Novel computational approaches for nuclear reactions

Kazuhiro Yabana

Center for Computational Sciences and Institute of Physics
Univ. of Tsukuba

Recent progresses in computational reaction theories:

Scattering calculation without scattering boundary condition

Time-dependent treatment for time-independent problem

Why? How?

Nuclear direct reactions: curiosity in dynamics, tool for spectroscopy

Elastic scattering

optical potential: real-part = nuclear mean-field
imaginary-part = mean-free path in nuclear matter

Inelastic scattering

Excited states, response of nuclei to external field

Rearrangement reaction (transfer, pickup,...)

Spectroscopic properties of excited states

Fusion reaction

large part of the cross section at low energy, multidimensional tunneling dynamics

Recent progress: secondary beam experiments with radioactive nuclei

Structure and reactions of weakly-bound system

halo structure, resonances, breakup reactions,...

Reactions of astrophysical interest

Low energy fusion cross section, inverse method with Coulomb breakup reaction

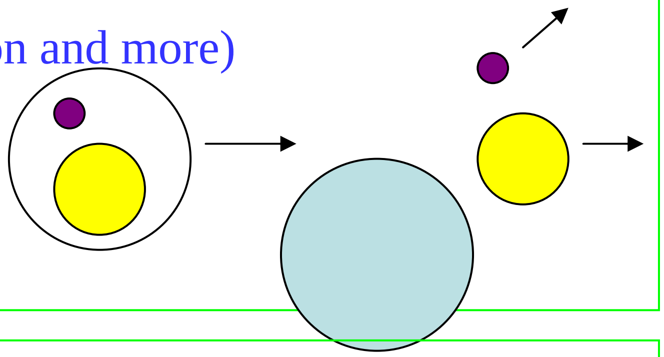
⇒ Demand to develop reaction theories for reactions of weakly-bound nuclei, breakup reactions, coupling to the continuum, ...

Orthodox nuclear reaction theories

Optical model (potential scattering, imaginary potential to describe nuclear excitations)
Distorted wave Born approx.
Coupled channels (A few nuclear excitations treated explicitly, potential scattering for nucleus-nucleus relative motion)

Developments for more than 2-body systems (3-body reaction and more)

Coupled Discretized Continuum Channels method
Faddeev theory
Glauber, eikonal theories for high energy reactions



New trends utilizing computational progresses, mainly developed in atomic and molecular collision theories

Efficient computational methods developed for linear algebraic problem with large dimension

$$\mathbf{A}\vec{x} = \vec{b} \qquad \mathbf{A}\vec{x} = a\vec{x} \qquad \frac{d\vec{y}(t)}{dt} = \mathbf{A}\vec{y}(t)$$

Make the best use of them for reaction problems

Absorbing boundary instead of scattering (outgoing) boundary
Real-time propagation for static problem

they avoid the standard procedure solving the differential equation from origin.

Purpose of my lecture

In the 1st lecture, I will introduce

Absorbing boundary instead of scattering (outgoing) boundary

Real-time propagation method for static problem

taking a simple one-dimensional potential scattering problems

1.scattering, 2.resonance, 3.dipole response, 4.fusion

Scattering calculation without outgoing boundary condition

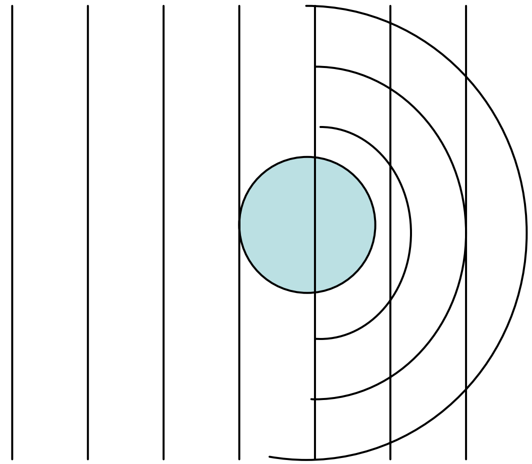
Time-dependent treatment for static problem

In the 2nd lecture, I will show some illustrative examples showing usefulness of the absorbing boundary and real-time wave-packet method

1. Low energy reactions of halo nuclei (3-body reaction)
2. E1 response of neutron-rich nuclei (3D time-dependent mean-field dynamics)
3. Applications to other field

Let's start with elements of scattering theory

Potential scattering in quantum mechanics



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\phi(\vec{r}) = E\phi(\vec{r})$$

$$\phi(\vec{r}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\Omega)\frac{e^{ikr}}{r}$$

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2$$

For spherically symmetric potential, partial wave expansion

$$\phi(\vec{r}) = \sum_l \frac{u_l(r)}{r} P_l(\cos\theta)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right]u_l(r) = E u_l(r)$$

$$u_l(0) = 0, \qquad u_l(r) \underset{r\to\infty}{\longrightarrow} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

solve differential equation from origin

Scattering amplitude is expressed with phase shift δ_l

Integral equation for scattering: Lipmann-Schwinger equation

$$\phi(\vec{r}) = e^{ikz} + \frac{1}{E+i\varepsilon-T}V(r)\phi(\vec{r}) \qquad T = -\frac{\hbar^2}{2m}\nabla^2$$

$$= e^{ikz} + \frac{1}{E+i\varepsilon-H}V(r)e^{ikz} \qquad H = T+V$$

$$\equiv \chi(\vec{r}) \underset{r\to\infty}{\longrightarrow} f(\Omega)\frac{e^{ikr}}{r}$$

Scattering amplitude obtainable
from the wave function of interaction region

$$f(\Omega) = -\frac{m}{2\pi\hbar^2}\int d\vec{r}\,' e^{-i\vec{k}_\Omega \vec{r}} V(r)\phi(\vec{r})$$

$$\frac{1}{E+i\varepsilon-T}V(r)\phi(\vec{r}) \underset{r\to\infty}{\longrightarrow} f(\Omega)\frac{e^{ikr}}{r}$$

$$\langle\vec{r}|\frac{1}{E+i\varepsilon-T}|\vec{r}\,'\rangle = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} \underset{r\to\infty}{\longrightarrow} -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}e^{-i\vec{k}_\Omega\cdot\vec{r}\,'}$$

Absorbing boundary condition: $\frac{1}{E+i\varepsilon-T} \qquad \frac{1}{E+i\varepsilon-H}$

$i\varepsilon$: infinitesimal imaginary number, specifying outgoing boundary condition

⇓

$i\varepsilon(r)$: absorb waves emitted outside

How justified?

Time-dependent treatment of scattering

$$\phi(\vec{r}) = e^{ikz} + \frac{1}{E+i\varepsilon-T}V(r)\phi(\vec{r}) = e^{ikz} + \frac{1}{E+i\varepsilon-H}V(r)e^{ikz}$$

For scattering wave $\chi(\vec{r}) = \frac{1}{E+i\varepsilon-H}V(r)e^{ikz} \xrightarrow[r\to\infty]{} f(\Omega)\frac{e^{ikr}}{r}$

Employing integral expression of Green function,

$$\frac{1}{i\hbar}\int_0^\infty dt e^{i(E+i\varepsilon-H)t/\hbar} = \left.\frac{-e^{i(E+i\varepsilon-H)t/\hbar}}{E+i\varepsilon-H}\right|_0^\infty = \frac{1}{E+i\varepsilon-H}$$

the scattering wave $\chi(\vec{r})$ is expressed as

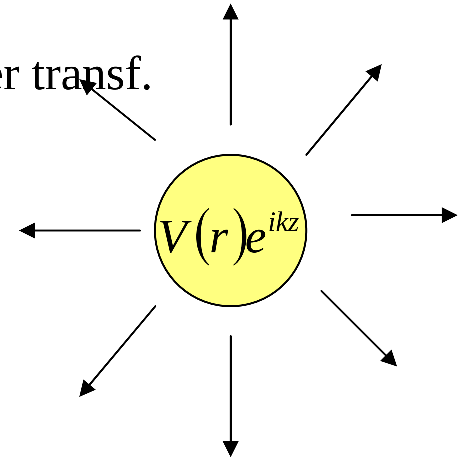
$$\chi(\vec{r}) = \frac{1}{E+i\varepsilon-H}V(r)e^{ikz} = \frac{1}{i\hbar}\int_0^\infty dt\, e^{i(E+i\varepsilon)t/\hbar}\boxed{e^{-iHt/\hbar}V(r)e^{ikz}} \Rightarrow \psi(\vec{r},t)$$

then, the scattering wave can be obtained by
solving the time-dependent Schroedinger equation + Fourier transf.

$$\psi(\vec{r},t=0) = V(r)e^{ikz} \quad \text{(Initial wave packet)}$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t) \quad \text{(Propagation)}$$

$$\chi(\vec{r}) = \frac{1}{i\hbar}\int_0^\infty dt\, e^{iEt/\hbar}\psi(\vec{r},t) \quad \text{(Fourier transform)}$$



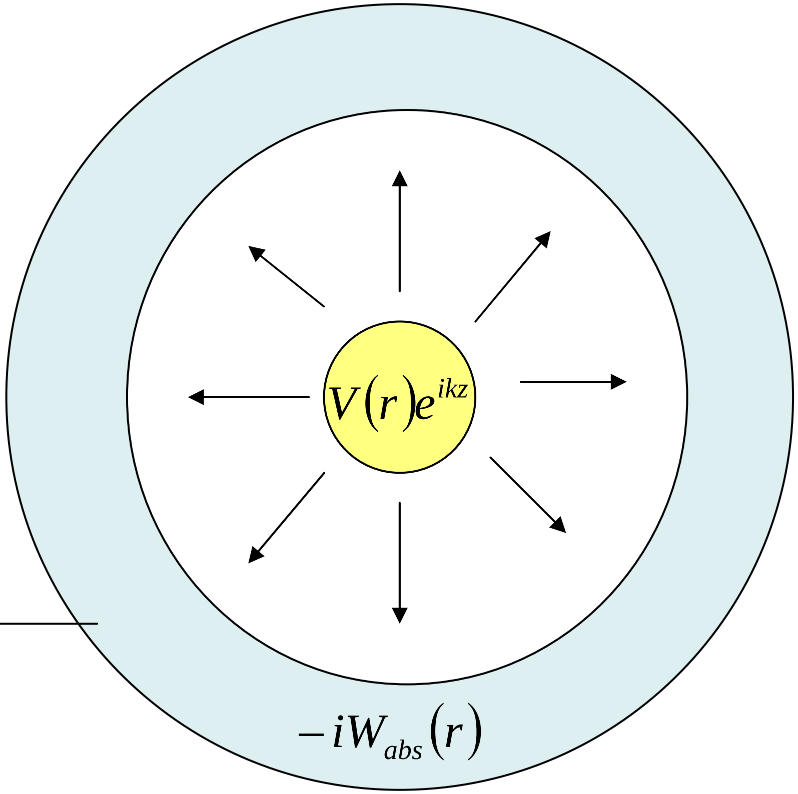
Introducing absorbing potential

$$\psi(\vec{r}, t=0) = V(r)e^{ikz}$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

One cannot solve in infinite spatial region.
approximate outgoing boundary condition
⇨ absorbing boundary condition

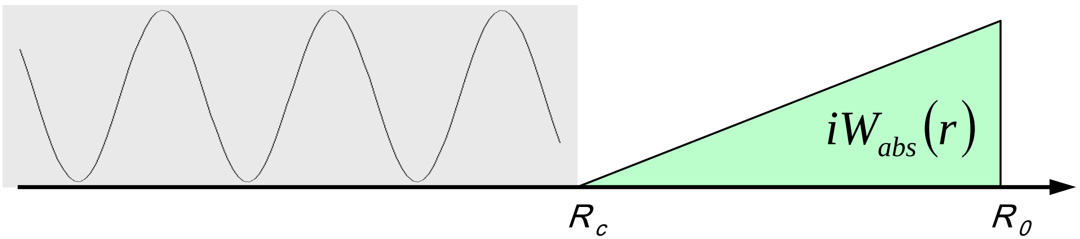
$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = (H - iW_{abs}(r))\psi(\vec{r},t)$$



Is it possible to absorb the emitted wave completely?
No, we can at most do as good as possible.

Example: linear absorber

$$-iW_{abs}(r) = \begin{cases} 0 & \text{for } r < R_c \\ -iW_0(r - R_c)/(R_0 - R_c) & \text{for } r > R_c \end{cases}$$



criteria for good absorber: No reflection at $r = R_c$, Complete absorption at $r = R_0$

$$7\frac{E^{1/2}}{(R_0 - R_c)(8m)^{1/2}} < W_0 < \frac{1}{10}(R_0 - R_c)(8m)^{1/2}E^{3/2}$$

Summary of time-dependent procedure

$$\psi(\vec{r}, t=0) = V(r) e^{ikz}$$

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[H - iW_{abs}(r) \right] \psi(\vec{r}, t)$$

$$\chi(\vec{r}) = \frac{1}{i\hbar} \int_0^\infty dt\, e^{iEt/\hbar} \psi(\vec{r}, t)$$

$$\phi(\vec{r}) = e^{ikz} + \chi(\vec{r}) \to e^{ikz} + f(\Omega) \frac{e^{ikr}}{r}$$

$\mathbf{A}\vec{x} = \vec{b}$ $\quad$ $\mathbf{A}\vec{x} = a\vec{x}$ $\quad$ $\frac{d\vec{y}(t)}{dt} = \mathbf{A}\vec{y}(t)$

Returning back to the differential equation for scattering wave, absorbing potential can be introduced in static form.

$$\chi(\vec{r}) = \frac{1}{E + i\varepsilon - H} V(r) e^{ikz} \quad \underset{r\to\infty}{\to} f(\Omega) \frac{e^{ikr}}{r}$$

$$\Updownarrow$$

$$\left[E - \left(H - iW_{abs}(r) \right) \right] \chi(\vec{r}) = V(r) e^{ikz} \qquad \chi(\vec{r}) \underset{r\to\infty}{\to} 0$$

$\mathbf{A}\vec{x} = \vec{b}$ $\quad$ $\mathbf{A}\vec{x} = a\vec{x}$ $\quad$ $\frac{d\vec{y}(t)}{dt} = \mathbf{A}\vec{y}(t)$

Scattering wave can be calculated by solving
Schroedinger-like equation with source term and with vanishing boundary condition

Example 1: Potential scattering

Time-dependent Schroedinger equation with absorbing potential

$$\psi(\vec{r},t) = \sum_l \frac{v_l(r,t)}{r} P_l(\cos\theta)$$

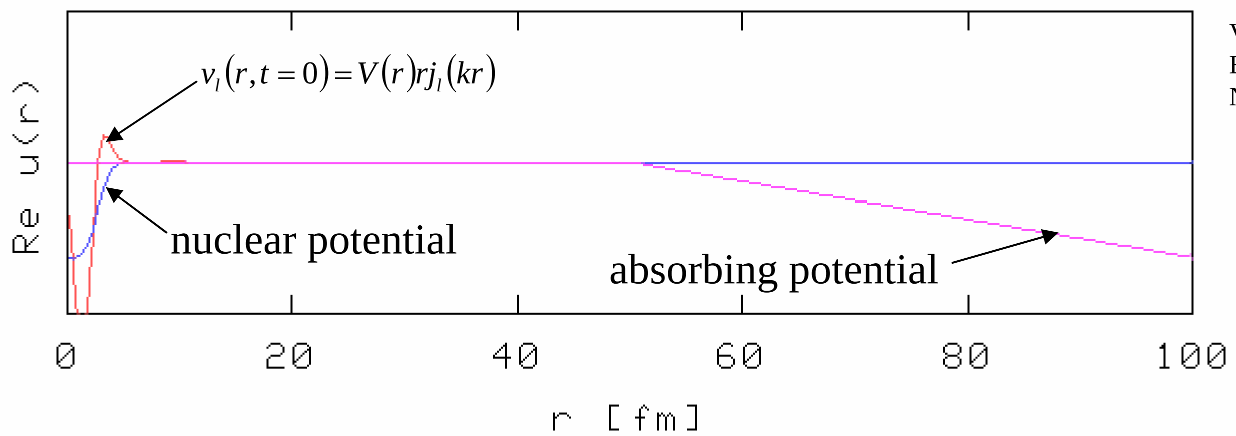
$$i\hbar \frac{\partial}{\partial t} v_l(r,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r) \right] v_l(r,t)$$

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

$$\psi(\vec{r},t=0) = V(r) e^{ikz}$$

$$v_l(r,t=0) = V(r) r j_l(kr)$$

l=0



V0=-51.1, R=2.691, a=0.52
Ecm=30
Nr=400, dr=0.25, Nt=12000, dt=0.0005

$$V(r) r j_l(kr) = \sum_i c_i y_i(r) + \int dE c(E) y_E(r)$$

3 ways to obtain scattering wave valid inside absorbing potential

from Fourier transformation (extract on-shell component with energy E)

$$w_l(r) = \frac{1}{i\hbar}\int_0^\infty dt e^{iEt/\hbar} v_l(r,t)$$

or directly solving the equation with source term

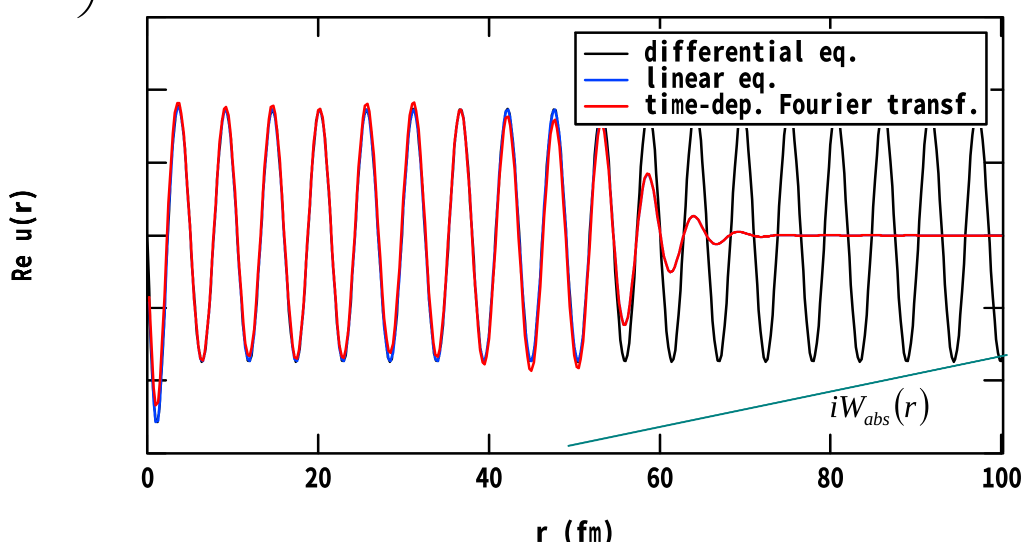
$$\left[E - \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r)\right)\right] w_l(r) = V(r) r j_l(kr)$$

or ordinary way (solving radial Schroedinger equation from origin)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right] u_l(r) = E u_l(r)$$

$$u_l(0) = 0, \qquad u_l(r) \underset{r\to\infty}{\to} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

Of course, different methods give the same wave function inside absorbing potential. (r < 50fm)



Computational aspects: Hamiltonian operation is a matrix multiplication in the finite difference

finite difference for space grid (radial coordinate): $r_i = i \cdot \Delta r \qquad f_i = f(r_i)$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r) \right] f(r) \to -\frac{\hbar^2}{2m}\frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta r^2} + [V_i + iW_i] f_i$$

(in practice, discrete variables representation is used)

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then, Hamiltonian operation is a matrix multiplication

$$Hu(r) \to \sum_j H_{ij} u_j$$

$$H_{ij} = -\frac{\hbar^2}{2m\Delta r^2}\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} + \begin{bmatrix} V(r_1) & 0 & 0 & 0 \\ 0 & V(r_2) & 0 & 0 \\ 0 & 0 & V(r_3) & 0 \\ 0 & 0 & 0 & V(r_4) \end{bmatrix}$$

Schroedinger-like equation with source term → linear algebraic equation

$$\left[E - \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r) \right) \right] w_l(r) = V(r) r j_l(kr)$$

$$\Rightarrow \sum_j \left(E\delta_{ij} - H_{ij} \right) w_j = V_i r_i j_l(kr_i)$$

Time evolution: Taylor expansion method works efficiently → Matrix multiplication to a vector

$$i\hbar\frac{\partial}{\partial t} u(r,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r) \right] u(r,t) \quad \Rightarrow i\hbar\frac{d}{dt} u_i(t) = \sum_j H_{ij} u_j(t)$$

$$\vec{u}(t+\Delta t) = \exp[-i\mathbf{H}\Delta t/\hbar]\vec{u}(t) \cong \sum_{k=0}^{k_{\max}} \frac{1}{k!}\left(\frac{-i\Delta t}{\hbar} \right)^k \mathbf{H}^k \vec{u}(t) \qquad k_{\max} = 3, 4$$

Fortran90 code: time evolution

```
      implicit none
      real(8),parameter :: PI=3.141592653589793d0
      complex(8),parameter :: zI=(0.d0,1.d0)
      real(8),parameter :: PM=931.494320d0,HC=197.3270530d0
      real(8),parameter :: V0=-51.1d0,RV=2.691d0,AV=0.52d0
      integer,parameter :: Nr=400,Nt=12000
      real(8),parameter :: dr=0.25d0,dt=5.d-4
      integer :: i,i1,i2,it,l,n
      real(8) :: AC,AT,rmu,Einc,rk,r
      complex(8) :: zV(Nr),zVabs(Nr),zh(Nr,Nr),zu(Nr),zhx(Nr),zx(Nr)
      complex(8) :: fact,zwf(Nr)

      AC=1  ! projectile mass number
      AT=10 ! target mass number
      rmu=AC*AT/(AC+AT)*PM ! reduced mass

      Einc=30.d0 ! incident energy
      rk=sqrt(2*rmu*Einc)/HC ! incident wave number
      l=0 ! angular momentum

      open(7,file='pot.dat')
      do i=1,Nr
        r=i*dr
        zV(i)=V0/(1+exp((r-RV)/AV))+HC**2*l*(l+1)/(2*rmu*r**2)
        if(r.gt.50.d0) then
          zVabs(i)=-zI*50.d0*(r-50.d0)/50.d0
        else
          zVabs(i)=0.d0
        endif
        write(7,"(3f15.6)") r,real(zV(i)),imag(zVabs(i))
      enddo
      close(7)

! construct Hamiltonian matrix
! kinetic energy by discrete variables representation
      do i1=1,Nr
      do i2=1,Nr
        if (i1.eq.i2) then
          zh(i1,i2)=PI**2/3.d0-0.5d0/i1**2
        else
          zh(i1,i2)=2.d0/(i1-i2)**2-2.d0/(i1+i2)**2
        endif
        zh(i1,i2)=zh(i1,i2)*0.5d0*HC**2*(-1)**(i1-i2)/(rmu*dr**2)
        if(i1.eq.i2) then
          zh(i1,i2)=zh(i1,i2)+zV(i1)+zVabs(i1)
        endif
      enddo
      enddo
```

Hamiltonian matrix

```
! initial wave packet
      do i=1,Nr
        r=i*dr
        zu(i)=zV(i)*sin(rk*r)
      enddo

! time evolution of the wave packet
      open(8,file='wf_scattering.dat')
      zwf=zu*(dt/2)/zI
      do it=1,Nt
        fact=1.d0
        zx=zu
        do n=1,4
          fact=fact*(-zI*dt)/n
          zhx=0.d0
          do i1=1,Nr
          do i2=1,Nr
            zhx(i1)=zhx(i1)+zh(i1,i2)*zx(i2)
          enddo
          enddo
          zu=zu+fact*zhx
          zx=zhx
        enddo
        zwf=zwf+exp(zI*Einc*it*dt)*zu*dt/zI

        write(*,*) it,sum(abs(zu)**2)*dr

        if((it-1)/40*40.eq.it-1) then
          do i=1,Nr
            write(8,"(3f15.5)") i*dr,real(zu(i)),imag(zu(i))
          enddo
          write(8,*) ' space'
        endif
      enddo
      close(8)

      open(9,file='wf_ft.dat')
      do i=1,Nr
        write(9,"(3f15.6)") i*dr,real(zwf(i)),imag(zwf(i))
      enddo
      close(9)
      stop
      END
```

time evolution

Making animation in linux

script to be run on perl

```
#!/usr/bin/perl
open(INPUT01,"wf_scattering.dat");
@lines=<INPUT01>;
open(OUTPUT01,">wf_gnu.dat");
$fnumb=1;
foreach $line (@lines){
  $_=$line;
  if(/space/){
    close(OUTPUT01);
    $bashr=`gnuplot wf_abc.gnu`;
    $fnameadd=&change_number_to_character($fnumb);
$bashr=`convert wf.pbm wf$fnameadd.bmp`;
    $fnumb++;
    open(OUTPUT01,">wf_gnu.dat");
  }else{
    print OUTPUT01 $line;
  }
}
$bashr=`convert wf*.bmp wf_animation.mpg`;
exit 0;

sub change_number_to_character {
    local($number45)=@_;
    $moji="moji";
    if($number45 >= 1000){
        $suji45=substr "$number45", -4,4;
        $moji="0".$suji45;
    }elsif($number45 >= 100){
        $suji45=substr "$number45", -3,3;
        $moji="00".$suji45;
    }elsif($number45 >= 10){
        $suji45=substr "$number45", -2,2;
        $moji="000".$suji45;
    }else{
        $suji45=substr "$number45", -1,1;
        $moji="0000".$suji45;
    }
    $moji;
}
```

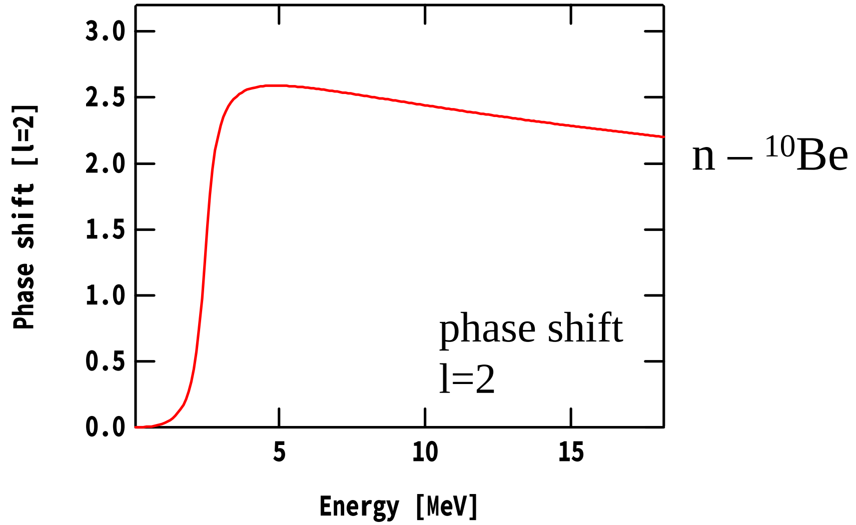
gnuplot file (wf_abc.gnu)

```
set terminal pbm medium color
set output 'wf.pbm'
set nokey
set size 1.0,0.5
set xlabel 'r [fm]'
set ylabel 'Re u(r)'
set linestyle 1 linetype 10 linewidth 5
set xrange [0:100]
set yrange [-80:80]
set format y ""
set noytics
set linestyle 1 lt 1 lw 3
set linestyle 2 lt 2 lw 3
set linestyle 3 lt 3 lw 3
set linestyle 4 lt 4 lw 3
plot 'wf_gnu.dat' u 1:($2*2) w l ls 1, 'pot.dat' u 1:2 w l ls 3,
'pot.dat' u 1:3
 w l ls 4
```

Example 3: Resonance in potential scattering

When the potential V(r) has a resonance,
phase shift crosses π/2

$$\delta_l(E_r) = \frac{\pi}{2} \qquad \left.\frac{d\delta_l}{dE}\right|_{E=E_r} = \frac{2}{\Gamma}$$



Resonance in time-domain:
as an initial condition,
place a Gaussian wave packet

$$u_{l=2}(r, t=0) = r^3 \exp\left[-\gamma (r - r_0)^2\right]$$

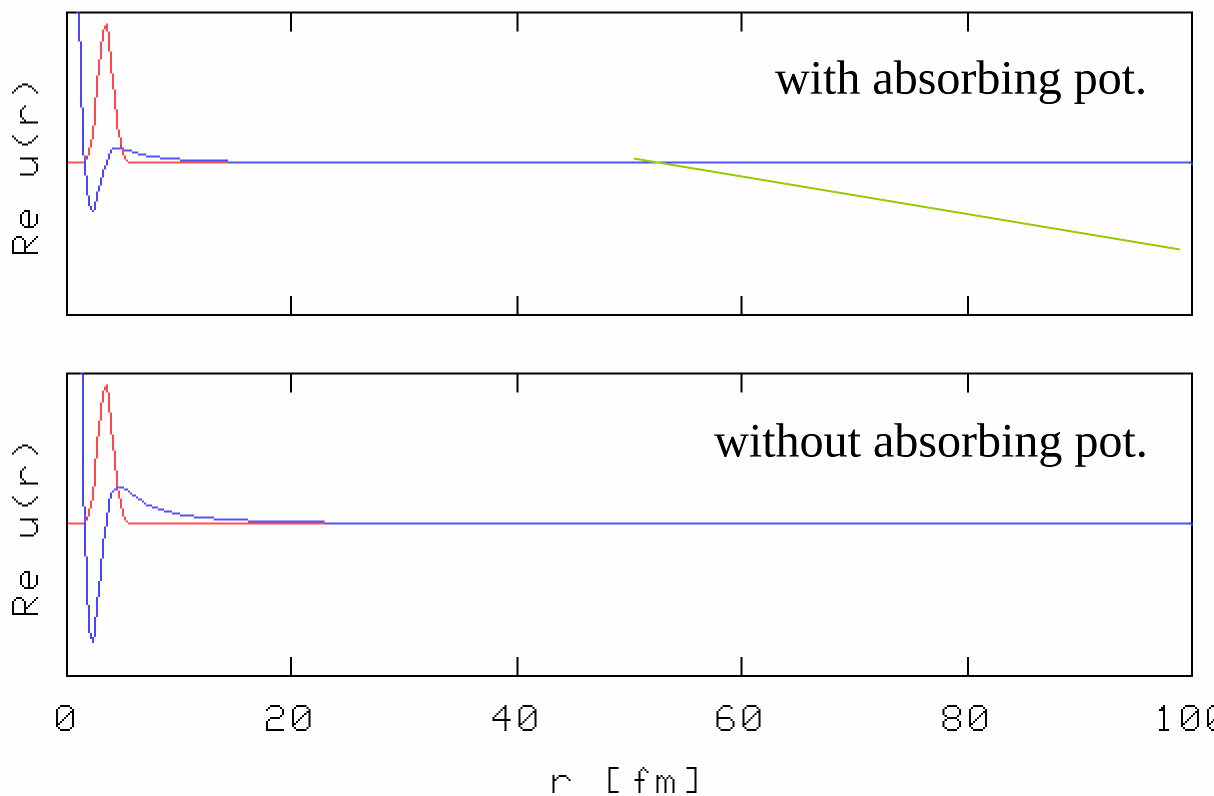
r_0=3fm, γ=1fm^{-2}

quasi-stationary behavior

⟶ Gamow state

$$u(r,t) \approx c(t) w(r)$$

V0=-61.1, R=2.691, a=0.52
Nr=400, dr=0.25, NT=12000, dt=0.0005



Eigenvalue problem for resonance

$\mathbf{A}\vec{x} = \vec{b}$ $\mathbf{A}\vec{x} = a\vec{x}$ $\frac{d\vec{y}(t)}{dt} = \mathbf{A}\vec{y}(t)$

Outgoing boundary condition

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2mr^2}+V(r)\right]u_l(r)=Eu_l(r)$$

$$u_l(0)=0, \qquad u_l(r)\underset{r\to\infty}{\to}\exp(ikr)$$

Absorbing boundary condition

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2mr^2}+V(r)-iW_{abs}(r)\right]u_l(r)=Eu_l(r)$$

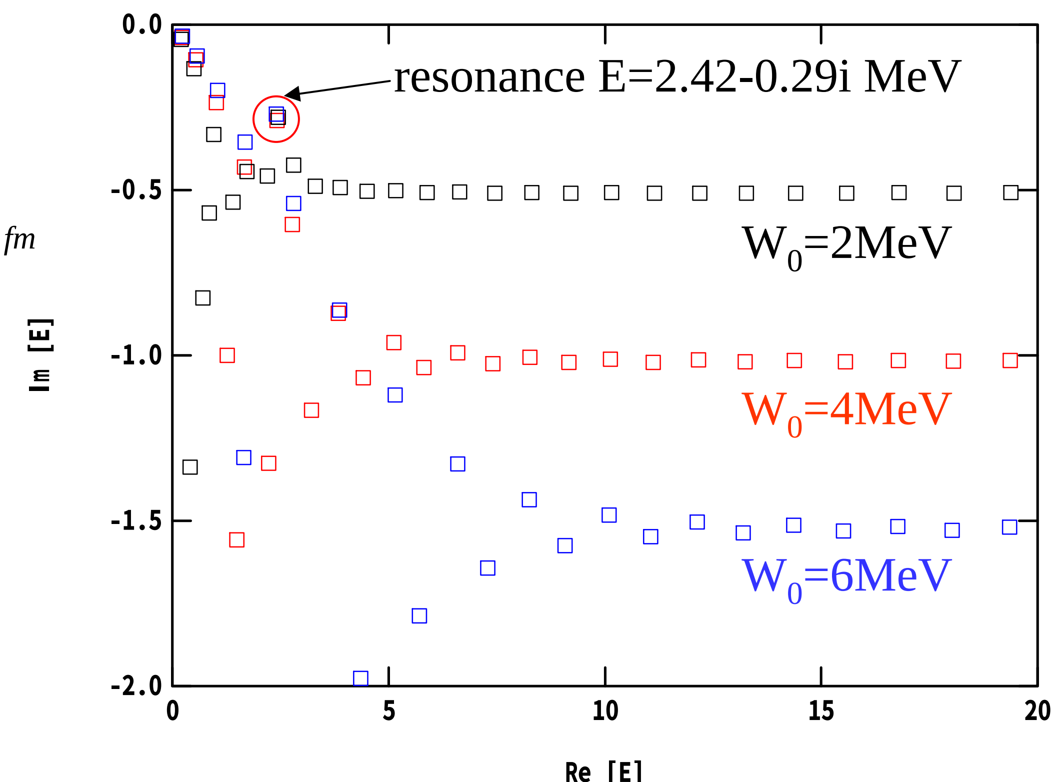
$$u_l(0)=0, \qquad u_l(r)\underset{r\to\infty}{\to}0$$

Complex eigenvalue, imaginary part represents decay width

Eigenvalue distribution
for various absorbing potential

$$-iW_{abs}(r)=\begin{cases}0 & r<50\,fm\\ -iW_0\dfrac{r-50\,fm}{50\,fm} & 50\,fm<r<100\,fm\end{cases}$$

Resonances appear as
stable complex eigenvalue

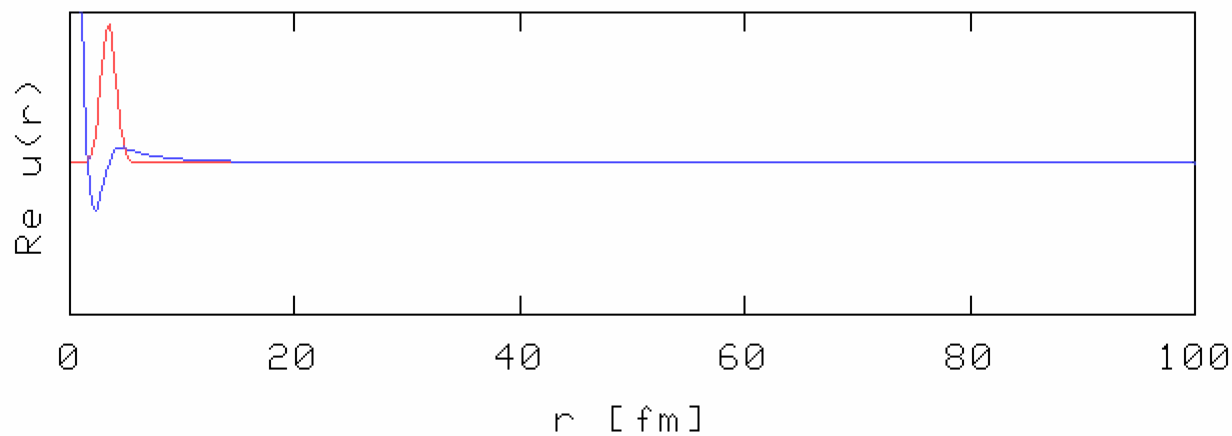


quasi-stationary behavior
⟶ Gamow state

$$u_{l=2}(r,t=0) = r^3 \exp\left[-\gamma (r-r_0)^2\right]$$

r_0=3fm, γ=1fm^{-2}

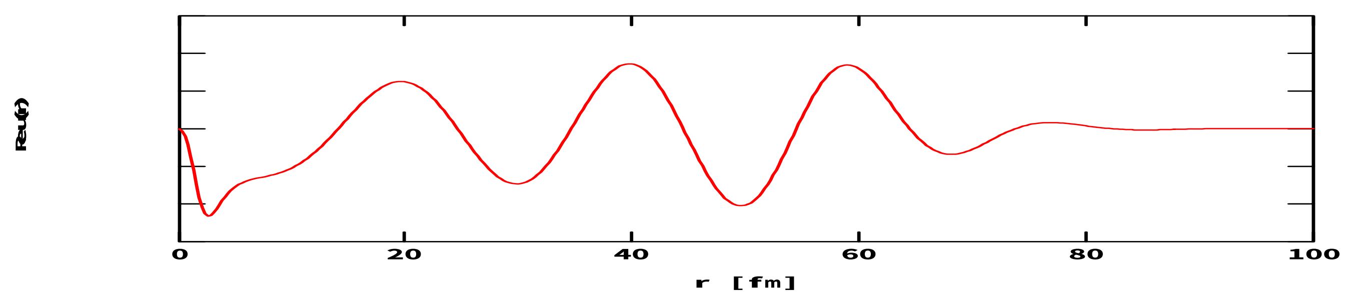
V0=-61.1, R=2.691, a=0.52
Nr=400, dr=0.25, NT=12000, dt=0.0005



$$u(r,t) \approx c(t) w(r)$$

$$|c(t)|^2 \approx \exp\left[-2(\mathrm{Im}\, E) t / \hbar\right]$$

Eigenfunction for E=2.42-0.29i MeV

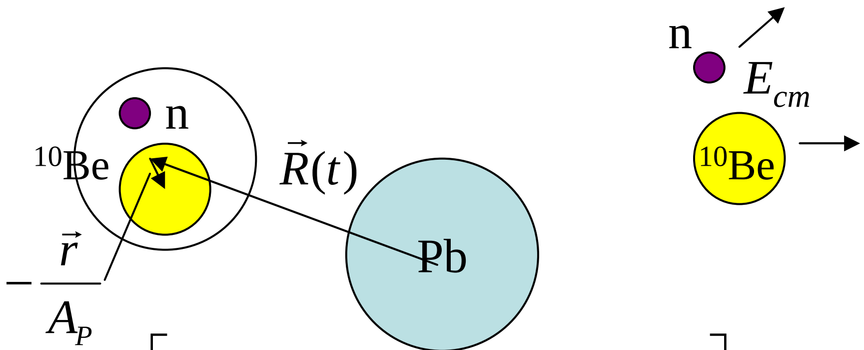


Absorbing boundary condition

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - iW_{abs}(r)\right] u_l(r) = E u_l(r)$$

$$u_l(0) = 0, \qquad u_l(r) \underset{r\to\infty}{\longrightarrow} 0$$

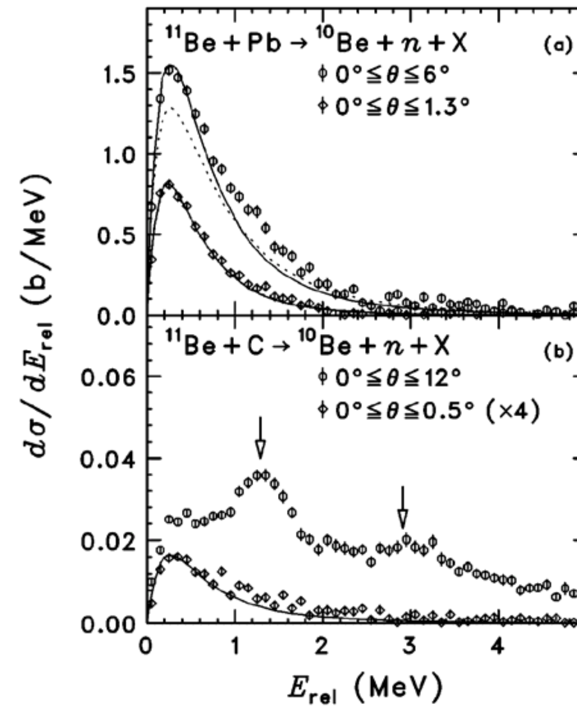
Example 4: Response to external field
Dipole strength of halo nuclei around threshold



$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)+\frac{Z_C Z_T e^2}{\left|\vec{R}(t)-\frac{\vec{r}}{A_P}\right|}\right]\psi(\vec{r},t)$$

$$\approx\frac{Z_C Z_T e^2}{R(t)}+\frac{Z_C Z_T e^2}{A_P}\hat{R}(t)\vec{r}$$

halo neutron feels uniform force field (dipole field), which induces breakup of ^{11}Be



N. Fukuda, et.al,
Phys. Rev. C60(2004)054606

Transition to continuum (breakup) state at energy *E*

$$\frac{dB(E1)}{dE}=\sum_m\left|\langle\phi_{E,l=1,m}|M_{1m}|\phi_0\rangle\right|^2,\quad M_{1m}=-\frac{Z_C}{A_P}erY_{1m}(\hat{r}),\quad \phi_{Elm}(\vec{r})\rightarrow\sqrt{\frac{2m}{\pi\hbar^2k}}\frac{\sin\left(kr-\frac{1}{2}l\pi+\delta_l\right)}{r}Y_{lm}(\hat{r})$$

x,y,z

$\phi_0(\vec{r})$ Initial bound orbital in ^{11}Be = ^{10}Be + n, weakly-bound s-orbital (l=0)

$\phi_{Elm}(\vec{r})$ Final continuum orbital of ^{11}Be = ^{10}Be + n

Dipole response function with absorbing boundary condition

$$\frac{dB(E1)}{dE} = -\frac{1}{\pi}\,\mathrm{Im}\sum_m \left\langle \phi_0 \left| M_{1m}^{+} \frac{1}{E+i\varepsilon-H} M_{1m} \right| \phi_0 \right\rangle \qquad M_{1m} = -\frac{Z_C}{A_P}\, e r Y_{1m}(\hat{r})$$

$$-\frac{1}{\pi}\,\mathrm{Im}\left\langle \phi_0 \left| M_{1m}^{+} \frac{1}{E+i\varepsilon-H} M_{1m} \right| \phi_0 \right\rangle \qquad \frac{1}{E+i\varepsilon-H} = \frac{P}{E+i\varepsilon-H} - i\pi\delta(E-H)$$

$$= \left\langle \phi_0 \left| M_{1m}^{+} \delta(E-H) M_{1m} \right| \phi_0 \right\rangle$$

$$= \sum_{lm'} \int dE' \delta(E-E') \left| \left\langle \phi_{E,l=1,m} \left| M_{1m} \right| \phi_0 \right\rangle \right|^2$$

Real-time propagation

$$\frac{dB(E1)}{dE} = -\frac{1}{\pi}\,\mathrm{Im}\sum_m \frac{1}{i\hbar}\int_0^\infty dt\, e^{iEt/\hbar} \left\langle \phi_0 \left| M_{1m}^{+} e^{-iHt/\hbar} M_{1m} \right| \phi_0 \right\rangle$$

$$= \frac{1}{\pi\hbar}\,\mathrm{Re}\int_0^\infty dt\, e^{iEt/\hbar} \sum_m \psi_{1m}^{*}(\vec{r},0)\,\psi_{1m}(\vec{r},t)$$

$$\psi(\vec{r},t=0) = M_{1m}\phi_0(\vec{r})$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

$$\frac{1}{i\hbar}\int_0^\infty dt\, e^{i(E+i\varepsilon-H)t/\hbar} = \left.\frac{-e^{i(E+i\varepsilon-H)t/\hbar}}{E+i\varepsilon-H}\right|_0^\infty = \frac{1}{E+i\varepsilon-H}$$

In the partial wave expansion,

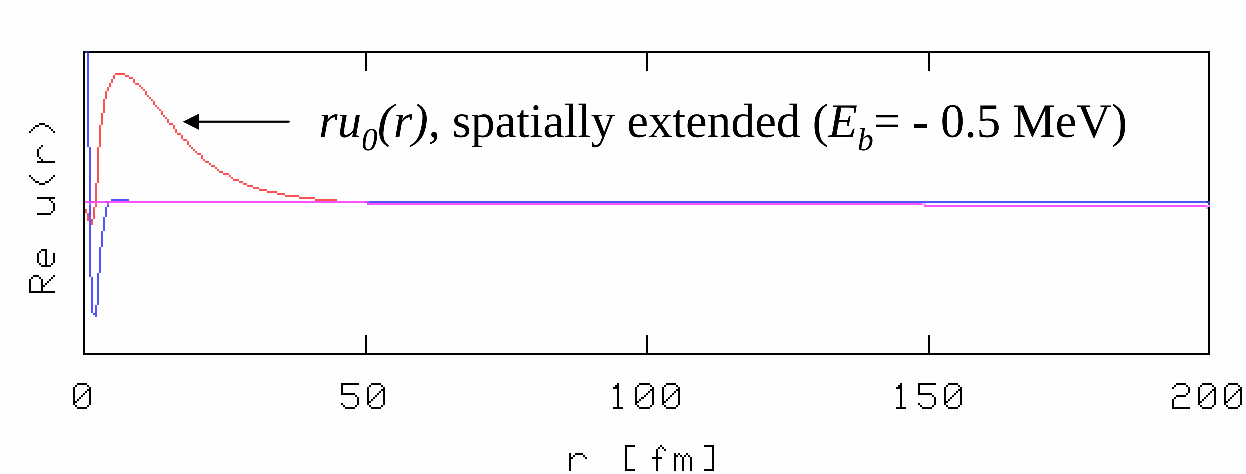
$$\psi\left(\vec{r}, t=0\right) = M_{1m}\phi_0\left(\vec{r}\right)$$

$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{r}, t\right) = H\psi\left(\vec{r}, t\right)$$

$$v_{l=1}\left(r, t=0\right) = ru_{l=0}\left(r\right)$$

Initial condition:
r multipled to s-wave ground state in [11]Be

$$i\hbar\frac{\partial}{\partial t}v_{l=1}\left(r, t\right) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V\left(r\right) - iW_{abs}\left(r\right)\right]v_{l=1}\left(r, t\right)$$

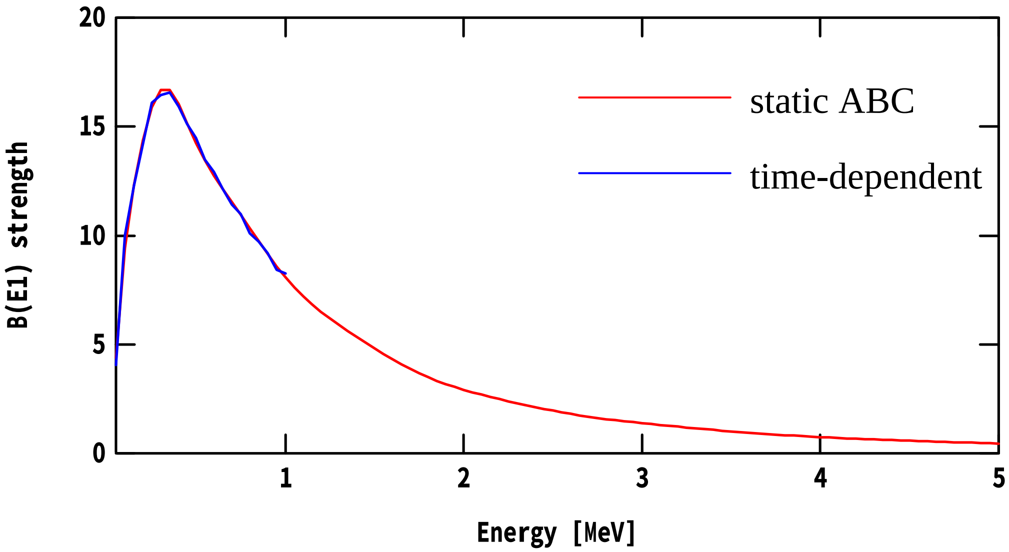


V0=-62.1, R=2.691, a=0.52
E_bound=-0.5MeV
Nr=400, dr=0.5, Nt=100000, dt=0.0005

$$ru_{l=0}(r) = \sum_i c_i y_i\left(r\right) + \int dEc\left(E\right)y_E\left(r\right)$$

Time-dependent calculation

$$\frac{dB(E1)}{dE} = \frac{1}{\pi\hbar} \mathrm{Re} \int_0^\infty dt e^{iEt/\hbar} \sum_m \psi_{1m}^*(\vec{r},0) \psi_{1m}(\vec{r},t)$$



Time-independent calculation

Scattering wave

$$\frac{dB(E1)}{dE} = -\frac{1}{\pi} \mathrm{Im} \sum_m \left\langle \phi_0 \middle| M_{1m}^+ \boxed{\frac{1}{E + i\varepsilon - H} M_{1m} \middle| \phi_0 \right\rangle} \qquad M_{1m} = -\frac{Z_C}{A_P} e r Y_{1m}(\hat{r})$$

$$\equiv \chi(\vec{r})$$

$$\left[E - H - iW_{abs}(r)\right] \chi(\vec{r}) = M_{1m} \phi_0(\vec{r}) \qquad \chi(\vec{r}) \underset{r \to \infty}{\longrightarrow} 0$$

Linear problem in the partial wave expansion

$$\left[E - \left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r) \right) \right] w_{l=1}(r) = r u_0(r)$$

Summary

Quantum mechanics textbook

For time-dependent Schroedinger equation, $i\hbar \frac{\partial}{\partial t}\psi(r,t) = H\psi(r,t)$
make a separation of variables and
solve time-independent Schroeginer equation. $H\phi(r) = E\phi(r)$
Then find a solution with scattering boundary condition

$$\phi(\vec{r}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\Omega)\frac{e^{ikr}}{r}$$

Today I showed

Employing Absorbing boundary condition
Real-time propagation of wave packet,
we can treat scattering problem with vanishing boundary condition

---

Tomorrow I will apply them to some problems of current interests
.
real-time calculation for static problems
efficient for calculation
useful for intuitive understanding of dynamics

Novel computational approaches for nuclear reactions
(2nd day)

Kazuhiro Yabana

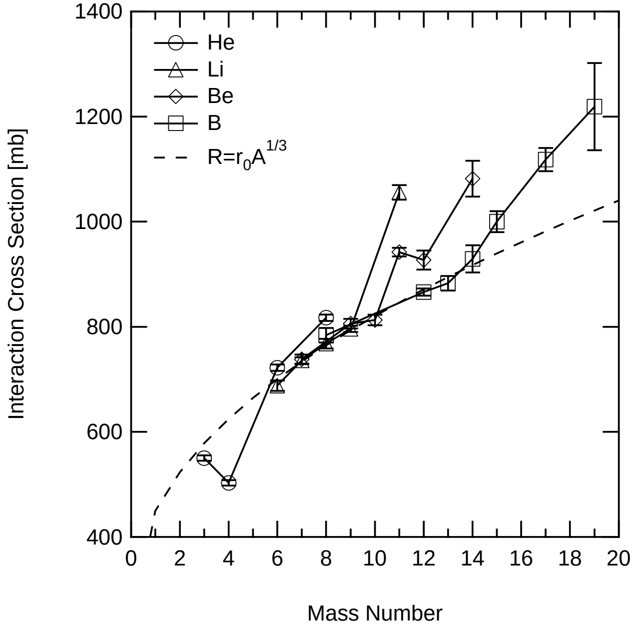
Center for Computational Sciences
Univ. of Tsukuba

1. Basics:
   Absorbing boundary, real-time propagating,
   taking potential scattering as example.

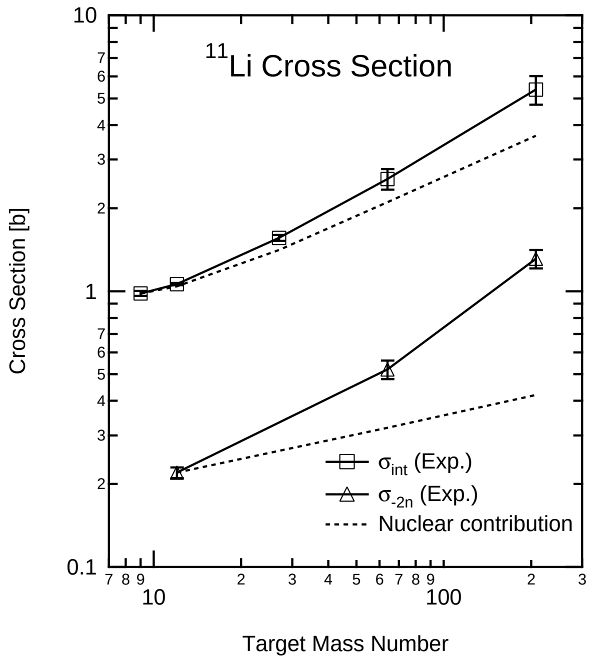
2. Applications:
   Reactions of halo nuclei at low energy — M. Ito, T. Nakatsukasa, M. Ueda
   Giant dipole resonances of neutron rich nuclei — T. Nakatsukasa
   Other field in sciences — G.F. Bertsch, T. Otobe, J.-I. Iwata, T. Nakatsukasa

Reactions of halo nuclei at low incident energy

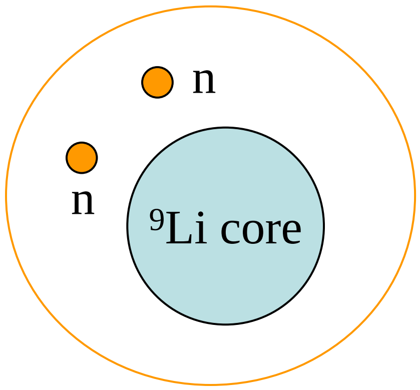
Interaction cross section of light unstable nuclei



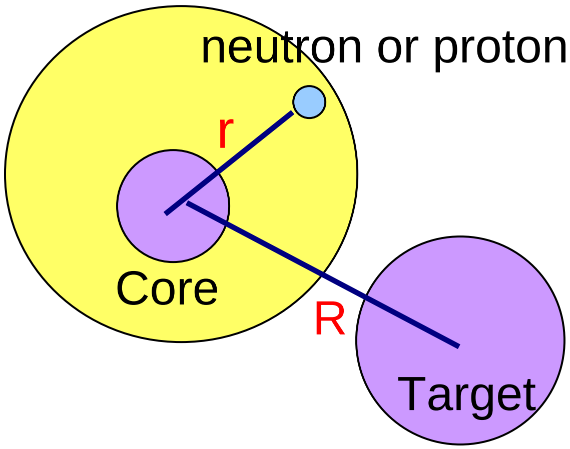
Interaction cross section and two-neutron removal cross section of ^{11}Li



Large enhancement at drip line ⇨ halo structure



3-body reaction: Fusion reactions of halo nuclei



$$\left(-\frac{\hbar^2}{2\mu}\nabla_R^{\ 2} - \frac{\hbar^2}{2m}\nabla_r^{\ 2} + V_{nC}(r_{nC}) + V_{CT}(r_{CT}) + V_{nT}(r_{nT}) \right)\Phi(\vec{R},\vec{r}) = E\Phi(\vec{R},\vec{r})$$

Scattering boundary condition?

time-dependent wave-packet calculation

⟶ fusion probability without boundary condition.

Example 2: Fusion reaction (potential scattering with absorption inside a Coulomb barrier)
Wave packet dynamics, no absorbing potential.

Radial Schroedinger equation for l=0

$$i\hbar \frac{\partial}{\partial t} u(r,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + iW(r) \right] u(r,t)$$

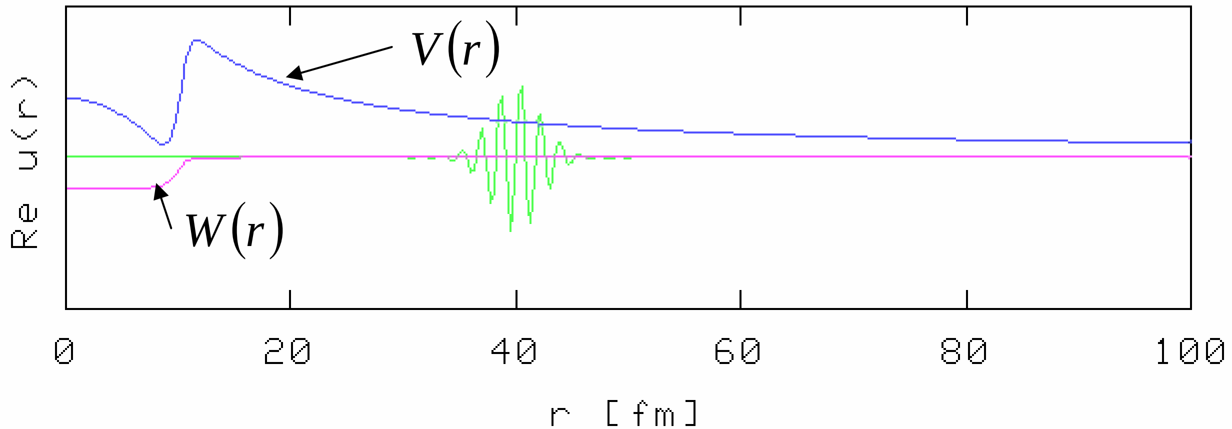
with incident Gaussian wave packet

$$u(r,t_0) = \exp\left[-ikr - \gamma (r-r_0)^2 \right]$$

10Be-208Pb (A,Z=10,4 and 208,82)
V0=-50 W0=-10, RV=1.26,RW=1.215, AV=0.44, AW=0.45
E_inc=28 MeV (+Coulomb at R_0), R_0=40fm, gamma=0.1fm-2
Nr=400, dr=0.25, Nt=10000, dt=0.001

Flux absorbed by W(r) represents fusion.

^{10}Be – ^{208}Pb



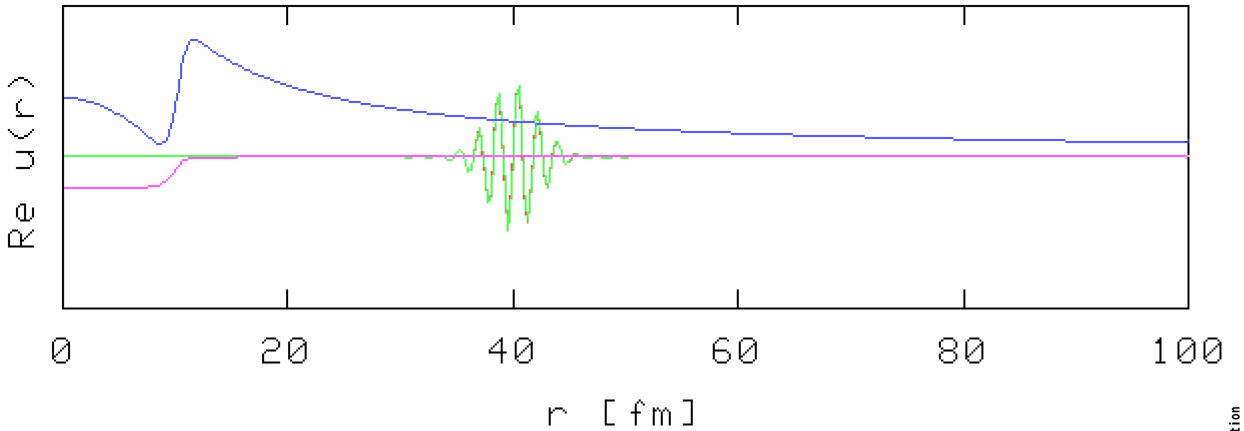
High energy component goes over barrier and absorbed
Low energy component is reflected at the barrier.

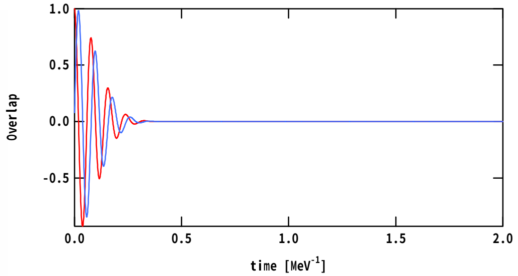
Wave packet dynamics includes scattering information for wide energy region.
How to extract reaction information for a fixed energy?

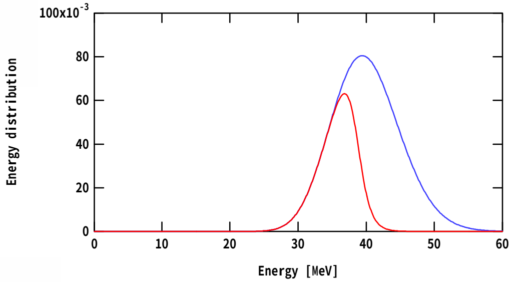
Extract static (fixed-E) information from wave-packet dynamics:

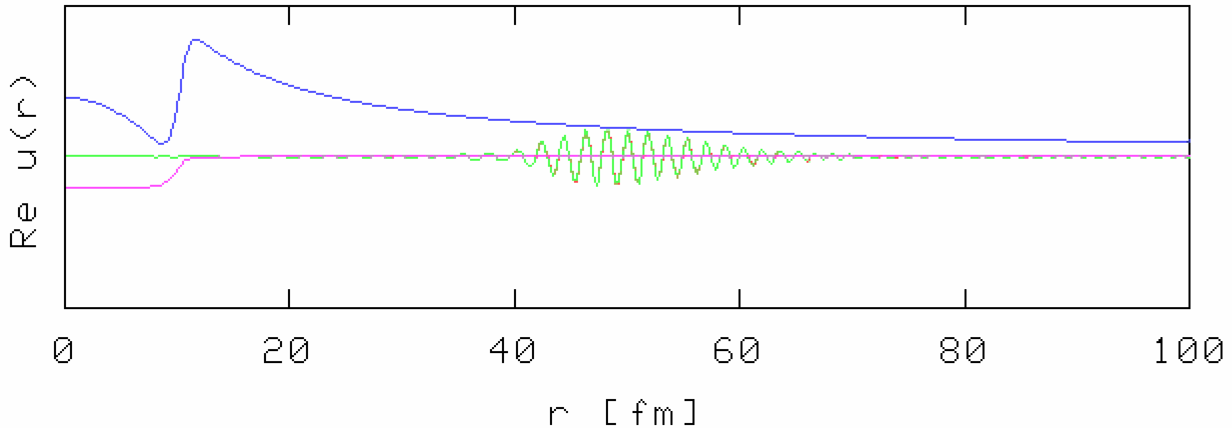
define energy distribution

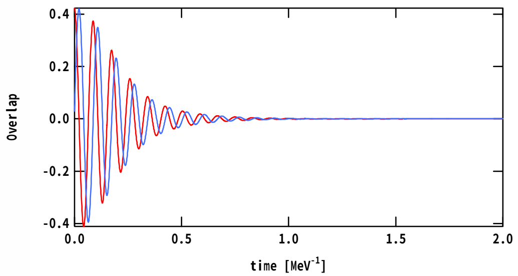
$$P_a(E) = \langle u_a | \delta(E-H) | u_a \rangle = \frac{1}{2\pi\hbar}\int_0^\infty dt\, e^{iEt/\hbar} \left\langle u_a\left(-\frac{t}{2}\right) \middle| u_a\left(\frac{t}{2}\right) \right\rangle$$



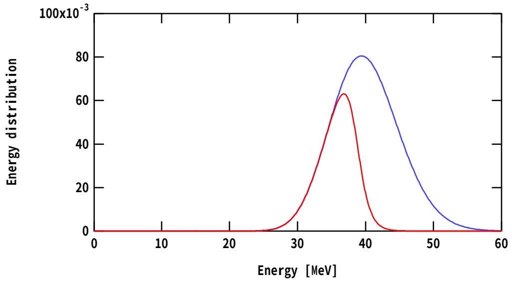


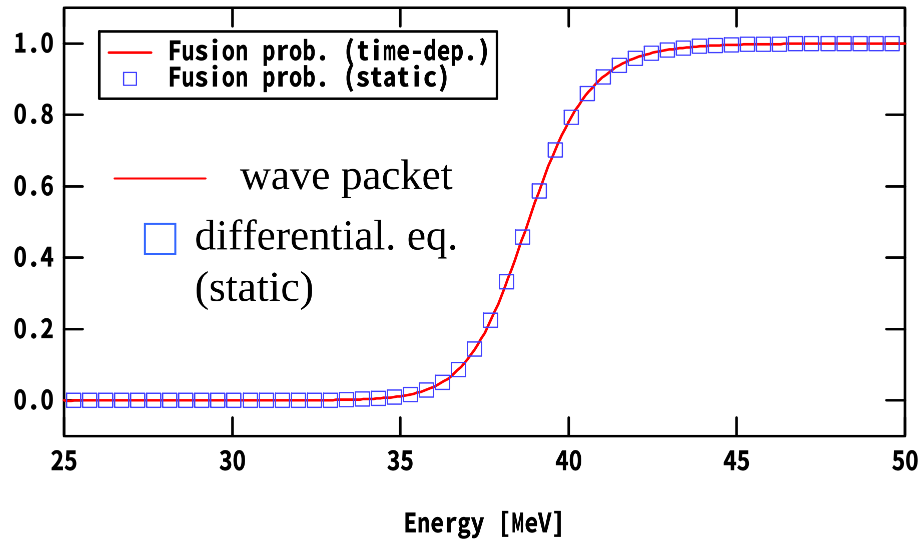






$$P_{fusion}(E) = \frac{P_{init}(E) - P_{final}(E)}{P_{init}(E)}$$

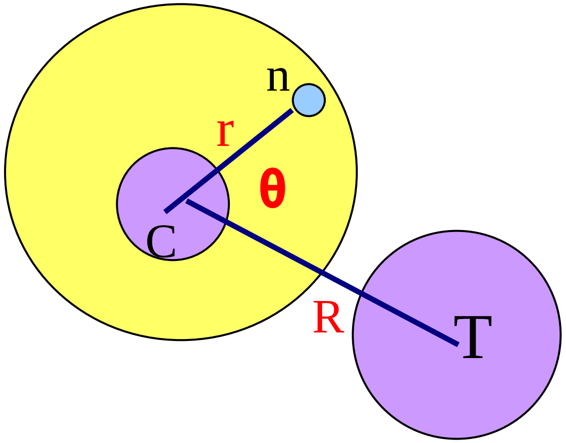




Fusion probability for whole barrier region from single wave-packet calculation.
No boundary condition required in the wave packet calculation.

Tomorrow, application for 3-body reaction.

3-body reaction
(n-C)-T



$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{R},\vec{r},t\right)=\left(-\frac{\hbar^2}{2\mu}\nabla_R^{\ 2}-\frac{\hbar^2}{2m}\nabla_r^{\ 2}+V_{nC}\left(r_{nC}\right)+V_{CT}\left(r_{CT}\right)+V_{nT}\left(r_{nT}\right)\right)\psi\left(\vec{R},\vec{r},t\right)$$

real potential,
weakly bound 2s bound orbital

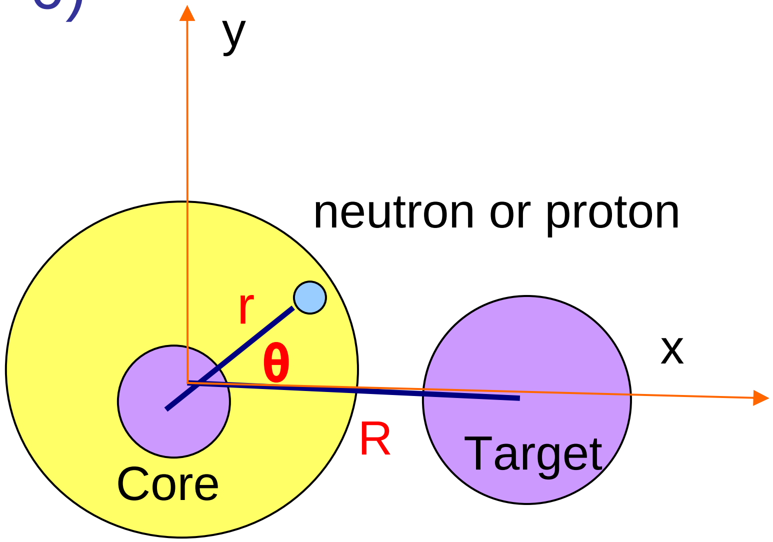
real nuclear potential
(+Coulomb for n=proton)

Coulomb + Nuclear potential
Absorption => C-T fusion

$$\psi_{J=0}\left(\vec{R},\vec{r},t\right)=\sum_l\frac{u_l^{J=0}\left(R,r,t\right)}{Rr}P_l\left(\cos\theta\right)$$

(n+Core)-Target head-on collision (J=0)

3-body dynamics
Tightly-bound projectile (E_b=-3.5MeV)
(n-^{10}Be)-^{40}Ca

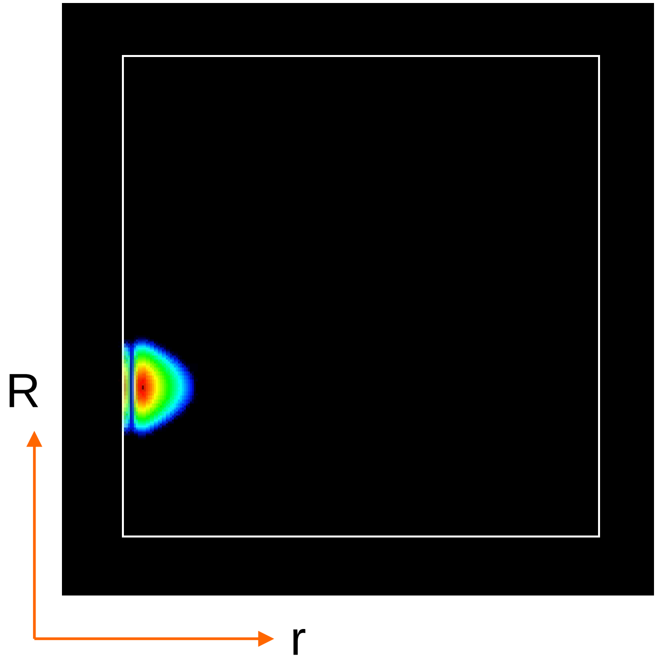


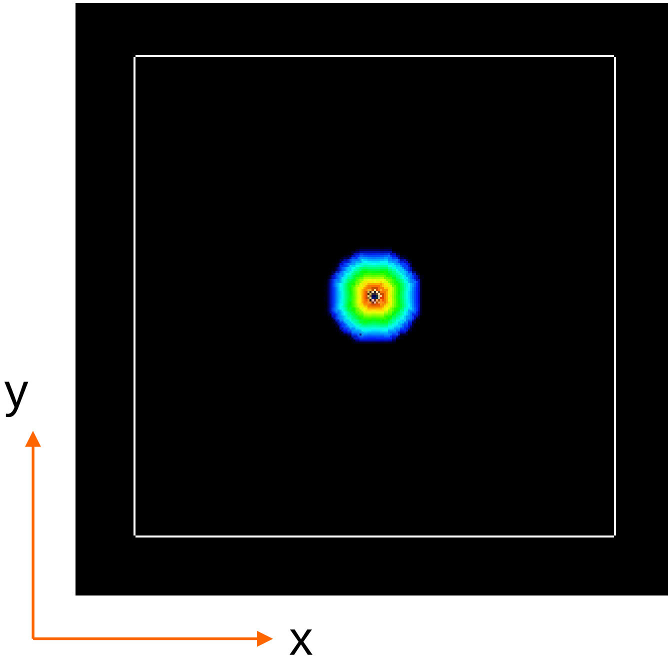
Initial wave packet:

$$u_l(R,r,t_0)=\delta_{l0}\exp\left[-iKR-\gamma(R-R_0)^2\right]u_0(r)$$

$$\rho(R,r,t)=\int d(\cos\theta)\left|\psi(R,r,\theta,t)\right|^2$$

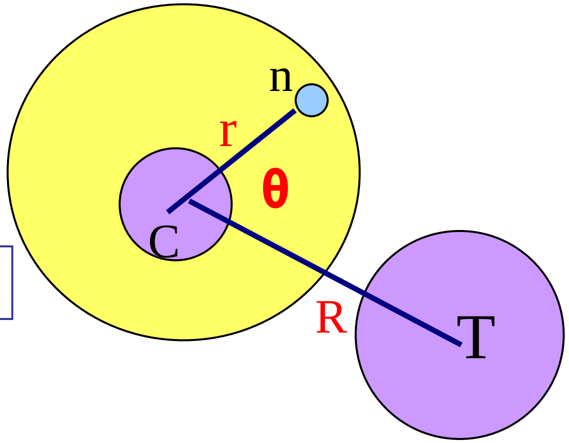
$$\rho(r,\theta,t)=\int dR\left|\psi(R,r,\theta,t)\right|^2$$





Fusion probability of 3-body system

$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{R},\vec{r},t\right)=\left(-\frac{\hbar^2}{2\mu}\nabla_R^{\ 2}-\frac{\hbar^2}{2m}\nabla_r^{\ 2}+V_{nC}\left(r_{nC}\right)+\underline{V_{CT}\left(r_{CT}\right)}+\underline{V_{nT}\left(r_{nT}\right)}\right)\psi\left(\vec{R},\vec{r},t\right)$$



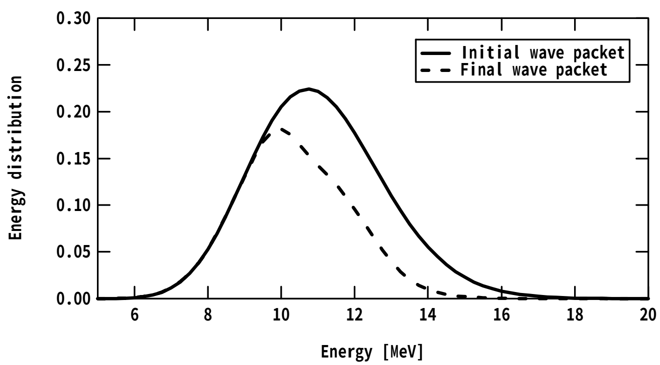
Coulomb + Nuclear potential
Absorption => C-T fusion

real nuclear potential

When core-target gets inside Coulomb barrier,
flux is absorbed (= fusion)

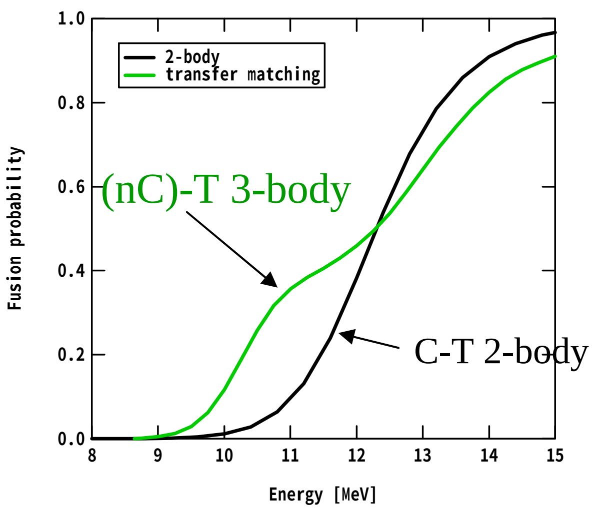
Energy distribution

$$P_a(E)=\left\langle u_a\left|\delta\left(E-H\right)\right|u_a\right\rangle$$
$$=\frac{1}{2\pi\hbar}\int_0^\infty dt\, e^{iEt/\hbar}\left\langle u\left(\frac{t}{2}\right)\middle| u\left(-\frac{t}{2}\right)\right\rangle$$



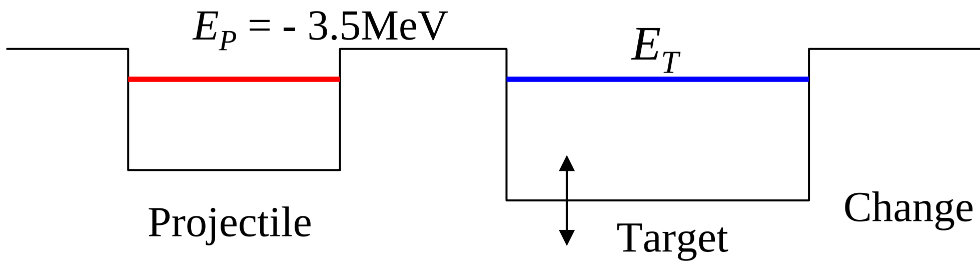
Fusion probability

$$P_{fusion}\left(E\right)=\frac{P_i\left(E\right)-P_f\left(E\right)}{P_i\left(E\right)}$$



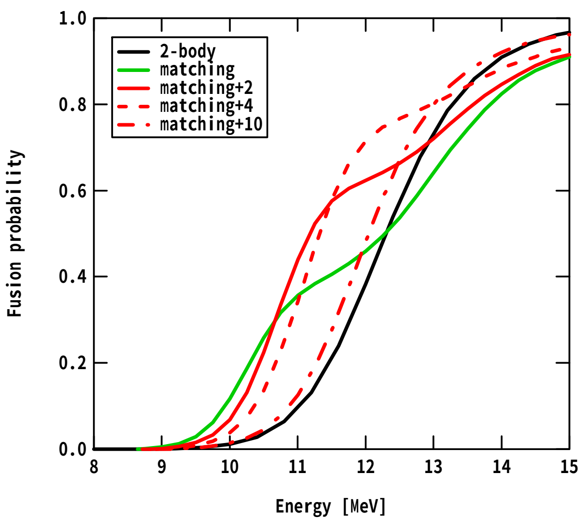
Large subbarrier enhancement

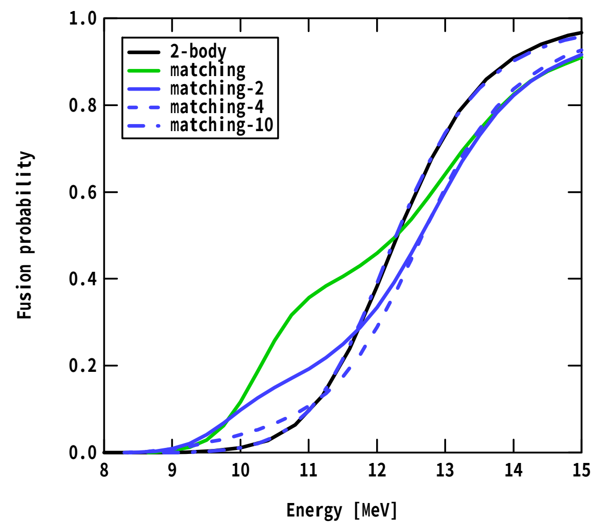
Transfer probability and Q-value matching



Change n-T potential depth

$E_P \approx E_T$ Strong mixing of projectile-target orbitals,
large transfer probability
energy-dependent barrier for fusion





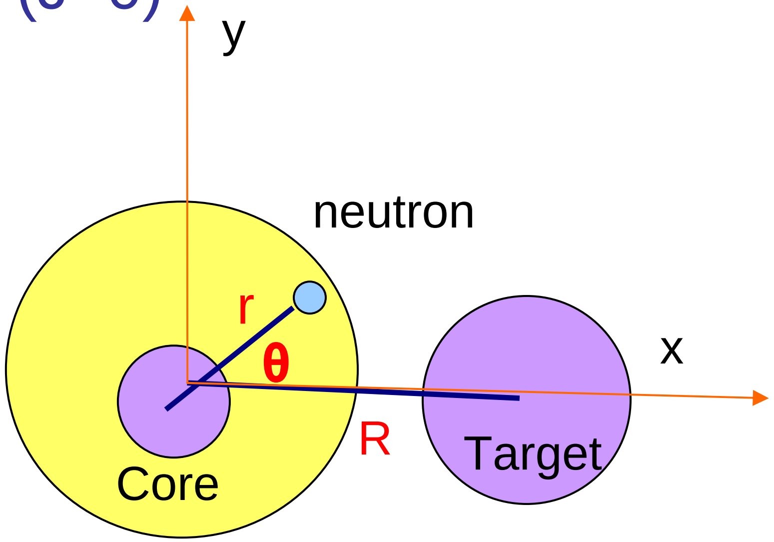
$E_P < E_T$
fusion enhancement

$E_P \approx E_T$
energy-dependent barrier

$E_P > E_T$
fusion suppression

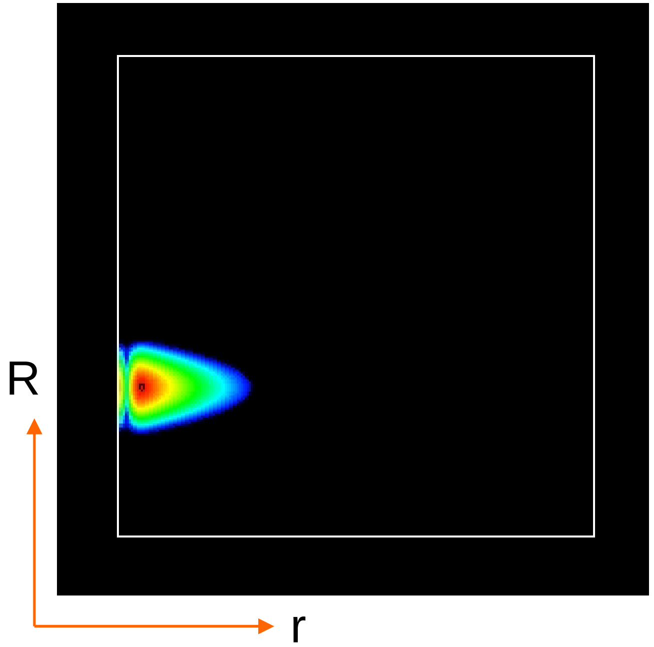
^{11}Be(n+^{10}Be)-^{208}Pb head-on collision (J=0)

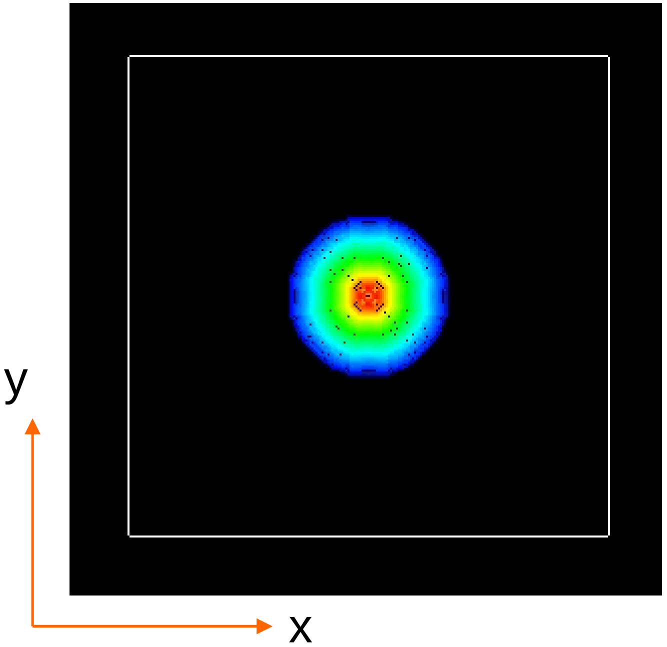
- n-C orbital energy: -0.6 MeV (Halo)



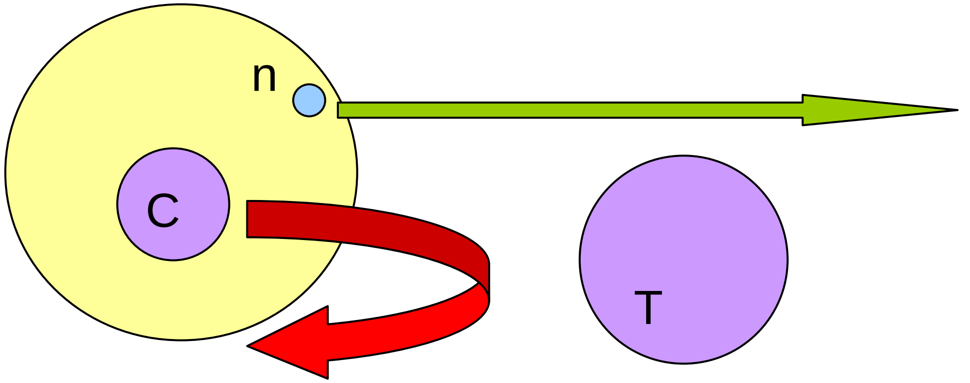
$$\rho(R,r,t)=\int d(\cos\theta)\left|\psi(R,r,\theta,t)\right|^2$$

$$\rho(r,\theta,t)=\int dR\left|\psi(R,r,\theta,t)\right|^2$$

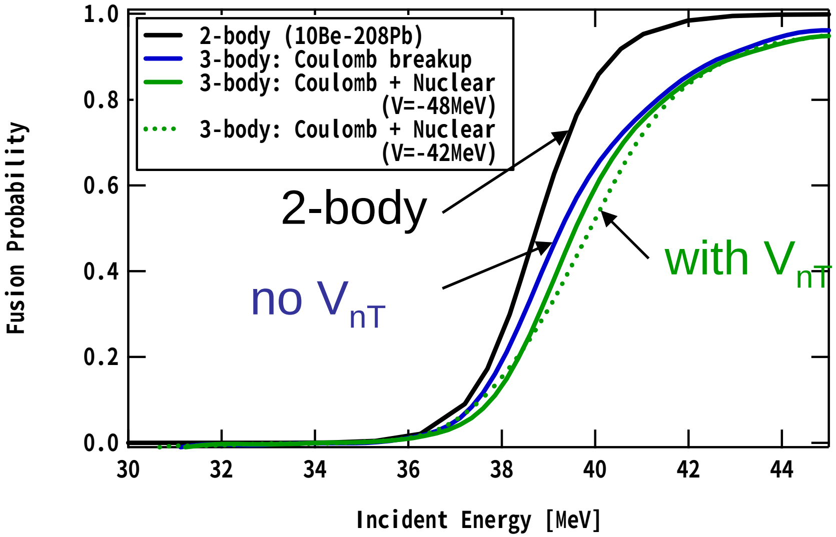




Coulomb breakup of halo neutron



Fusion probability of neutron-halo nuclei is suppressed

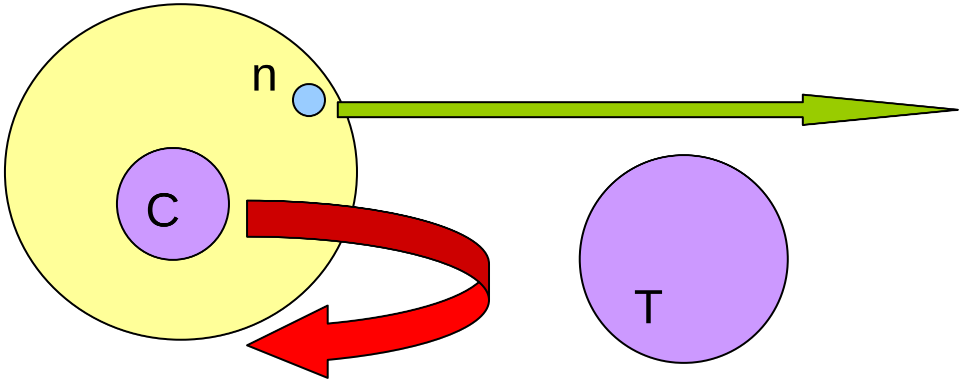


Why fusion probability suppressed by the Coulomb breakup?

Possible Reason:

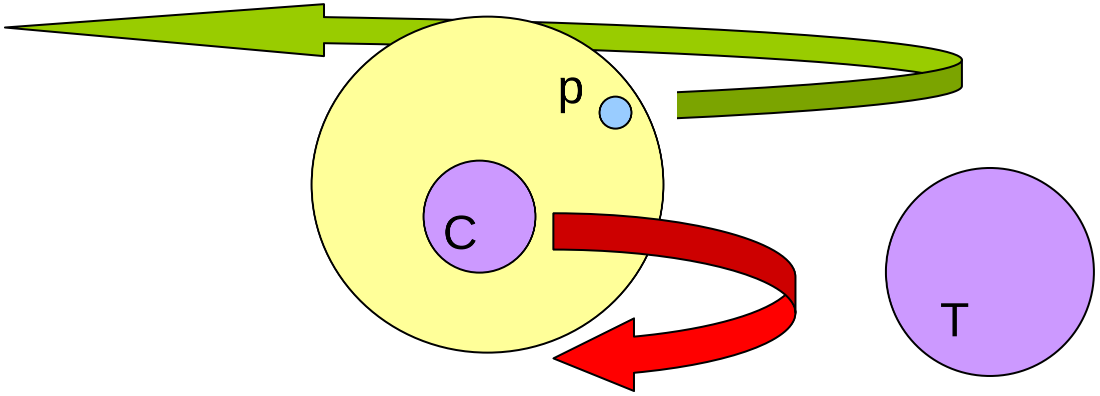
Core incident energy decreases effectively by neutron breakup

$$E_{core} \approx \frac{M_{core}}{M_{core} + M_n} E_{projectile}$$



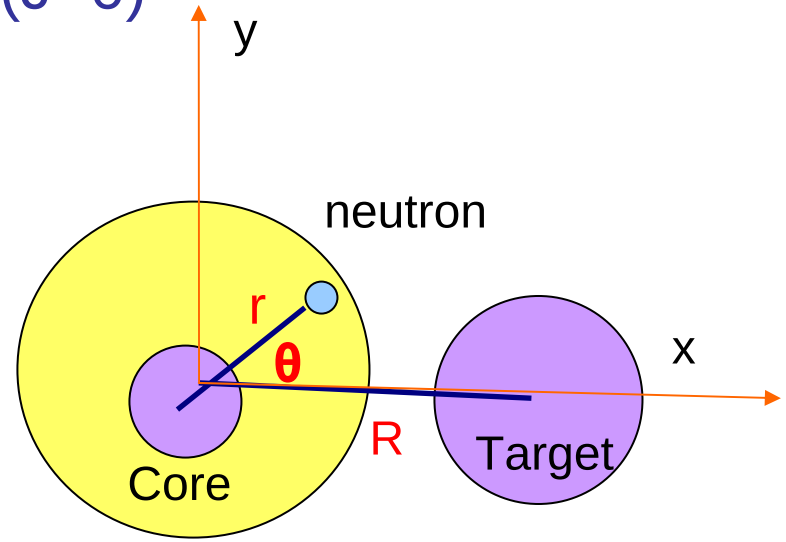
Then, What happens for proton-halo nuclei?

Stronger backward acceleration by [charge/mass] ratio

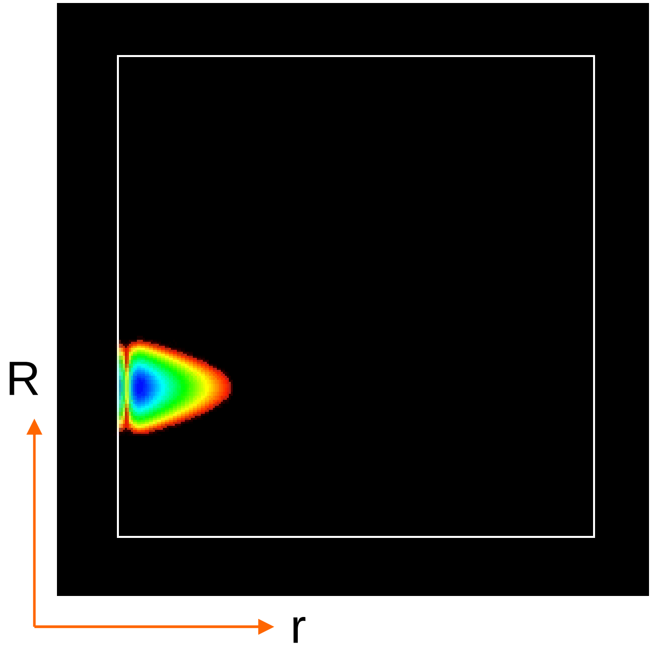


$^{11}Be(p+^{10}Li)$-^{208}Pb head-on collision (J=0)

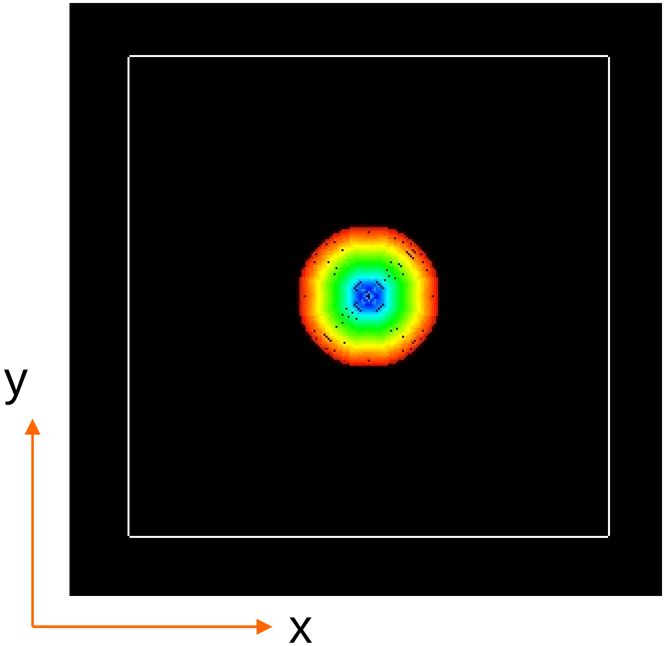
- p-C orbital energy: -0.3 MeV (Halo)
- p-T Coulomb only. (No nuclear potential)



$$\rho(R,r,t)=\int d(\cos\theta)\left|\psi(R,r,\theta,t)\right|^2$$

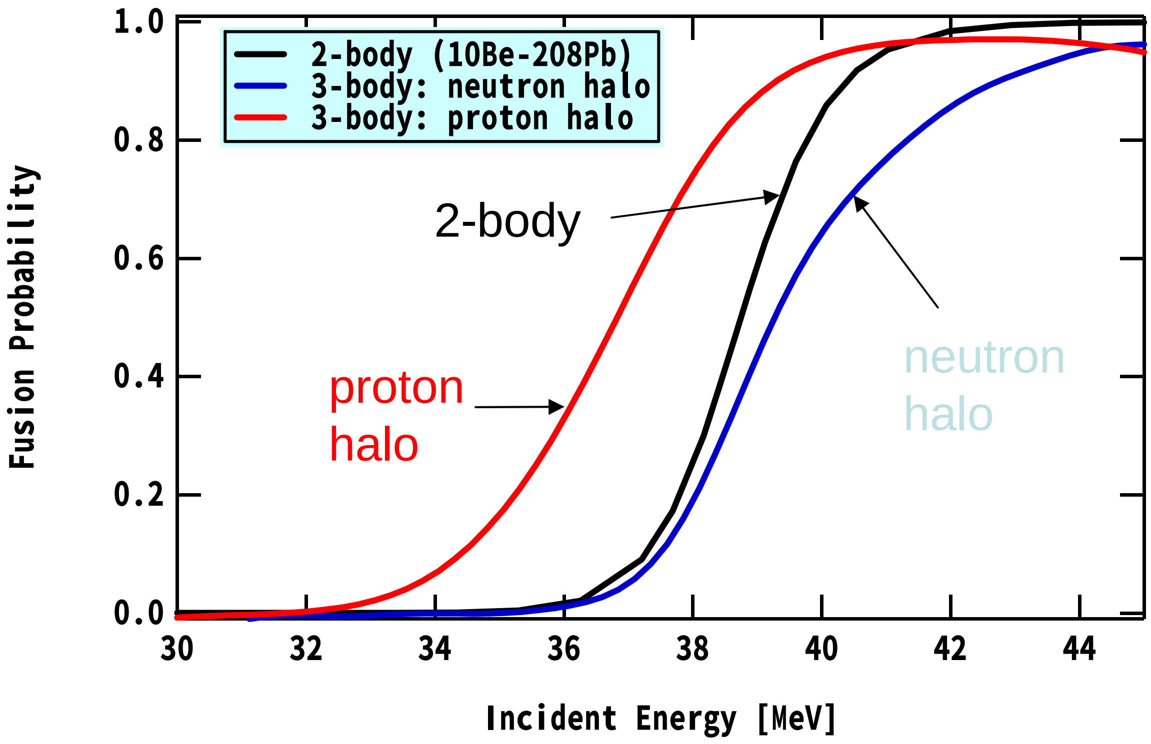


$$\rho(r,\theta,t)=\int dR\left|\psi(R,r,\theta,t)\right|^2$$



^{11}Be-^{208}Pb fusion probability

Comparison between
Proton halo (p-^{10}Li) -^{208}Pb
and Neutron halo (n-^{10}Be)-^{208}Pb

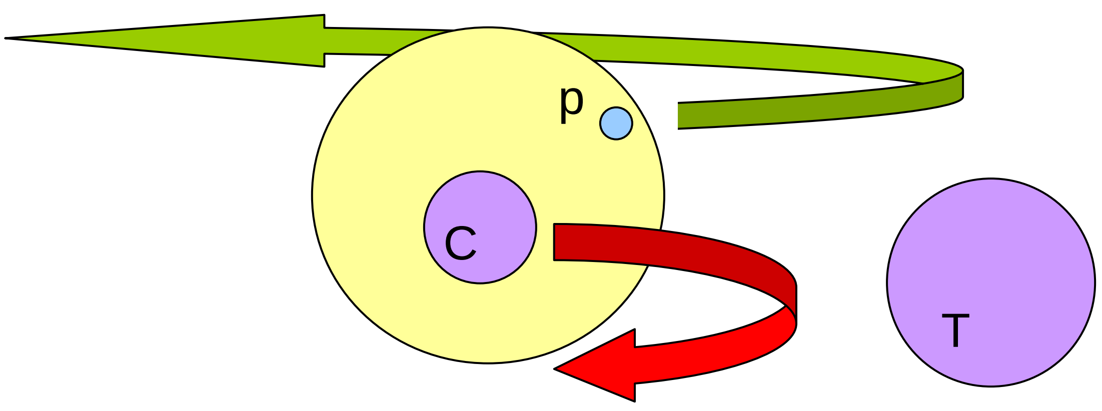


Strong enhancement of Fusion Probability for Proton-Halo case
Why?

Strong enhancement of Fusion Probability for Proton-Halo case
Why?

Proton breakup :

Core charge number smaller than Projectile (Z_C=Z_P-1)
⇒ Decrease of Coulomb barrier height



Current experimental situation

6He + 238U   R. Raabe et.al, Nature 431(2004, Oct.) 823.

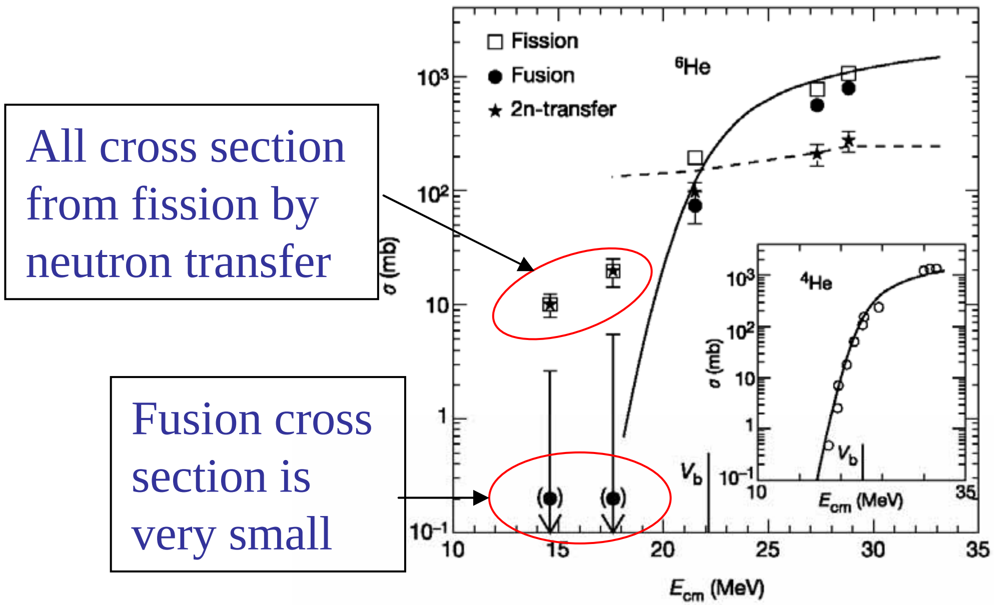
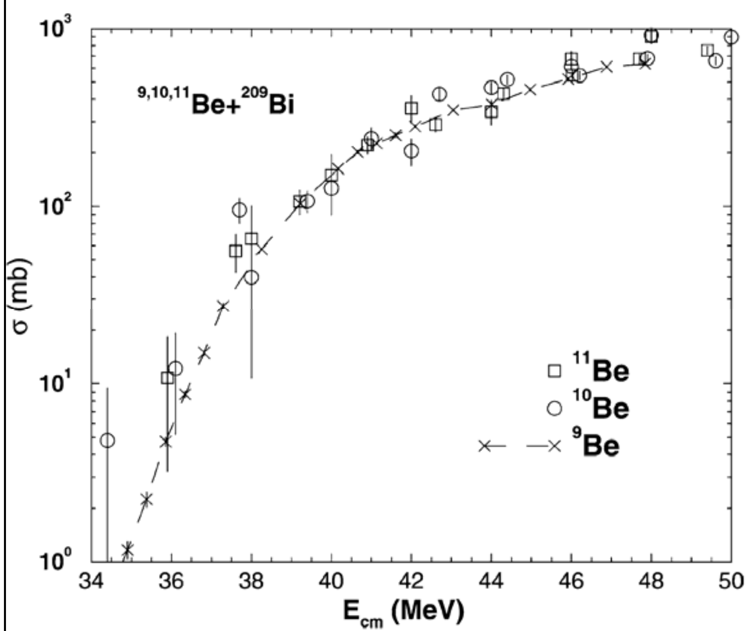


Figure 4 Fusion and two-neutron transfer cross-section for ^{6}He on ^{238}U (error bars are one standard deviation). Below the Coulomb barrier V_b there is no enhancement of the fusion cross-section. The curves are results of calculations performed using an effective optical potential, which accounts for the breakup of ^{6}He. The dotted curve is the two-neutron transfer cross-section in excited states of ^{240}U. The solid curve is the fusion cross-section obtained by employing a short-range imaginary potential to reproduce the incoming wave boundary condition[12]. The inset shows the data for ^{4}He on ^{238}U; the curve is the fusion cross-section obtained using a short-range imaginary potential.

Fusion cross section for ^{9,10,11}Be-^{209}Bi

Cross sections are similar among three projectiles



C. Signorini et.al, Nucl. Phys. 735 (2004) 329.

Recent measurements seem to suggest
No enhancement of fusion cross section by adding halo neutrons

Time-dependent Mean-Field dynamics

$$i\hbar \frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[\rho(t)]\psi_i(\vec{r},t) \qquad \Psi(\vec{r}_1,\cdots,\vec{r}_N,t) = \det\{\psi_i(\vec{r}_j,t)\}$$

Small amplitude oscillation around ground state
= RPA (Random phase approximation), Linear response theory)
Giant resonances

Initial value problem, Nonlinear and nonperturbative dynamics
Heavy ion collision

3D TDHF dynamics
in Cartesian grid representation

H. Flocard, S.E. Koonin, M.S. Weiss, 1978
P. Bonche, B. Grammaticos, S.E. Koonin, 1978

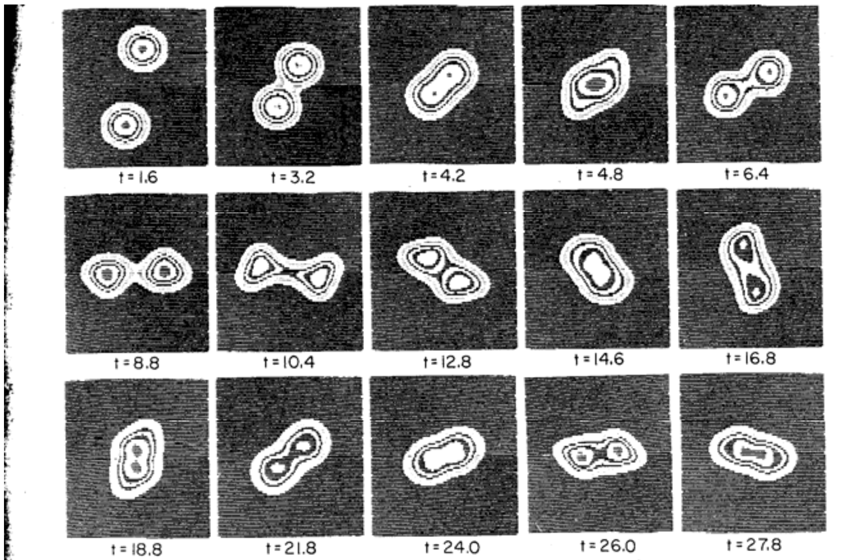


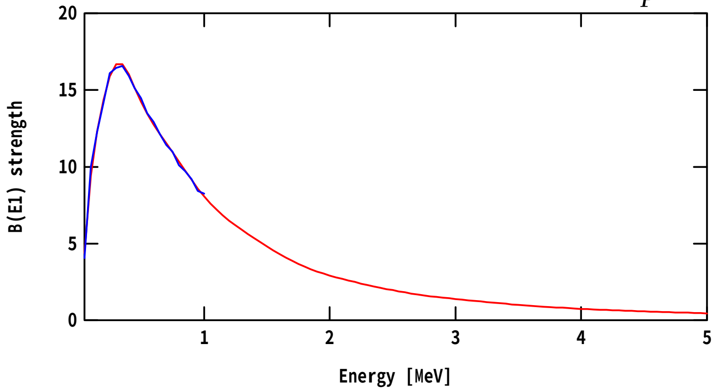
FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{lab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

Continuum RPA for Giant resonance

Dipole response function

$$\frac{dB(E1)}{dE} = -\frac{1}{\pi}\mathrm{Im}\sum_m \left\langle \phi_0 \left| M_{1m}^{+} \frac{1}{E+i\varepsilon-H} M_{1m} \right| \phi_0 \right\rangle \qquad M_{1m} = -\frac{Z_C}{A_P} erY_{1m}(\hat{r})$$

Single-particle response around threshold



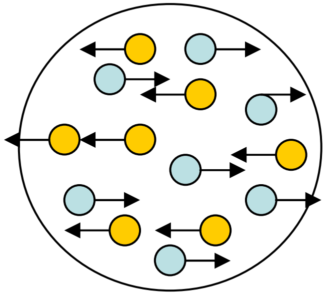
Response function with correlation: RPA (Random phase approx.)

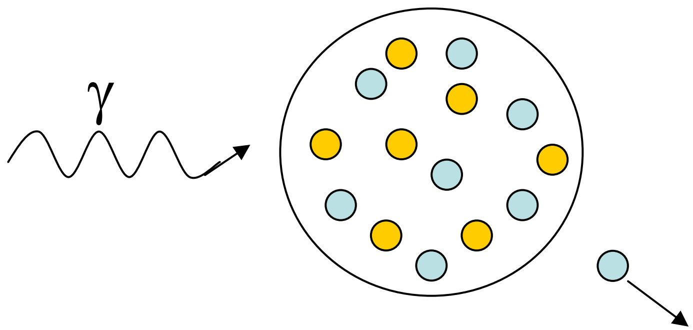
Time-dependent mean-field equation,
start with distortion in the ground state orbital

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[\rho(t)]\psi_i(\vec{r},t)$$

$$\psi_i(\vec{r},t=0) = \exp[-ikF(\vec{r})]\phi_i(\vec{r})$$

$$\frac{dB(F)}{dE} \propto -\frac{1}{\pi k}\mathrm{Im}\int_0^\infty dt F(\vec{r})\rho(\vec{r},t)$$





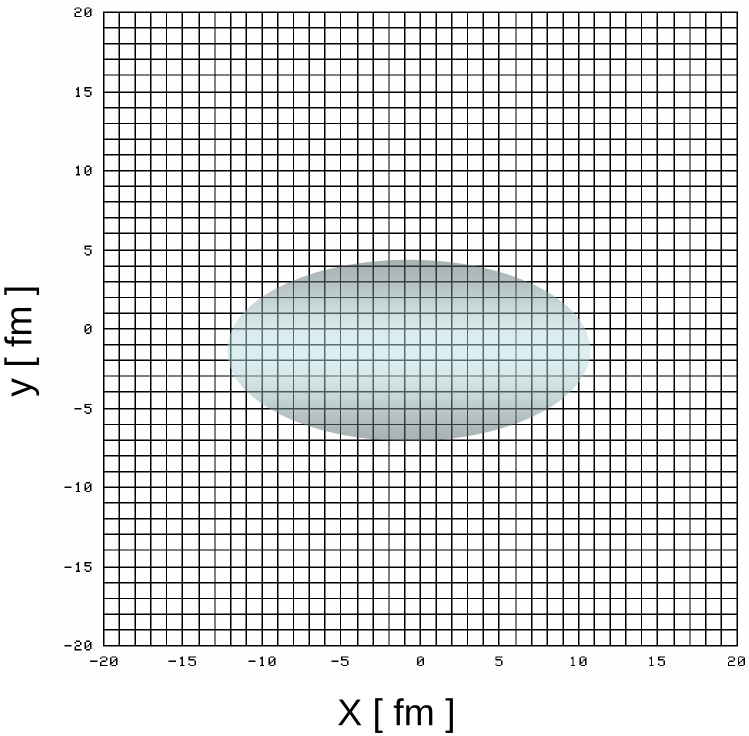
How to impose boundary condition?

Spherical nuclei

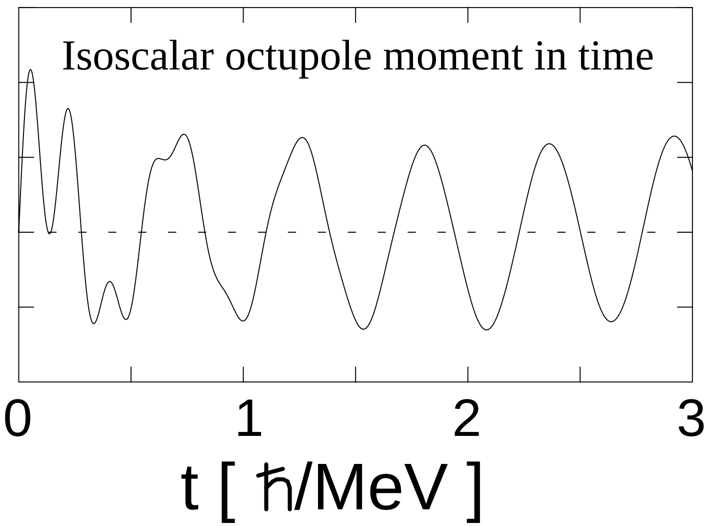
radial Hartree-Fock equation (1D problem)
continuum RPA (Shlomo and Bertsch, 1975)

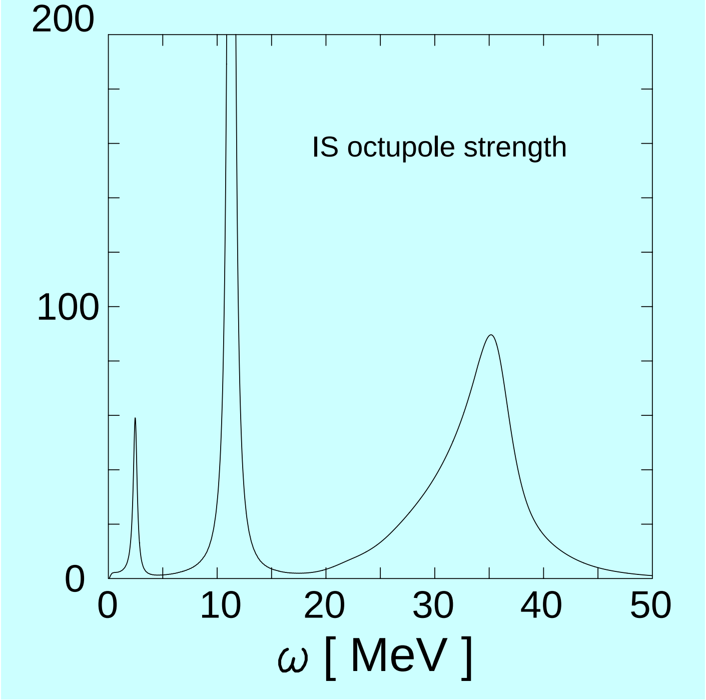
3D Cartesian grid for spherical and deformed nuclei

TDHF with absorbing potential

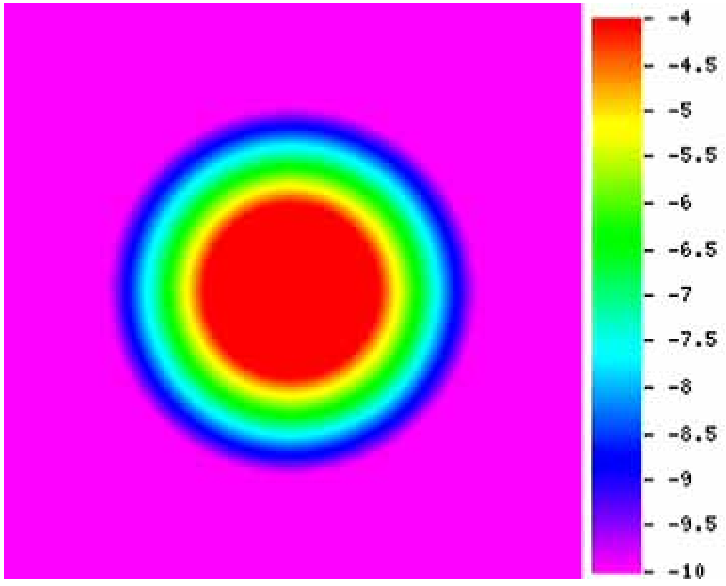


Isoscalar octupole resonance in ^{16}O (BKN interaction)

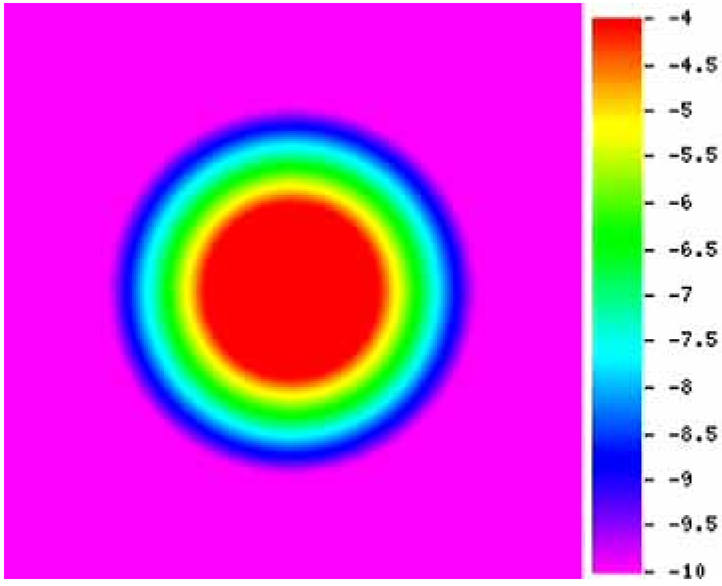




TDHF with absorbing potential

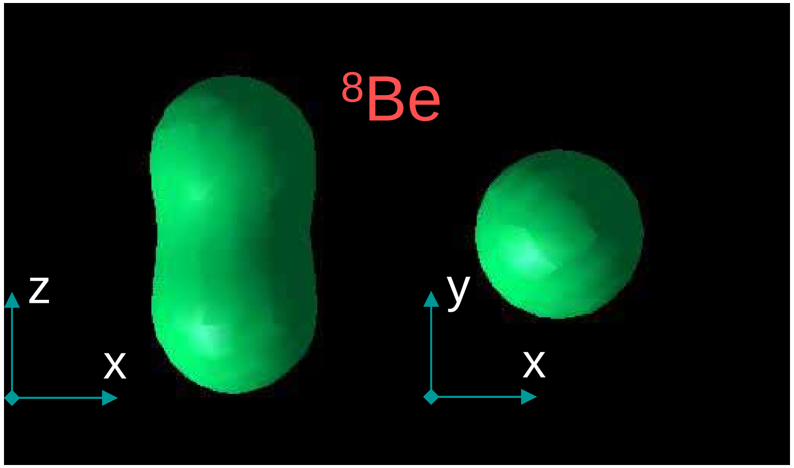


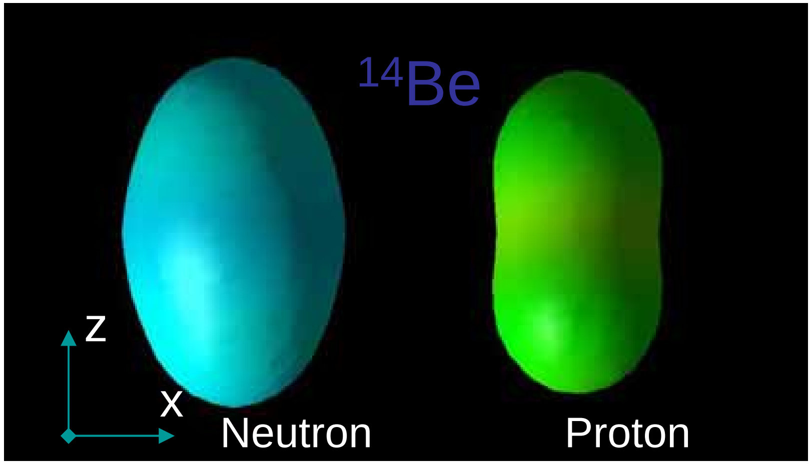
without absorbing potential



Isovector dipole response of Be isotopes with Skyrme interaction

Nakatsukasa, Yabana, Phys. Rev. C71 (2005) 024301





Density Functional Theory in Nuclei and Electronic systems

Nuclear physics

1972 Nuclear DFT, Skyme HF
(Negele, Vautherin, Brink)

1975 Continuum RPA for nuclear GR
(Bertsch, Shlomo)

1978 3D TDHF
(Flocard, Koonin, Weiss,
Bonche, Grammaticos, Koonin)

Electronic systems

Atomic, molecular, and condensed matter physics,
Quantum chemistry

1964 Foundation of DFT (Kohn)
1965 Kohn-Sham theory

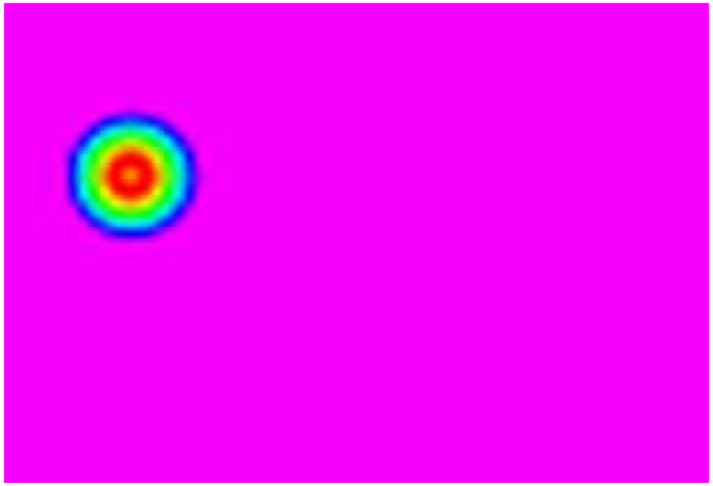
1980 Continuum RPA for rare-gas atom
(Zangwill, Soven)
1984 Continuum RPA for metallic cluster
(Ekardt)

1996 3D TDLDA for electrons
(Yabana, Bertsch)

Quantum dynamics simulation for Fermion many-body systems

Applications of time-dependent mean-field theory for electronic systems

Atomic physics:
Collision of highly-charged ion with atom

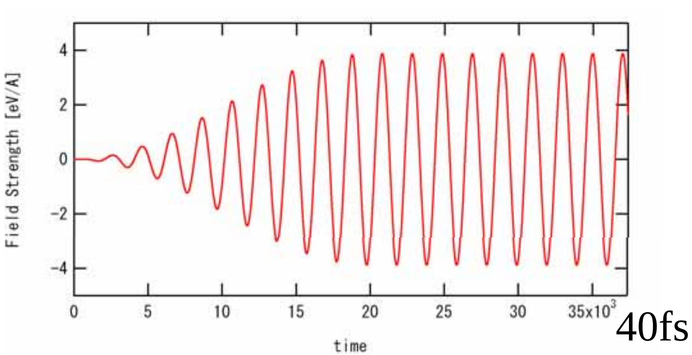


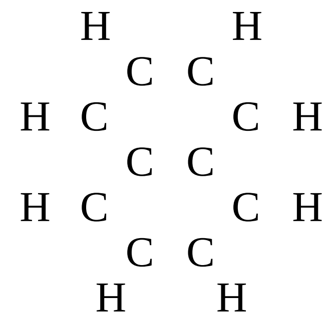
Ar^{8+} - Ar at E=18keV

Formation of highly excited ion (hollow atom)

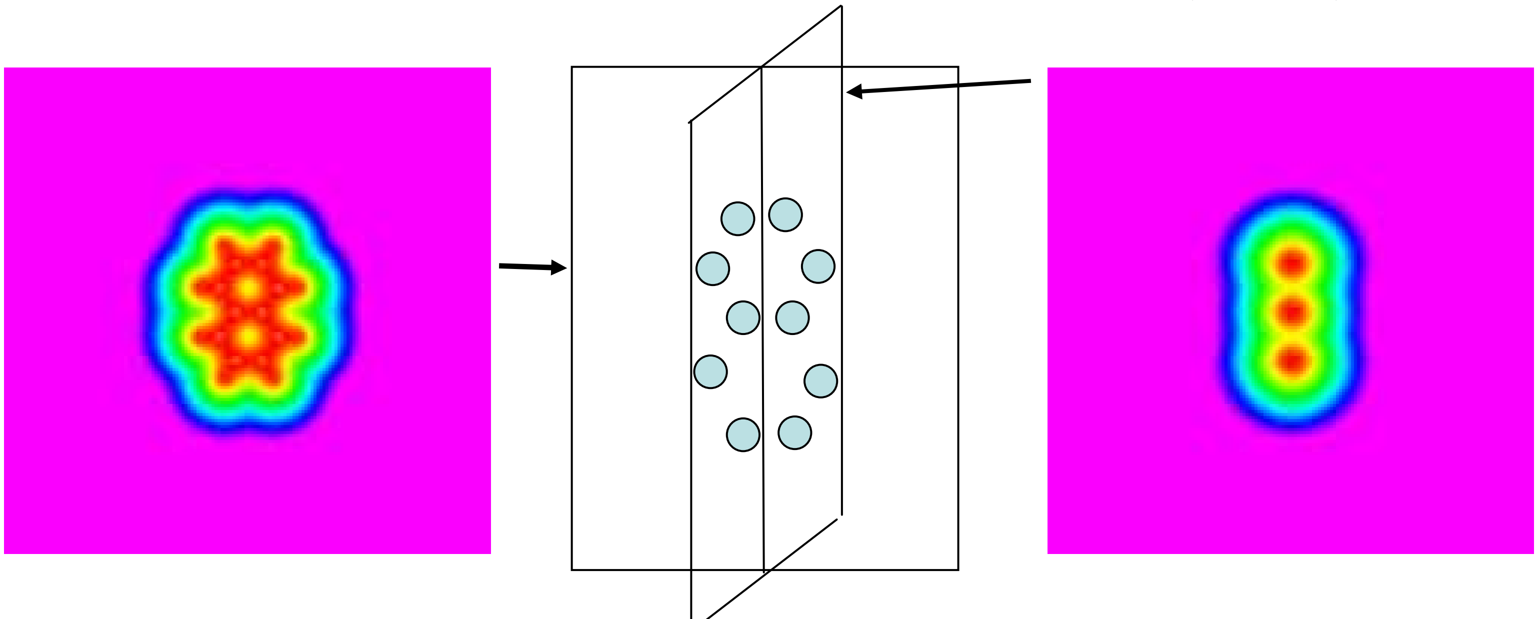
Intense Laser Science   moderate intensity laser: 10^{14}W/cm$_2$ 1-10eV/Å

Napthalene ($C_{10}H_8$) molecule in laser field



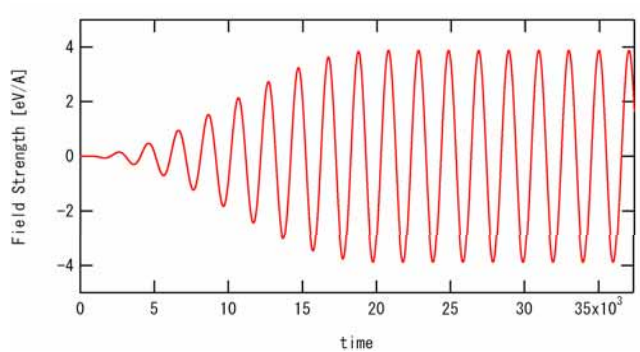


2.5x10^{13}W/cm^2, 800nm (1.55eV)



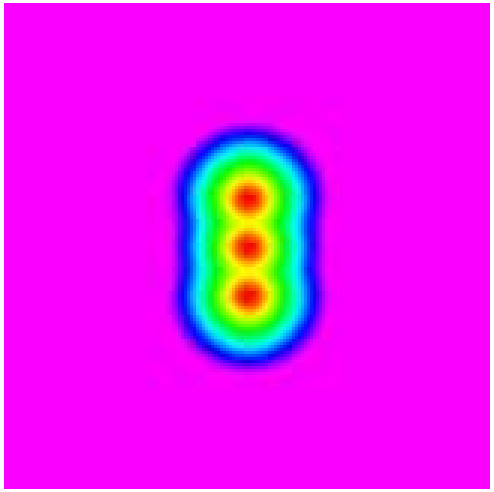
Laser frequency dependence of Electron Dynamics

$2.5\mathrm{x}10^{13}\mathrm{W/cm}^2$

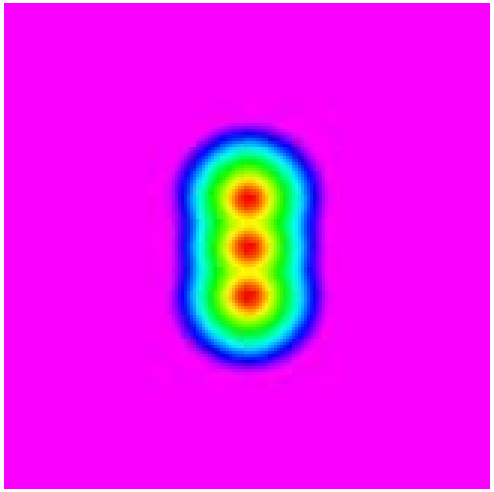


40fs

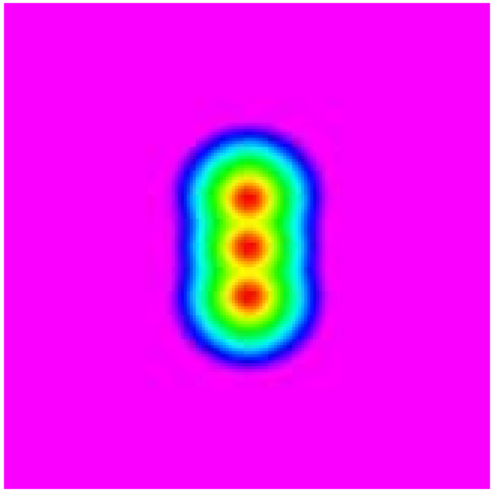
1600nm (0.78eV)



800nm (1.55eV)



400nm (3.1eV)

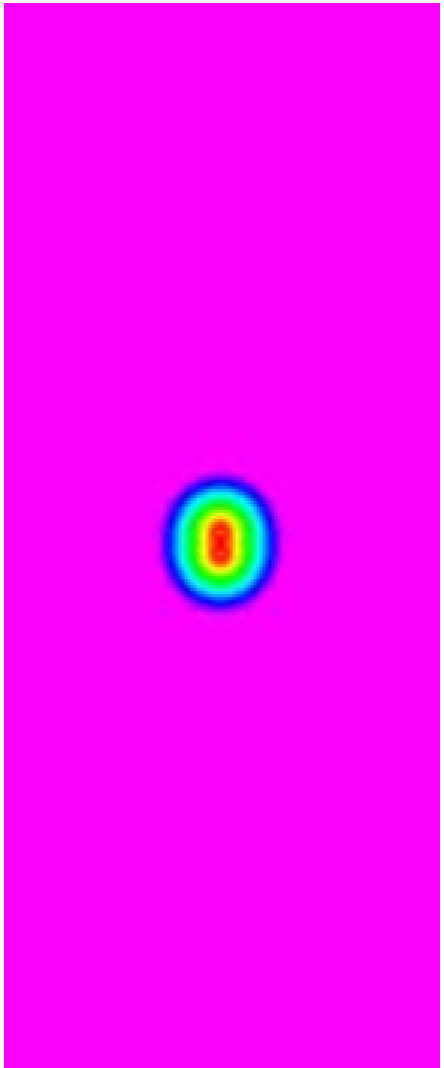


Quantum tunneling ←

(Ti:sapphire laser)

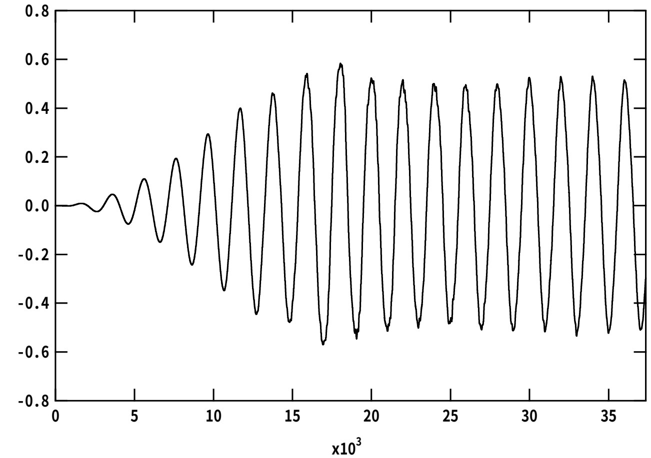
→ Multiphoton absorption

N_2 molecule in $2x10^{14}W/cm^2$, 800nm laser



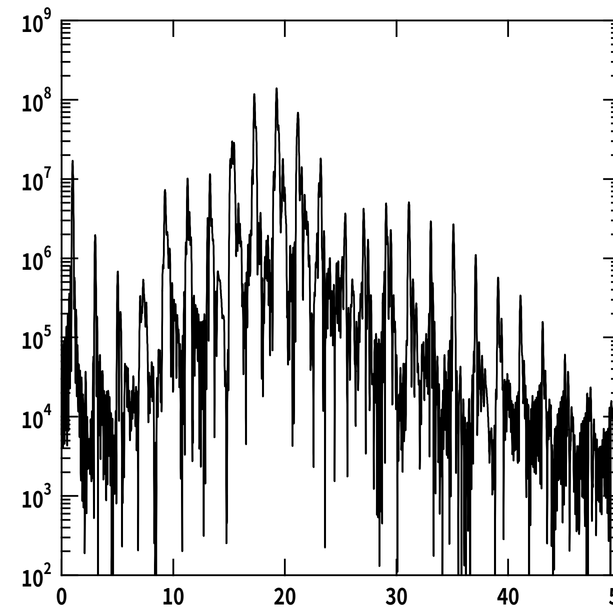
dipole moment

$$d(t)=\sum_i \langle\psi_i(t)|z|\psi_i(t)\rangle$$



radiation emission
(high harmonic generation)

$$I(\omega)\propto\left|\int dt e^{i\omega t}d_A(t)\right|^2$$

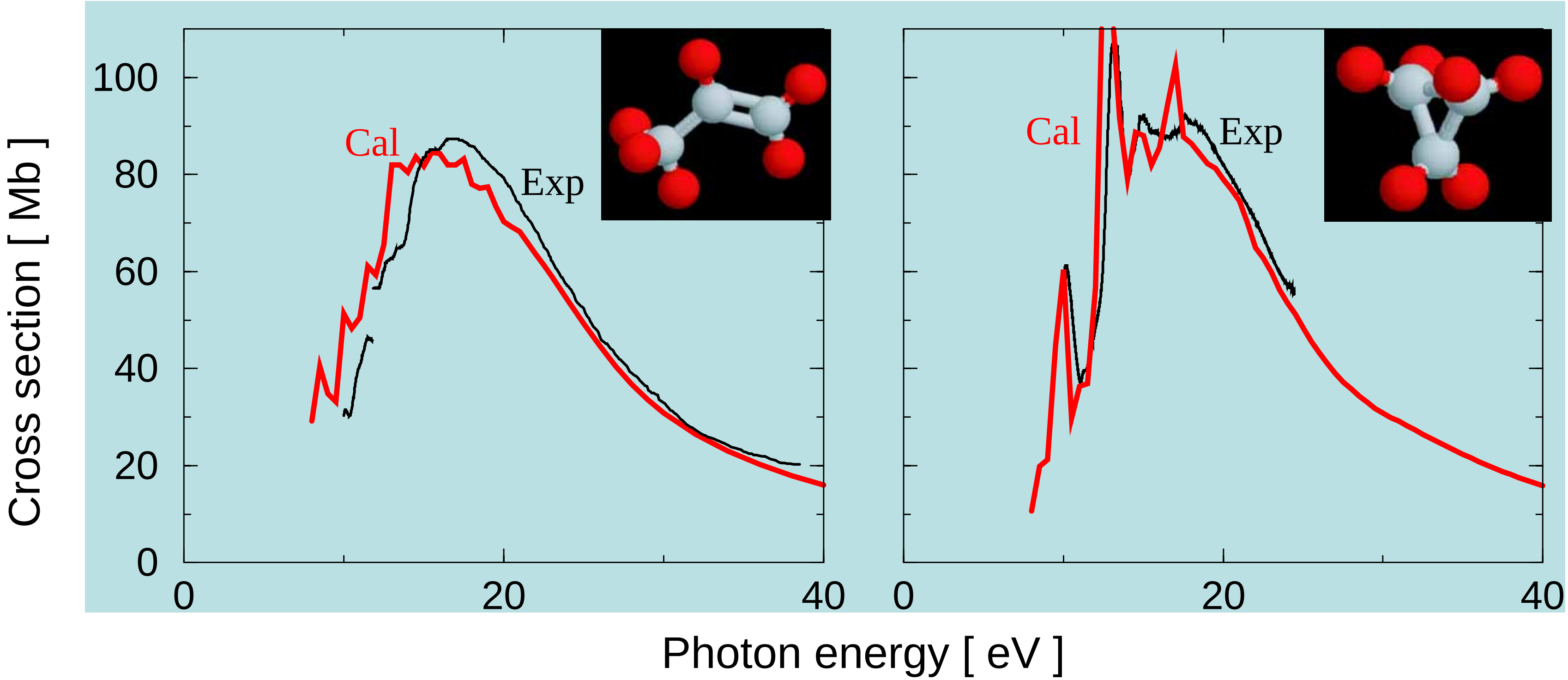


Linear optical absorption: from organic molecules to biomolecules

C_3H_6 isomer molecules

T. Nakatsukasa & K. Yabana, Chem. Phys. Lett. 374 (2003) 613.

- TDLDA cal with LB94 in 3D real space
- 33401 lattice points (r < 6 Å)
- Isomer effects can be understood in terms of symmetry and anti-screening effects on bound-to-continuum excitations.



Exp: K. Kameta, K. Muramatsu, S. Machida, N. Kouchi, Y. Hatano, J. Phys. B32(1999)2719.