.7500000	8.11878417E-05	3.02483817E-03	8.48753192E-03
-48.5000000	8.37276530E-05	4.62769996E-03	7.89379794E-03
-48.2500000	8.52661542E-05	6.15607155E-03	6.88250922E-03
-48.0000000	8.65038237E-05	7.52407406E-03	5.46736922E-03
-47.7500000	8.83546600E-05	8.64779390E-03	3.68379219E-03
-47.5000000	9.17651269E-05	9.44703538E-03	1.58702326E-03
-47.2500000	9.75877483E-05	9.85029712E-03	-7.47931248E-04
-47.0000000	1.06456144E-04	9.79940034E-03	-3.22922552E-03
-46.7500000	1.18670869E-04	9.25225951E-03	-5.75035345E-03
-46.5000000	1.34186004E-04	8.18734709E-03	-8.19471478E-03
-46.2500000	1.52631736E-04	6.60495553E-03	-1.04406076E-02
-46.0000000	1.73423046E-04	4.53073671E-03	-1.23650907E-02
-45.7500000	1.95925590E-04	2.01440044E-03	-1.38516352E-02
-45.5000000	2.19618625E-04	-8.67994619E-04	-1.47940936E-02
-45.2500000	2.44244642E-04	-4.01895726E-03	-1.51027357E-02
-45.0000000	2.69948883E-04	-7.31897354E-03	-1.47099122E-02
-44.7500000	2.97317951E-04	-1.06324060E-02	-1.35746058E-02
-44.5000000	3.27306130E-04	-1.38114765E-02	-1.16854291E-02
-44.2500000	3.61102109E-04	-1.67018082E-02	-9.06375702E-03
-44.0000000	3.99954821E-04	-1.91496704E-02	-5.76584507E-03
-43.7500000	4.44861274E-04	-2.10077558E-02	-1.88028580E-03
-43.5000000	4.96436493E-04	-2.21435502E-02	2.46975827E-03
-43.2500000	5.54633385E-04	-2.24444978E-02	7.13287760E-03
-43.0000000	6.18779508E-04	-2.18262710E-02	1.19328713E-02
-42.7500000	6.87542197E-04	-2.02368461E-02	1.66736990E-02

-42.5000000	7.59166374E-04	-1.76626258E-02	2.11470556E-02
-42.2500000	8.31750222E-04	-1.41301081E-02	2.51414049E-02
-42.0000000	9.03629640E-04	-9.71046370E-03	2.84488406E-02
-41.7500000	9.73681279E-04	-4.51691356E-03	3.08752116E-02
-41.5000000	1.04165531E-03	1.29624316E-03	3.22486460E-02
-41.2500000	1.10842264E-03	7.53587764E-03	3.24288942E-02
-41.0000000	1.17590069E-03	1.39767462E-02	3.13137546E-02
-40.7500000	1.24702416E-03	2.03675032E-02	2.88476888E-02
-40.5000000	1.32536935E-03	2.64405254E-02	2.50253454E-02
-40.2500000	1.41476106E-03	3.19203436E-02	1.98960491E-02
-40.0000000	1.51880877E-03	3.65348384E-02	1.35651864E-02
-39.7500000	1.64052797E-03	4.00270075E-02	6.19407417E-03
-39.5000000	1.78196223E-03	4.21656929E-02	-2.00418197E-03
-39.2500000	1.94406696E-03	4.27564979E-02	-1.07679572E-02
-39.0000000	2.12683622E-03	4.16527316E-02	-1.97961163E-02
-38.7500000	2.32949387E-03	3.87631059E-02	-2.87561417E-02
-38.5000000	2.55105319E-03	3.40603143E-02	-3.72954160E-02
-38.2500000	2.79075885E-03	2.75851320E-02	-4.50535156E-02
-38.0000000	3.04869516E-03	1.94496233E-02	-5.16759828E-02
-37.7500000	3.32612381E-03	9.83738527E-03	-5.68273664E-02
-37.5000000	3.62580363E-03	-9.99222975E-04	-6.02063537E-02
-37.2500000	3.95175675E-03	-1.27440859E-02	-6.15576580E-02
-37.0000000	4.30907169E-03	-2.50263419E-02	-6.06856942E-02
-36.7500000	4.70315013E-03	-3.74297015E-02	-5.74644916E-02
-36.5000000	5.13906637E-03	-4.95071150E-02	-5.18469997E-02
-36.2500000	5.62049542E-03	-6.07937984E-02	-4.38703634E-02
-36.0000000	6.14928734E-03	-7.08252192E-02	-3.36611867E-02
-35.7500000	6.72455505E-03	-7.91526288E-02	-2.14340165E-02
-35.5000000	7.34266499E-03	-8.53614360E-02	-7.48931477E-03
-35.2500000	7.99756218E-03	-8.90889466E-02	7.79240625E-03
-35.0000000	8.68107937E-03	-9.00388882E-02	2.39599366E-02
-34.7500000	9.38394945E-03	-8.79963562E-02	4.05042097E-02
-34.5000000	1.00970156E-02	-8.28404799E-02	5.68724088E-02
-34.2500000	1.08124306E-02	-7.45537356E-02	7.24856555E-02
-34.0000000	1.15246875E-02	-6.32275492E-02	8.67580846E-02
-33.7500000	1.22313322E-02	-4.90646362E-02	9.91160572E-02
-33.5000000	1.29336873E-02	-3.23789082E-02	0.109019697
-33.2500000	1.36364633E-02	-1.35887824E-02	0.115981929
-33.0000000	1.43475989E-02	6.79147011E-03	0.119588777
-32.7500000	1.50774391E-02	2.81644873E-02	0.119516529
-32.5000000	1.58378147E-02	4.98665795E-02	0.115547128
-32.2500000	1.66410562E-02	7.11870566E-02	0.107580006
-32.0000000	1.74995102E-02	9.13899839E-02	9.56419334E-02
-31.7500000	1.84248574E-02	0.109737672	7.98905417E-02
-31.5000000	1.94284152E-02	0.125515372	6.06160499E-02
-31.2500000	2.05216613E-02	0.138056397	3.82373072E-02
-31.0000000	2.17168089E-02	0.146765426	1.32935783E-02
-30.7500000	2.30280850E-02	0.151142314	-1.35678239E-02

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33.5000000	3.41337430E-03	-4.99988981E-02	-3.02239023E-02
33.7500000	3.21407593E-03	-4.24858741E-02	-3.75369973E-02
34.0000000	3.02455202E-03	-3.40108722E-02	-4.32181992E-02
34.2500000	2.84444378E-03	-2.49024481E-02	-4.71626110E-02
34.5000000	2.67341733E-03	-1.54955760E-02	-4.93285358E-02
34.7500000	2.51114182E-03	-6.11969689E-03	-4.97362167E-02
35.0000000	2.35727243E-03	2.91231833E-03	-4.84643243E-02
35.2500000	2.21148250E-03	1.13139851E-02	-4.56451140E-02
35.5000000	2.07344349E-03	1.88343842E-02	-4.14573215E-02
35.7500000	1.94283889E-03	2.52649616E-02	-3.61181460E-02
36.0000000	1.81934843E-03	3.04451883E-02	-2.98737157E-02
36.2500000	1.70266768E-03	3.42659019E-02	-2.29894668E-02
36.5000000	1.59250724E-03	3.66710722E-02	-1.57397483E-02
36.7500000	1.48856069E-03	3.76568809E-02	-8.39762110E-03
37.0000000	1.39055762E-03	3.72700393E-02	-1.22548896E-03
37.2500000	1.29822362E-03	3.56033407E-02	5.53405704E-03
37.5000000	1.21128664E-03	3.27901691E-02	1.16658220E-02
37.7500000	1.12949871E-03	2.89980359E-02	1.69886015E-02
38.0000000	1.05260930E-03	2.44205855E-02	2.13598758E-02
38.2500000	9.80380690E-04	1.92693155E-02	2.46794261E-02
38.5000000	9.12581163E-04	1.37650315E-02	2.68906131E-02
38.7500000	8.48987489E-04	8.12926143E-03	2.79803965E-02
39.0000000	7.89391284E-04	2.57591950E-03	2.79777758E-02
39.2500000	7.33579276E-04	-2.69599282E-03	2.69501563E-02
39.5000000	6.81357633E-04	-7.50931306E-03	2.49993559E-02
39.7500000	6.32527866E-04	-1.17140356E-02	2.22555455E-02
40.0000000	5.86911920E-04	-1.51915830E-02	1.88713465E-02
40.2500000	5.44333132E-04	-1.78577229E-02	1.50144883E-02
40.5000000	5.04613039E-04	-1.96636375E-02	1.08606806E-02
40.7500000	4.67591046E-04	-2.05962434E-02	6.58679148E-03
41.0000000	4.33109759E-04	-2.06766278E-02	2.36364175E-03
41.2500000	4.01019206E-04	-1.99573599E-02	-1.65013608E-03

41.5000000	3.71168629E-04	-1.85185429E-02	-5.31339552E-03
41.7500000	3.43424355E-04	-1.64636020E-02	-8.50729924E-03
42.0000000	3.17649014E-04	-1.39135094E-02	-1.11383684E-02
42.2500000	2.93717079E-04	-1.10013243E-02	-1.31410789E-02
42.5000000	2.71510566E-04	-7.86614418E-03	-1.44787552E-02
42.7500000	2.50909536E-04	-4.64736158E-03	-1.51430368E-02
43.0000000	2.31807731E-04	-1.47880171E-03	-1.51532469E-02
43.2500000	2.14101543E-04	1.51587930E-03	-1.45534761E-02
43.5000000	1.97694157E-04	4.22786828E-03	-1.34096714E-02
43.7500000	1.82495016E-04	6.56684255E-03	-1.18055744E-02
44.0000000	1.68417479E-04	8.46317131E-03	-9.83830355E-03
44.2500000	1.55378846E-04	9.86974686E-03	-7.61360303E-03
44.5000000	1.43307712E-04	1.07628535E-02	-5.24105877E-03
44.7500000	1.32132191E-04	1.11412527E-02	-2.82925414E-03
45.0000000	1.21787256E-04	1.10252183E-02	-4.81482100E-04
45.2500000	1.12214504E-04	1.04544619E-02	1.70843117E-03
45.5000000	1.03356506E-04	9.48500354E-03	3.65940086E-03
45.7500000	9.51617258E-05	8.18615966E-03	5.30551793E-03
46.0000000	8.75854676E-05	6.63661631E-03	6.59854384E-03
46.2500000	8.05809395E-05	4.92063584E-03	7.50788115E-03
46.5000000	7.41085241E-05	3.12396954E-03	8.02180450E-03
46.7500000	6.81304809E-05	1.33025553E-03	8.14621989E-03
47.0000000	6.26131805E-05	-3.82547092E-04	7.90359639E-03
47.2500000	5.75239283E-05	-1.94511819E-03	7.33078737E-03
47.5000000	5.28342462E-05	-3.29922186E-03	6.47683442E-03
47.7500000	4.85153796E-05	-4.39990917E-03	5.39964624E-03
48.0000000	4.45417172E-05	-5.21612167E-03	4.16338677E-03
48.2500000	4.08912201E-05	-5.73184993E-03	2.83498038E-03
48.5000000	3.75380732E-05	-5.94517495E-03	1.48086634E-03
48.7500000	3.44640721E-05	-5.86830452E-03	1.64543017E-04
49.0000000	3.16458754E-05	-5.52532263E-03	-1.05673494E-03
49.2500000	2.90670123E-05	-4.95122140E-03	-2.13363906E-03
49.5000000	2.67086161E-05	-4.18899208E-03	-3.02670826E-03
49.7500000	2.45537994E-05	-3.28746904E-03	-3.70760635E-03
50.0000000	2.25859767E-05	-2.29871925E-03	-4.15955111E-03
50.2500000	2.07900484E-05	-1.27538911E-03	-4.37760539E-03
50.5000000	1.91510662E-05	-2.68222910E-04	-4.36796527E-03
50.7500000	1.76562789E-05	6.75930351E-04	-4.14721575E-03
51.0000000	1.62920969E-05	1.51642074E-03	-3.74066341E-03
51.2500000	1.50459600E-05	2.22012261E-03	-3.18072550E-03
51.5000000	1.39078247E-05	2.76246527E-03	-2.50531663E-03
51.7500000	1.28667216E-05	3.12830973E-03	-1.75510696E-03
52.0000000	1.19132083E-05	3.31187923E-03	-9.71938483E-04
52.2500000	1.10383889E-05	3.31659243E-03	-1.96480338E-04
52.5000000	1.02348858E-05	3.15441191E-03	5.33452840E-04
52.7500000	9.49493551E-06	2.84453714E-03	1.18471228E-03
53.0000000	8.81298001E-06	2.41236528E-03	1.73016579E-03
53.2500000	8.18295757E-06	1.88759482E-03	2.14940519E-03

53.5000000	7.60058947E-06	1.30286685E-03	2.42963526E-03
53.7500000	7.06125365E-06	6.91540656E-04	2.56574061E-03
54.0000000	6.56130624E-06	8.65185284E-05	2.56004324E-03
54.2500000	6.09771769E-06	-4.81785974E-04	2.42190016E-03
54.5000000	5.66807194E-06	-9.86337429E-04	2.16684351E-03
54.7500000	5.26988970E-06	-1.40527904E-03	1.81523571E-03
55.0000000	4.90160483E-06	-1.72213721E-03	1.39134773E-03
55.2500000	4.56107364E-06	-1.92664238E-03	9.21478495E-04
55.5000000	4.24703057E-06	-2.01481208E-03	4.33085253E-04
55.7500000	3.95831739E-06	-1.98899349E-03	-4.71407257E-05
56.0000000	3.69336885E-06	-1.85712241E-03	-4.94433974E-04
56.2500000	3.45115473E-06	-1.63231161E-03	-8.86968686E-04
56.5000000	3.23069253E-06	-1.33176195E-03	-1.20710512E-03
56.7500000	3.02998728E-06	-9.75543051E-04	-1.44163205E-03
57.0000000	2.84875432E-06	-5.86027687E-04	-1.58282206E-03
57.2500000	2.68523104E-06	-1.85560435E-04	-1.62812718E-03
57.5000000	2.53796611E-06	2.03555363E-04	-1.58004160E-03
57.7500000	2.40564714E-06	5.61075518E-04	-1.44597411E-03
58.0000000	2.28684030E-06	8.69149750E-04	-1.23750523E-03
58.2500000	2.18004379E-06	1.11352035E-03	-9.69595916E-04
58.5000000	2.08418101E-06	1.28415588E-03	-6.59639831E-04
58.7500000	1.99751253E-06	1.37509475E-03	-3.26537789E-04
59.0000000	1.91825552E-06	1.38496910E-03	1.07686501E-05
59.2500000	1.84583598E-06	1.31707161E-03	3.33404052E-04
59.5000000	1.77886386E-06	1.17846020E-03	6.24576176E-04
59.7500000	1.71609474E-06	9.79659846E-04	8.69690382E-04
60.0000000	1.65675533E-06	7.34195753E-04	1.05721899E-03
60.2500000	1.60008653E-06	4.57279501E-04	1.17939897E-03
60.5000000	1.54523082E-06	1.65317382E-04	1.23203127E-03
60.7500000	1.49180823E-06	-1.25039660E-04	1.21497875E-03
61.0000000	1.43933858E-06	-3.97983909E-04	1.13178953E-03
61.2500000	1.38795008E-06	-6.39222562E-04	9.89618362E-04
61.5000000	1.33744049E-06	-8.36748630E-04	7.98305788E-04
61.7500000	1.28791748E-06	-9.81242862E-04	5.70157717E-04
62.0000000	1.23950031E-06	-1.06667459E-03	3.18913371E-04
62.2500000	1.19221420E-06	-1.09028269E-03	5.91419230E-05
62.5000000	1.14660247E-06	-1.05294399E-03	-1.94708467E-04
62.7500000	1.10284736E-06	-9.58667370E-04	-4.28724015E-04
63.0000000	1.06149491E-06	-8.14411498E-04	-6.31053816E-04
63.2500000	1.02220065E-06	-6.29625283E-04	-7.91057828E-04
63.5000000	9.86017994E-07	-4.15819057E-04	-9.01727472E-04
63.7500000	9.52671201E-07	-1.85376150E-04	-9.58283315E-04
64.0000000	9.22579659E-07	4.84978373E-05	-9.59284953E-04
64.2500000	8.95645258E-07	2.72924779E-04	-9.06177331E-04
64.5000000	8.71712871E-07	4.75869922E-04	-8.03281204E-04
64.7500000	8.50890217E-07	6.46751549E-04	-6.57725381E-04
65.0000000	8.32600733E-07	7.77036184E-04	-4.78346657E-04
65.2500000	8.17497892E-07	8.60961154E-04	-2.76122708E-04

65.5000000	8.04306239E-07	8.94653786E-04	-6.24569948E-05
65.7500000	7.93271283E-07	8.77814833E-04	1.50706299E-04
66.0000000	7.83613416E-07	8.12345650E-04	3.51721421E-04
66.2500000	7.75083890E-07	7.03064492E-04	5.29890764E-04
66.5000000	7.67190897E-07	5.56849758E-04	6.76098512E-04
66.7500000	7.59789145E-07	3.82554834E-04	7.83224707E-04
67.0000000	7.52100675E-07	1.90005696E-04	8.46166979E-04
67.2500000	7.44020213E-07	-9.82946949E-06	8.62510060E-04
67.5000000	7.35217043E-07	-2.06034339E-04	8.32326186E-04
67.7500000	7.25578332E-07	-3.87957814E-04	7.58331793E-04
68.0000000	7.14657517E-07	-5.46270981E-04	6.45170920E-04
68.2500000	7.02632406E-07	-6.72883703E-04	4.99859860E-04
68.5000000	6.89391982E-07	-7.61481584E-04	3.30964860E-04
68.7500000	6.75159754E-07	-8.08260520E-04	1.47900952E-04
69.0000000	6.59955504E-07	-8.11426551E-04	-3.92733491E-05
69.2500000	6.44039119E-07	-7.71705643E-04	-2.20248709E-04
69.5000000	6.27499276E-07	-6.91883382E-04	-3.85741674E-04
69.7500000	6.10634459E-07	-5.77153929E-04	-5.26809075E-04
70.0000000	5.93891286E-07	-4.34259069E-04	-6.36639888E-04
70.2500000	5.77401067E-07	-2.71414989E-04	-7.09742890E-04
70.5000000	5.61463480E-07	-9.77483578E-05	-7.42905599E-04
70.7500000	5.46513490E-07	7.73743959E-05	-7.35205249E-04
71.0000000	5.32602030E-07	2.44425057E-04	-6.87647029E-04
71.2500000	5.20218748E-07	3.94809089E-04	-6.03609544E-04
71.5000000	5.09047084E-07	5.20398433E-04	-4.88090678E-04
71.7500000	4.99472378E-07	6.15238445E-04	-3.47784488E-04
72.0000000	4.91516062E-07	6.74632378E-04	-1.90754363E-04
72.2500000	4.85039209E-07	6.95979863E-04	-2.55195191E-05
72.5000000	4.80055860E-07	6.78784680E-04	1.38950418E-04
72.7500000	4.76357087E-07	6.24515756E-04	2.93831865E-04
73.0000000	4.73656655E-07	5.36622712E-04	4.30920743E-04
73.2500000	4.71931088E-07	4.20409604E-04	5.43311005E-04
73.5000000	4.70956223E-07	2.82444933E-04	6.25444693E-04
73.7500000	4.70227178E-07	1.30374683E-04	6.73223287E-04
74.0000000	4.69496285E-07	-2.76037026E-05	6.84641767E-04
74.2500000	4.68805212E-07	-1.83052209E-04	6.59770507E-04
74.5000000	4.67654587E-07	-3.27507558E-04	6.00327738E-04
74.7500000	4.65807375E-07	-4.53743269E-04	5.09827863E-04
75.0000000	4.63113281E-07	-5.55134378E-04	3.93623079E-04

Perhaps it's better to just see things graphically. gnuplot is a very good, universally available plotting program, and with just a few keystrokes we can generate good-looking graphs.

```
In [7]: %%file Vo.dat
        -75      0
        -1       0
        -1       1
```



```
1      1
1      0
75     0
```

Writing Vo.dat

```
In [8]: %%bash
gnuplot --persist
plot 'Vo.dat' with lines
```

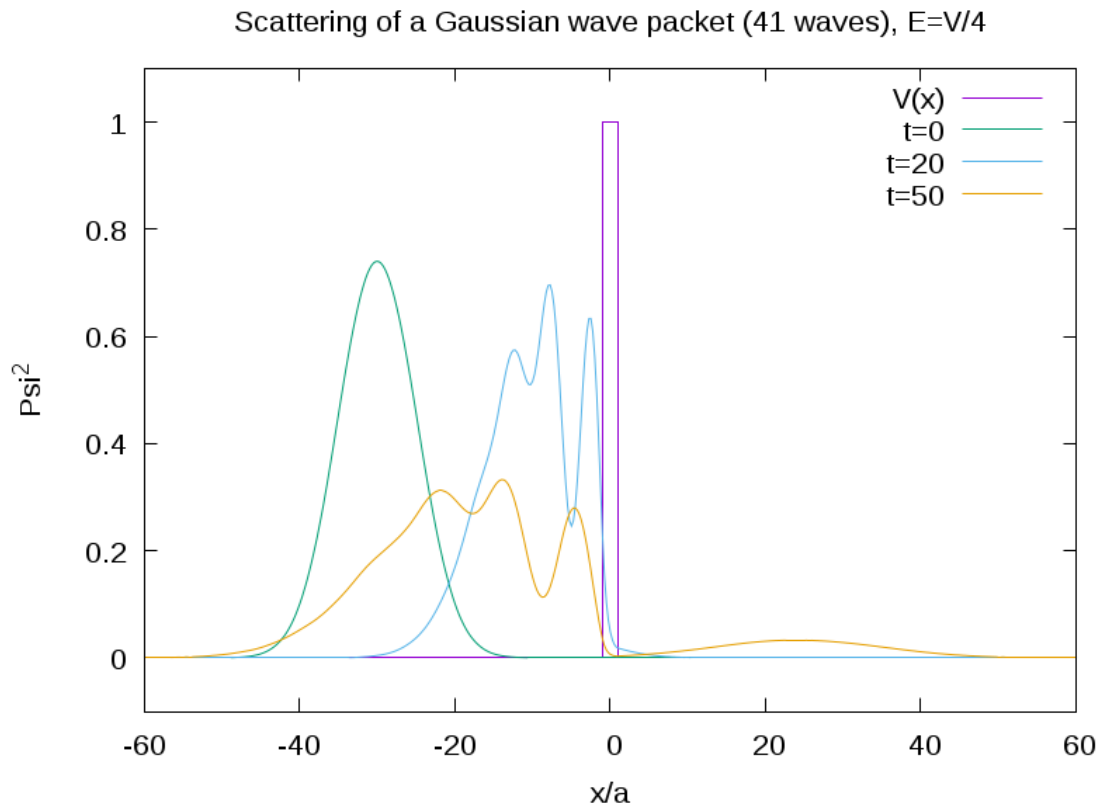
```
In [9]: %%bash
gnuplot --persist
set style data line
plot [-80:80] [-0.1:1.1] 'Vo.dat' title "energy barrier V", '<./packet 40' using 1:4 titl
```

Another way of using gnuplot is to load it right into the Jupyter notebook itself.

```
In [10]: %load_ext gnuplot_kernel
```

```
In [11]: %gnuplot inline pngcairo font "Arial,16" size 800,600
```

```
In [23]: %%gnuplot
set style data line
set yrange [-0.1:1.1]
set xrange [-60:60]
set xlabel "x/a"
set ylabel "Psi^2"
set title "Scattering of a Gaussian wave packet (41 waves), E=V/4"
plot \
  'Vo.dat' t "V(x)", \
  '<./packet 0' title "t=0", \
  '<./packet 20' title "t=20", \
  '<./packet 50' title "t=50"
```



```

set style data line
set yrange [-0.1:1.1]
set xrange [-60:60]
set xlabel "x/a"
set ylabel "Psi^2"
set title "Scattering of a Gaussian wave packet (41 waves), E=V/4"
set output '/tmp/gnuplot-inline-1517961252.4544995.585617581060.png'
plot 'Vo.dat' t "V(x)", '<./packet 0' title "t=0", '<./packet 20' title "t=20", '<./pa
gnuplot>
gnuplot>
unset output

```

Now we are ready to add the same computational functionality to the skeleton C program we introduced last time.

We already know how to compile (using a Makefile) and start a program, and how to pass command-line parameters to it at runtime.

In [13]: `%%file Makefile`

```
OBJ = packet.o
```

```

# these are pre-defined, but we can also change the default behaviour, if we have multi
CC = cc
#CC = icc
CFLAGS = -O -DVERSION="\`date +%Y-%b-%d-%H:%M'\`"
LIBS = -lm

# special abbreviations: $@ is the file to be made; $? is the changed dependent(s).

packet: $(OBJ)
        $(CC) $(CFLAGS) -o $@ $(OBJ) $(LIBS)

# this is the default implicit rule to convert xxx.c into xxx.o
.c.o:
        $(CC) $(CFLAGS) -c $<

clean:
        rm -f packet *.o *~ core

```

Writing Makefile

```

In [14]: %%file packet.c
/*
 * packet.c
 * packet - generate a Gaussian wavepacket impacting on an energy barrier.
 *
 * Completed: January.2018 (c) E.Sternin
 * Revisions:
 *
 */

#ifndef VERSION /* date-derived in Makefile */
#define VERSION "2018.01" /* default, that's when we first wrote the program */
#endif

#include <stdarg.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <ctype.h>
#include <unistd.h>
#include <sys/types.h>
#include <sys/stat.h>
#include <fcntl.h>
#include <math.h>
#include <complex.h>

```

```

#define MAX_STR 256
#define NPTS    601      /* these cannot be changed via command-line switches */
#define X_MIN   -75.0
#define X_MAX   75.0
#define NS      4       /* +/- NS * sigma is the extent of the Gaussian packet we call

/* Global variables */

static char whoami[MAX_STR] ;      /* argv[0] will end up here */
static int  verbosity;             /* Show detailed information */
static char options[] = "Vvhn:t:U:p:s:x:"; /* command-line options, : means takes a value
static char help_msg[] = "\
%s [<options>]\n\
\t-V      report version information\n\
\t-v      increase verbosity, may combine several\n\
\t-n #    number of waves making up the packet\n\
\t-t #    time since the beginning\n\
\t-U #    U[=16] height of the barrier U(x), in epsilon\n\
\t-p #    p0[=0.5] is the mean momentum of the packet\n\
\t-s #    s[=0.1] is the width of the packet in p-space\n\
\t-x #    x0[=-25] is the initial position of the packet\n\
\t-h      help message\n\
\n\
e.g.\tppacket -v -n 20 -t 20 -p 0.5 -s 0.1\n"
;

/*****service routines*****/

void __attribute__((noreturn)) die(char *msg, ...) {
    va_list args;
    va_start(args, msg);
    vfprintf(stderr, msg, args);
    fputc('\n', stderr);
    exit(1);
}

/***** main *****/
int main(int argc, char **argv) {
    int    i,j,n;
    double t,U,p0,s,x0,dx,x[NPTS],A0,p_step,p_now,E;
    double complex Psi[NPTS];

    double Pi = 2.*acos(0.);

/*
 * default values, may get changed by the command-line options
 */
    verbosity = 0; /* 0 = quiet by default, 1 = info, 2 = debug */

```

```

n = 20;          /* default to 41=(2*n+1) waves in the packet */
p0 = 0.5;       /* default to 0.5 in p-space */
s = 0.1;        /* keep to less than 1/4 of p0, so that (p0+/-4s) > 0, all */
                /* constituent waves travel to the right initially */
U = 1;          /* barrier height, in epsilon */
x0 = -25;       /* initial position of the packet */
t = 0;

strncpy(whoami, argv[0], MAX_STR);

while ((i = getopt(argc, argv, options)) != -1)
  switch (i) {
    case 'V':
      printf(" %s: version %s\n",whoami,VERSION);
      break;
    case 'v':
      verbosity++;
      if (verbosity > 1) printf(" %s: verbosity level set to %d\n",whoami,verbosity);
      break;
    case 'h':
      die(help_msg,whoami);
      break;
    case 'n':
      if ( ((n = atoi(optarg)) > 10000) || n < 10 )
        die(" %s: -n %d is not a valid number of points (10..10000)\n",whoami,n);
      if (verbosity > 1) printf(" %s: Number of points = %d\n",whoami,n);
      break;
    case 't':
      if ( ((t = atof(optarg)) < 0) )
        die(" %s: -t %d is not a valid time\n",whoami,t);
      if (verbosity > 1) printf(" %s: time = %f\n",whoami,t);
      break;
    case 'U':
      U = atof(optarg);
      if (verbosity > 1) printf(" %s: barrier height is = %f epsilon\n",whoami,U);
      break;
    case 'p':
      p0 = atof(optarg);
      if (verbosity > 1) printf(" %s: mean momentum of packet is p0 = %f\n",whoami,p0);
      break;
    case 's':
      if ( (s = atof(optarg)) < 1e-2 )
        die(" %s: -s %f is not a valid packet width, >= 1e-2\n",whoami,s);
      if (verbosity > 1) printf(" %s: width of packet, s = %f\n",whoami,s);
      break;
    case 'x':
      if ( ((x0 = atof(optarg)) < X_MIN) || x0 > 0 )
        die(" %s: -x %f is not a valid packet position, %d..0\n",whoami,x0,X_MIN);
  }

```

```

        if (verbosity > 1) printf(" %s: initial position of packet, x0 = %f\n",whoami,
            break;
    default:
        if (verbosity > 0) die(" try %s -h\n",whoami);          /* otherwise, die quietly
        return 0;
    }

/*
* when we get here, we parsed all user input, and are ready to calculate things
*/

if ((p0-NS*s) <= 0) /* is the smallest value of p still positive ? */
    die(" %s: some waves in the packet p=%f+/-%d*%f are not travelling to the right at

if ((p0+NS*s) >= sqrt(U)) /* is the largest value of p still below U of the barrier ?
    die(" %s: some waves in the packet p=%f+/-%d*%f have energy >= U=%f\n",whoami,p0,N

dx = (X_MAX-X_MIN)/(double)(NPTS-1);
for (j=0; j < NPTS; j++) {
    x[j]=X_MIN + j*dx;
    Psi[j] = (double complex)0.0; /* start with a blank Psi(x) */
}

A0 = 1./sqrt( sqrt(2.*Pi) * s ) /(double)(2*n+1);
p_step = NS*s/(double)n; /* calculate over p0 +/- NS*sigma_p */

double complex A,k1,k2,ce4,C1,b,c,d,f;

/* add (complex) waves to Psi[j]; each wave is calculated at x[j]*/
for (i=-n; i < n; i++) {
    p_now = p0 + (double)i * p_step;
    E = p_now*p_now;
    A = A0*exp(-pow((p_now-p0)/(2*s),2))*cexp(-I*(p_now*x0 + E*t));

    k1 = csqrt((double complex)(E));
    k2 = csqrt((double complex)(E-U));
    ce4 = cexp(4*I*k2);
    C1 = -2*k1*k2-k1*k1-2*k1*k2*ce4+ce4*(k1*k1+k2*k2)-k2*k2;

    b = (k1*k1-k2*k2)/ C1 *(cexp(2*I*(2*k2-k1))-cexp(-2*I*k1));
    c = -2*k1*(k2+k1)/ C1 *cexp(I*(k2-k1));
    d = (-2*k2+2*k1)*k1/ C1 *cexp(I*(-k1+3*k2));
    f = -4*k1*k2/ C1 *cexp(2*I*(k2-k1));

    for (j=0; j < NPTS; j++) {
        if (x[j] < -1.) { /* to the left of the barrier, x < -1 */
            Psi[j] += A*( cexp(I*k1*x[j]) + b*cexp(-I*k1*x[j]) );
        }
    }
}

```

```

        else if (x[j] > 1.) {      /* to the right of the barrier, x > 1 */
            Psi[j] += A*f*cexp(I*k1*x[j]);
        }
        else {                    /* inside the barrier, -1 < x < 1 */
            Psi[j] += A*( c*cexp(I*k2*x[j]) + d*cexp(-I*k2*x[j]) );
        }
    }
}

/* output the total Psi as is, without normalization */
for (j=0; j < NPTS; j++) {
    if (verbosity > 0) printf("\t%f\t%f\t%f\t%f\n",x[j],cabs(Psi[j]),creal(Psi[j]),cimag(Psi[j]));
}

return 0;
}

```

Writing packet.c

In [24]: %%bash

```

make clean; make
./packet -x -40 -t 0

```

rm -f packet \*.o \*~ core

cc -O -DVERSION=""`date +%Y-%b-%d-%H:%M`\`" -c packet.c

cc -O -DVERSION=""`date +%Y-%b-%d-%H:%M`\`" -o packet packet.o -lm

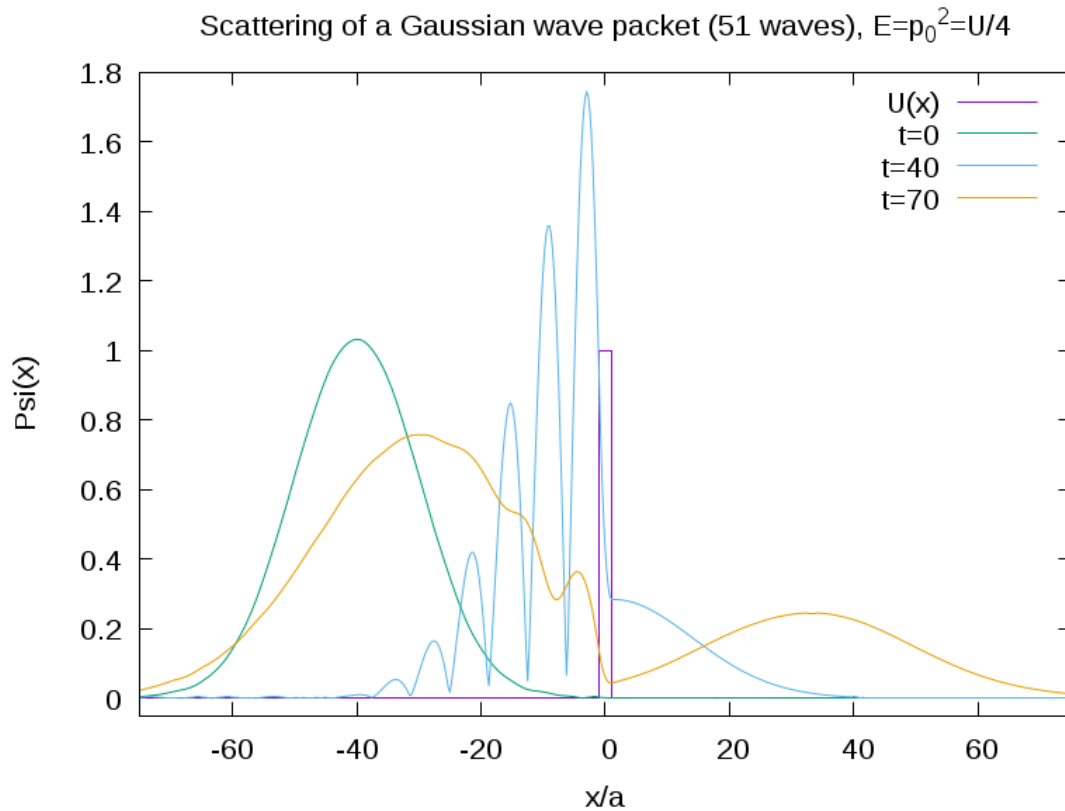
The homework for today was to convert the evolution expressions into dimensionless form, ready to be implemented in code. Today's session is to try to do just that.

In [27]: %%gnuplot

```

set style data line
set xrange [-75:75]
set yrange [-0.05:1.8]
set xlabel "x/a"
set ylabel "Psi(x)"
set title "Scattering of a Gaussian wave packet (51 waves), E=p_0^2=U/4"
plot \
    'Vo.dat' t "U(x)",\
    '<./packet -v -n 25 -x -40 -p .5 -s 0.07 -t 0' title "t=0",\
    '<./packet -v -n 25 -x -40 -p .5 -s 0.07 -t 40' title "t=40",\
    '<./packet -v -n 25 -x -40 -p .5 -s 0.07 -t 70' title "t=70"

```



```

set style data line
set xrange [-75:75]
set yrange [-0.05:1.8]
set xlabel "x/a"
set ylabel "Psi(x)"
set title "Scattering of a Gaussian wave packet (51 waves),  $E=p_0^2=U/4$ "
set output '/tmp/gnuplot-inline-1517961329.5172246.5513159542.png'
plot 'Vo.dat' t "U(x)", '<./packet -v -n 25 -x -40 -p .5 -s 0.07 -t 0' title "t=0", '<./p
gnuplot>
gnuplot>
unset output

```

## 1.2 Notes on Fortran-to-C conversion

Fortran:

C:

Fortran:

C:

Fortran:

C: