Visualizing Reaction Mechanism

A time-dependent Schrödinger equation approach

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Solve static quantum problem by time-dependent method:

- Intuitive understanding of the dynamics.
- Boundary condition is not necessary.
- Computationally demanding.

Examples (3-body dynamics):

- Low energy reaction of halo nuclei
- Dipole response of two-neutron halo nuclei

Wave packet calculation for fusion probability

Radial Schroedinger equation for l=0

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

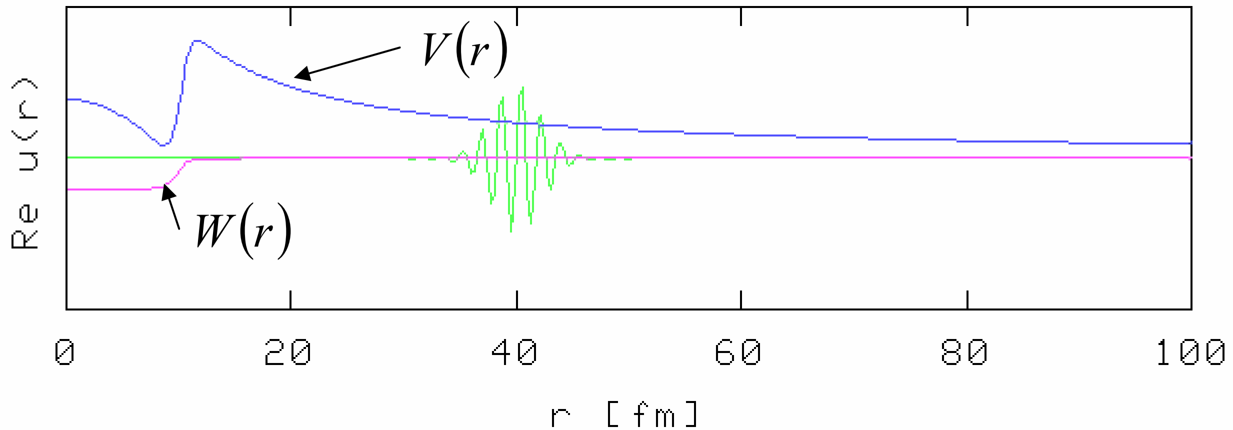
Flux absorbed by W(r) represents fusion.

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

$^{10}Be - ^{208}Pb$



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?

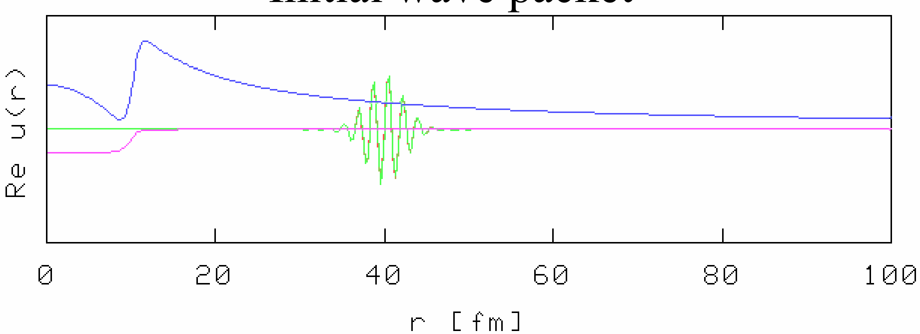
Extract static (fixed-E) information from wave-packet dynamics:

define energy distribution

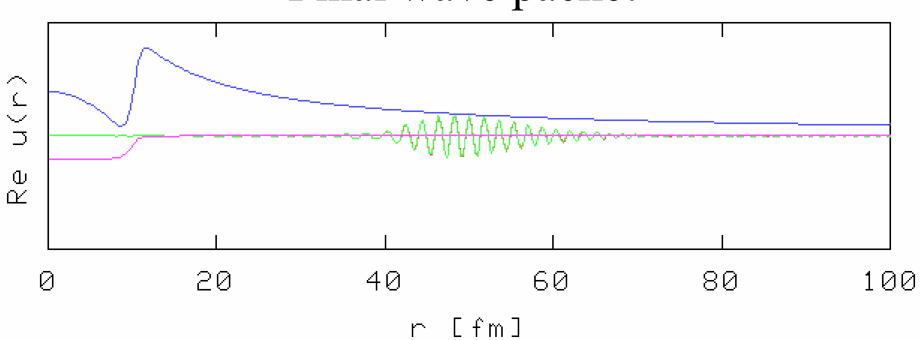
$$P_a(E) = \langle u_a | \delta(E-H) | u_a \rangle = \frac{1}{2\pi\hbar}\int_0^\infty dt\, e^{iEt/\hbar} \left\langle u_a\left(-\frac{t}{2}\right) \middle| u_a\left(\frac{t}{2}\right) \right\rangle$$

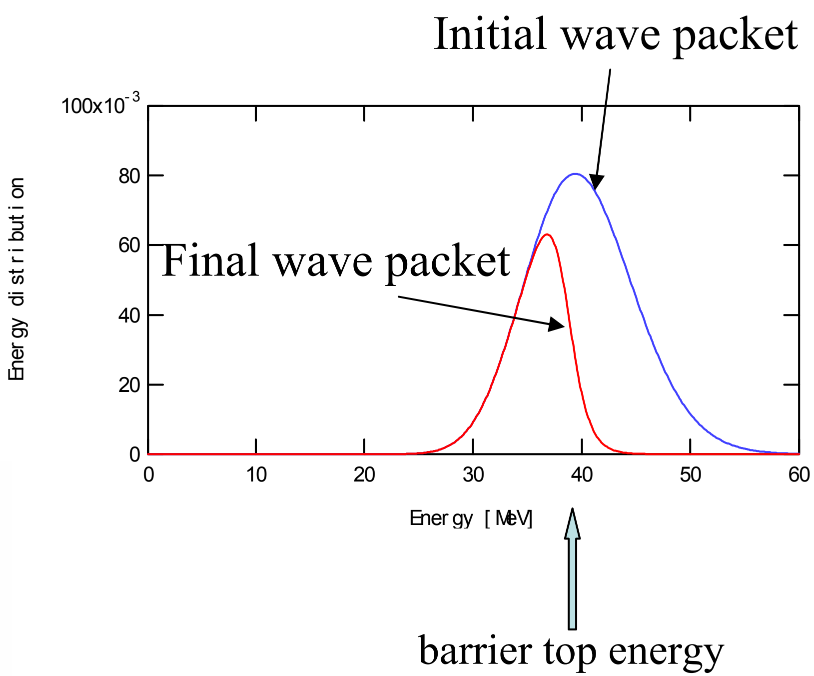
$$\delta(E-H) == \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{i(E-H)t/\hbar}$$

Initial wave packet

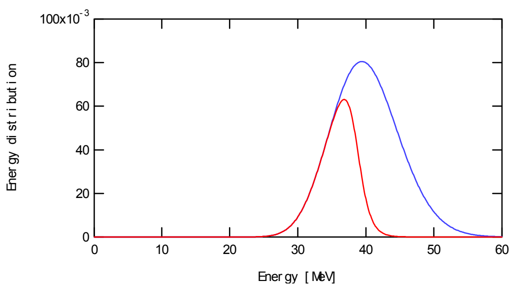


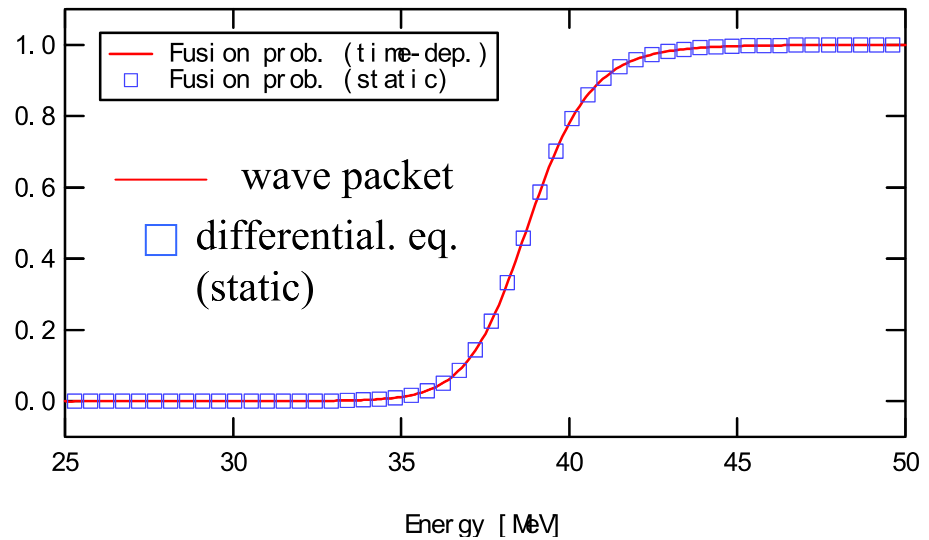
Final wave packet





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

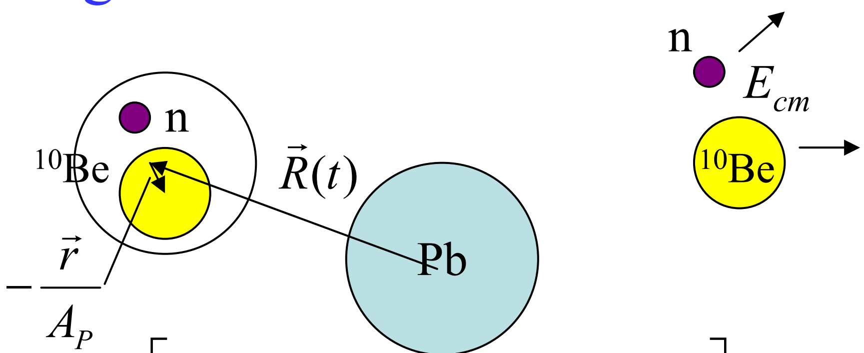


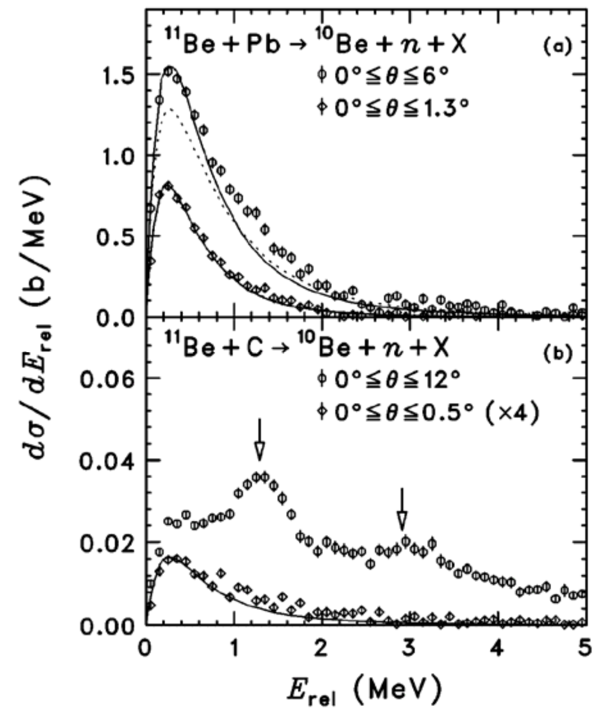


Fusion probability for whole barrier region from single wave-packet calculation.

No boundary condition required in the wave packet calculation.
(applicable to even 3-body reaction with 3 charged particles.)

1-Dimensional example:
Dipole strength of halo nuclei around threshold





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

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

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

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

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

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 by real-time propagation

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

$$\frac{1}{E + i\varepsilon - H} \rightarrow -i\pi\delta(E - H)$$

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

Time representation of response function

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

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

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

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

In the partial wave expansion,

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

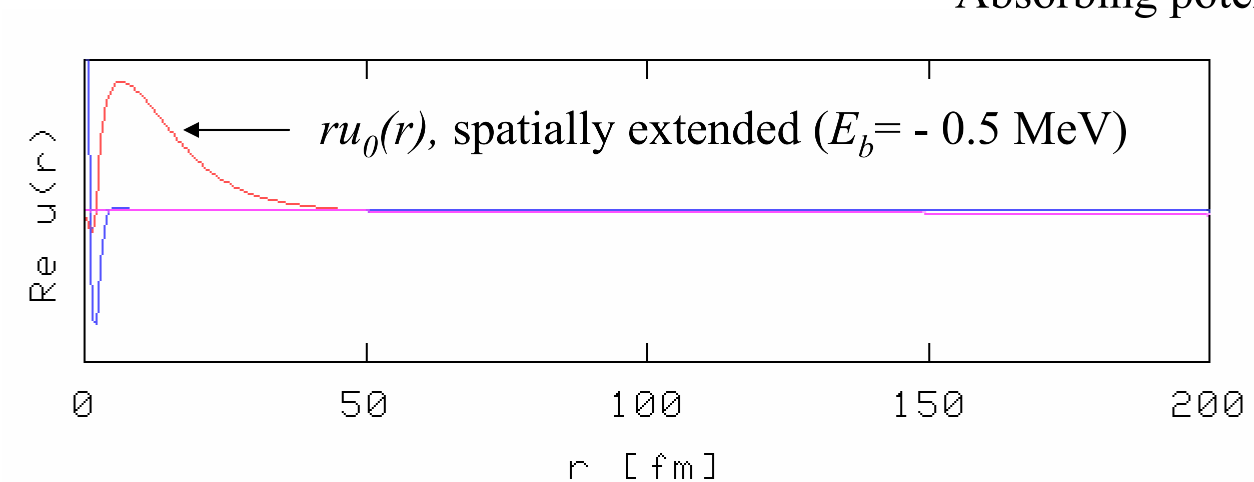
$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{r}, t\right) = H\psi\left(\vec{r}, t\right)$$

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

Initial condition:
r multipled to s-wave ground state in ^{11}Be

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

Absorbing potential to save spatial region

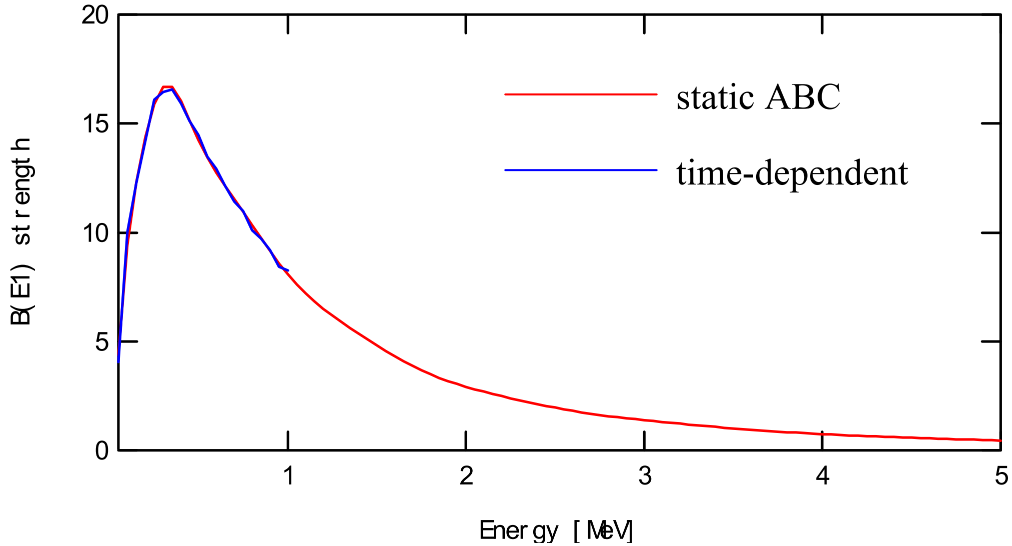


V0=-62.1, R=2.691, a=0.52
E_bound=-0.5MeV
Nr=400, dr=0.5, Nt=100000, dt=0.0005

$$r u_{l=0}\left(r\right) = \sum_i c_i y_i\left(r\right) + \int dE c\left(E\right) y_E\left(r\right)$$

Time-dependent calculation

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



Time-independent calculation

Scattering wave

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

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

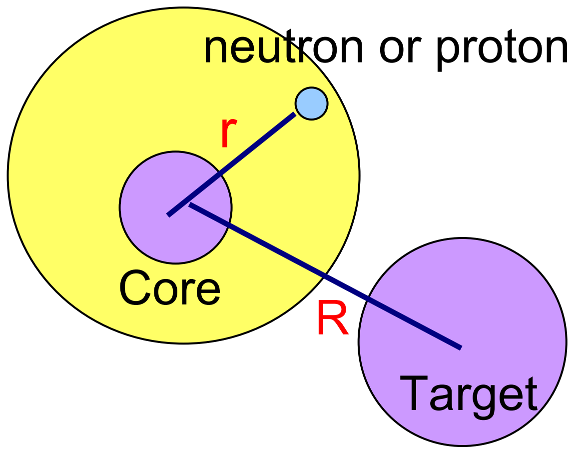
$$\left[E - H - iW_{abs}(r)\right]\chi(\vec{r}) = M_{1m}\phi_0(\vec{r}) \qquad \chi(\vec{r}) \underset{r\to\infty}{\longrightarrow} 0$$

Linear problem in the partial wave expansion

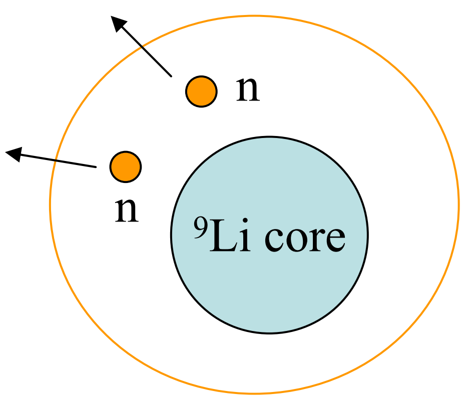
$$\left[E - \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) + iW_{abs}(r)\right)\right] w_{l=1}(r) = r u_0(r)$$

3-body dynamics in real-time

Low energy reaction of single-halo nucleus



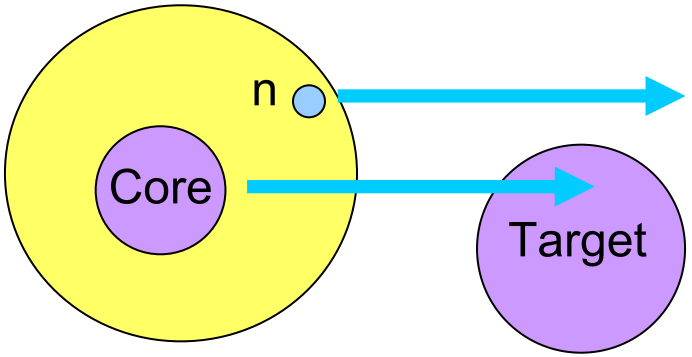
Dipole response function of ^{11}Li (just started)



Reactions of halo nuclei at high incident energy

Success of Glauber and eikonal picture
Core and nucleon are scattered independently from the target

$$\phi_n \cdot \Phi_C \Rightarrow \exp[i\chi_{nT}]\phi_n \cdot \exp[i\chi_{CT}]\Phi_C$$



Separation between:
- Fast nucleus-nucleus relative motion
- Slow internal halo motion

What is a basic picture at low incident energy?

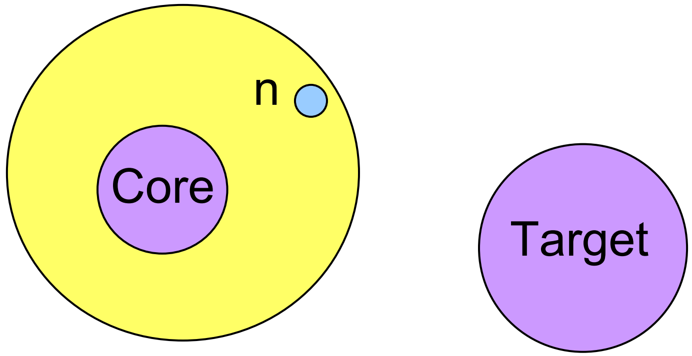
Controversial history on the role of halo nucleon

Both experimentally and theoretically.
Fusion enhancement or suppression?

Simple and intuitive argument.
(presented in early stage and still many people are thinking)

Fusion probability may be enhanced by long-range nuclear attraction.
but breakup hinders the enhancement of complete fusion.
breakup processes contributes to the incomplete fusion.

But …



^{6}He experiments: evidence of fusion enhancement was reported.

^{6}He + ^{209}Bi   J.J. Kolata et.al, PRL81(1998)4580.

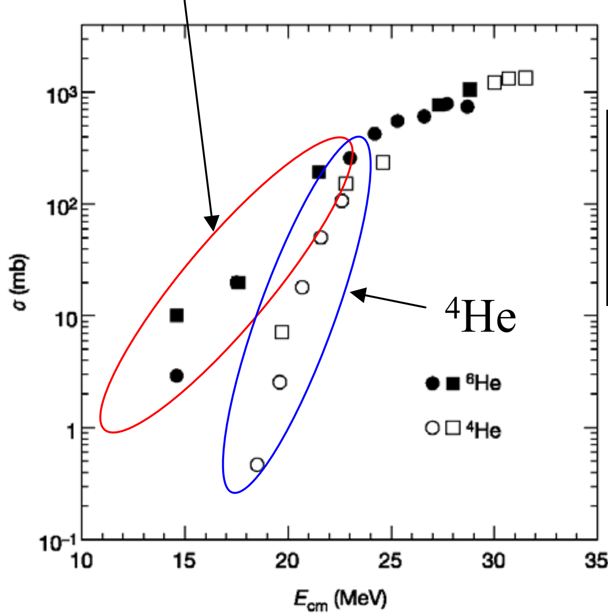
^{6}He + ^{238}U   M. Trotta et.al, PRL84(2000)2342.

However, recently …

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

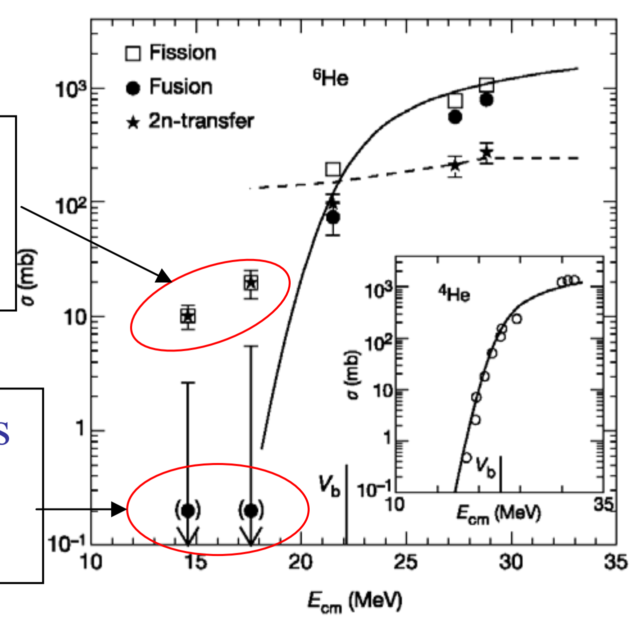
Fusion cross section of ^{6}He, ^{4}He on ^{238}U by measuring fission fragment.

^{6}He + ^{238}U, large cross section accompanying fission



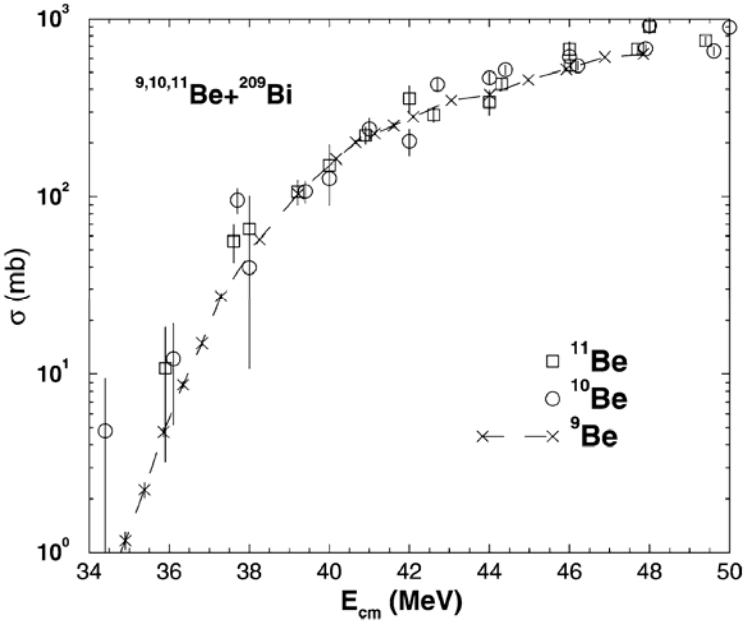
All cross section from fission by neutron transfer

Fusion cross section is very small



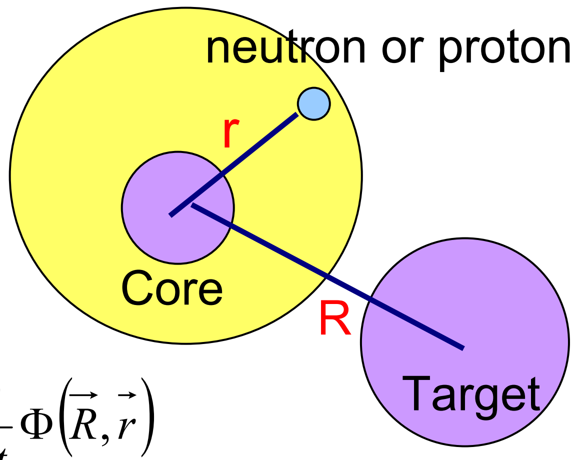
Fusion cross section for $^{9,10,11}Be$-^{209}Bi

Cross sections are similar among three projectiles



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

Solve 3-body problem accurately, and look what happens.

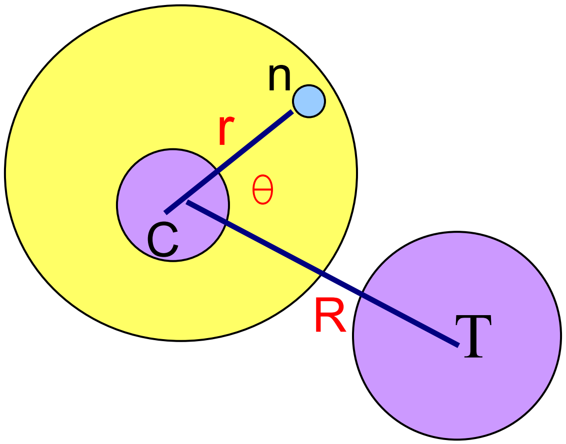


$$\left(-\frac{\hbar^2}{2\mu}\nabla_R{}^2 - \frac{\hbar^2}{2m}\nabla_r{}^2 + V_{nC}(r_{nC}) + V_{CT}(r_{CT}) + V_{nT}(r_{nT}) \right)\Phi(\vec{R},\vec{r}) = i\hbar\frac{\partial}{\partial t}\Phi(\vec{R},\vec{r})$$

We developed the time-dependent method,
and we found the fusion is hindered by adding the halo nucleon.

1-dim, 3-body: Yabana, Suzuki, Nucl. Phys. A588(1995)99c
3-dim, 3-body, J=0: Yabana, Prog. Theor. Phys. 97(1997)437
3-dim, 3-body, full J: Ito, Yabana, Nakatsukasa, Ueda, Phys. Lett submitted (2005).

3-body reaction (n-C)-T simulating $^{11}Be(=n+^{10}Be)$-^{209}Bi



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

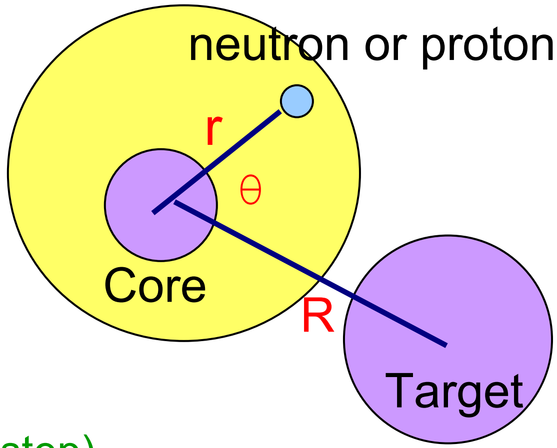
- $V_{nC}(r_{nC})$: real potential, weakly bound 2s bound orbital
- $V_{CT}(r_{CT})$: Coulomb + Nuclear potential
- $iW_{CT}(r_{CT})$: Core-Target fusion (=3-body fusion)
- $V_{nT}(r_{nT})$: real nuclear potential (+Coulomb for n=proton)

Computational aspects

- Partial wave expansion in body-fixed frame

$$\psi_{JM}\left(\vec{R},\vec{r},t\right)=\sum_{J\Omega l}\frac{u^{J}_{\Omega l}\left(R,r,t\right)}{Rr}\Theta^{\Omega}{}_{l}(\theta)D^{J}_{\Omega M}(\alpha\beta\gamma)$$

R.T.Pack, J. Chem. Phys. 60(1974)633



- Uniform grids for R and r (R<50fm 0.2fm step, r<60fm 1fm step)

- Large cutoff angular momentum, up to l_{max}=70 (maximum)

- Taylor expansion of time-evolution operator (as in TDHF calculations)

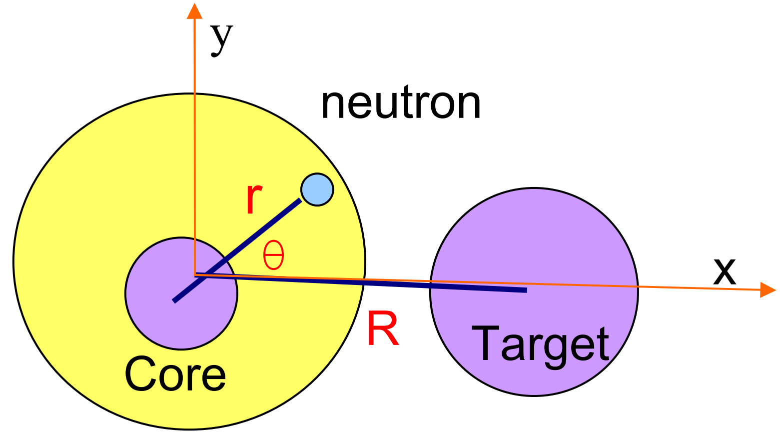
Initial wave packet: (s-wave n-C orbital)

$$u^{J}_{\Omega l}\left(R,r,t_0\right)=\delta_{\Omega 0}\delta_{lJ}\exp\left[-iKR-\gamma\left(R-R_0\right)^2\right]\phi_0(r)$$

Projectile-target relative motion
(incoming Gaussian wave packet)

Intial halo orbital (2s)

When a neutron is tightly bound in the projectile, two-center orbital and transfer process is significant.

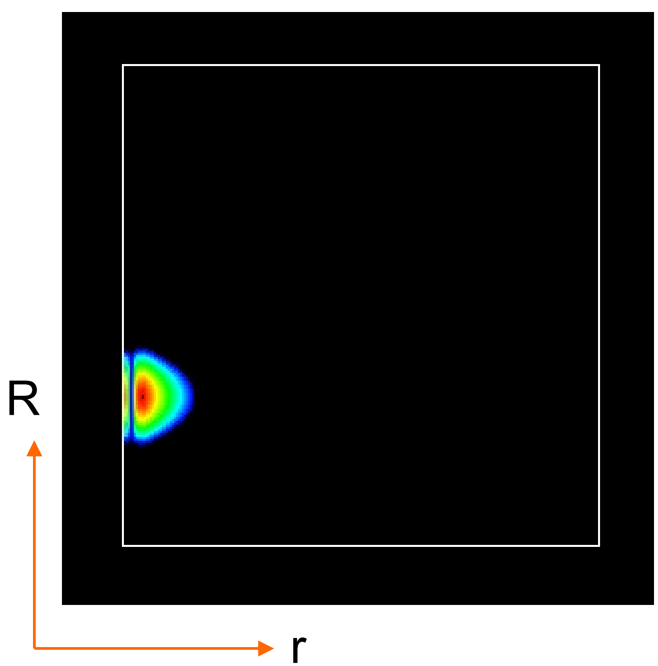


3-body dynamics
Tightly-bound projectile (E_b= - 3.5MeV)
(n-^{10}Be)-^{40}Ca

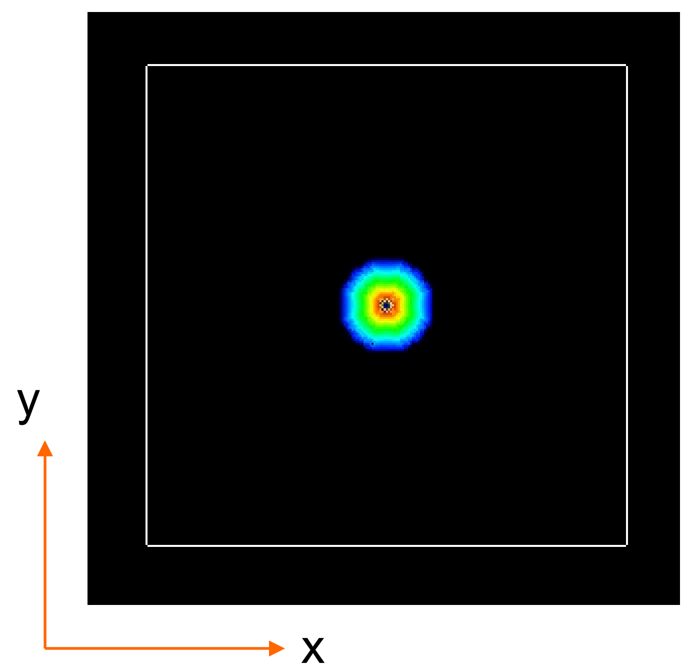
Initial wave packet:

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

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

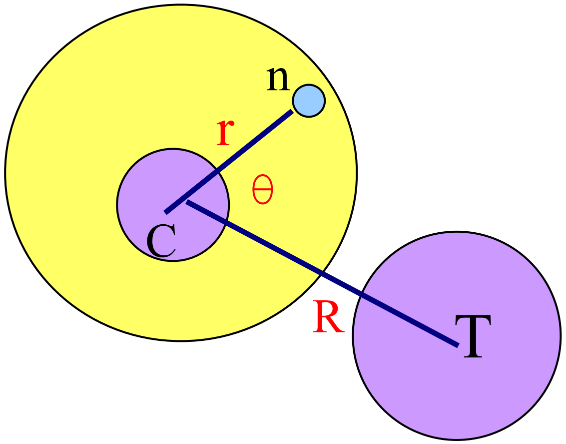


$$\rho\left(r,\theta,t\right)=\int dR\left|\psi\left(R,r,\theta,t\right)\right|^2$$



Fusion probability of 3-body system

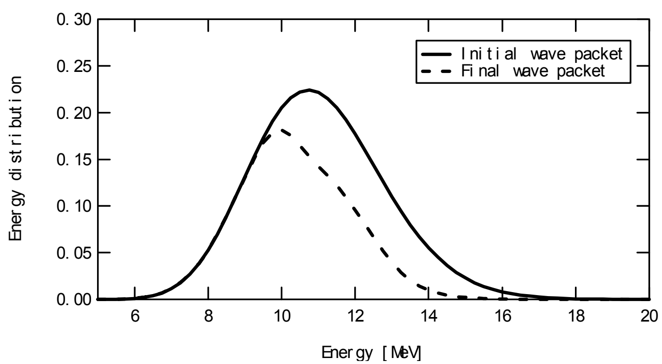
$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{R},\vec{r},t\right)=\left(-\frac{\hbar^2}{2\mu}\nabla_R^{\ 2}-\frac{\hbar^2}{2m}\nabla_r^{\ 2}+V_{nC}\left(r_{nC}\right)+V_{CT}\left(r_{CT}\right)+\underline{iW_{CT}\left(r_{CT}\right)}+V_{nT}\left(r_{nT}\right)\right)\psi\left(\vec{R},\vec{r},t\right)$$



Fusion = core-target gets over the barrier.
(flux absorbed by iW_{CT})

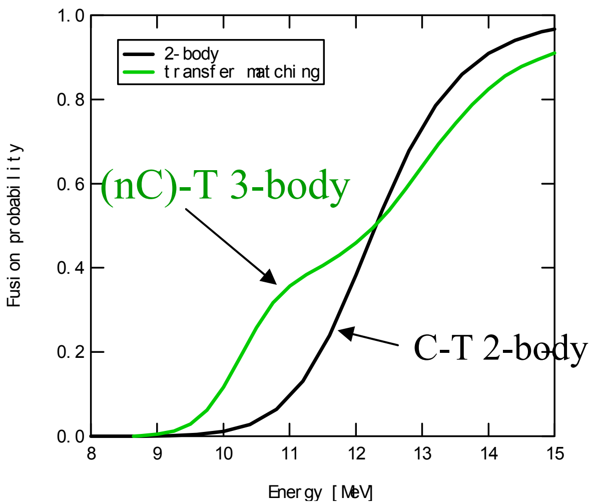
Energy distribution

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



Fusion probability

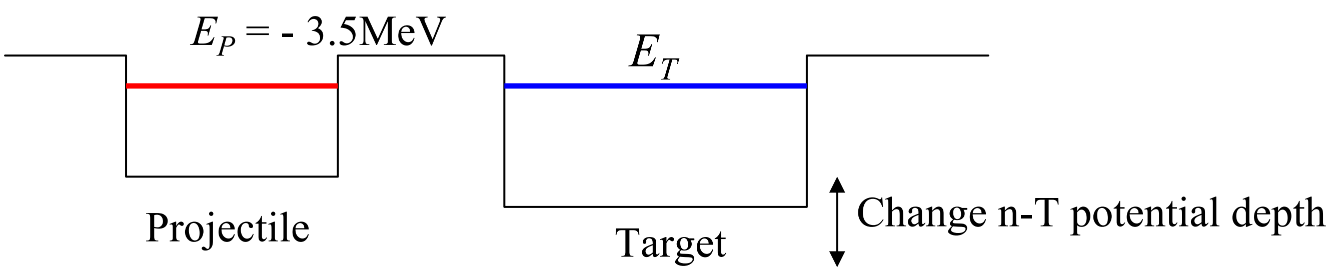
$$P_{fusion}(E)=\frac{P_i(E)-P_f(E)}{P_i(E)}$$

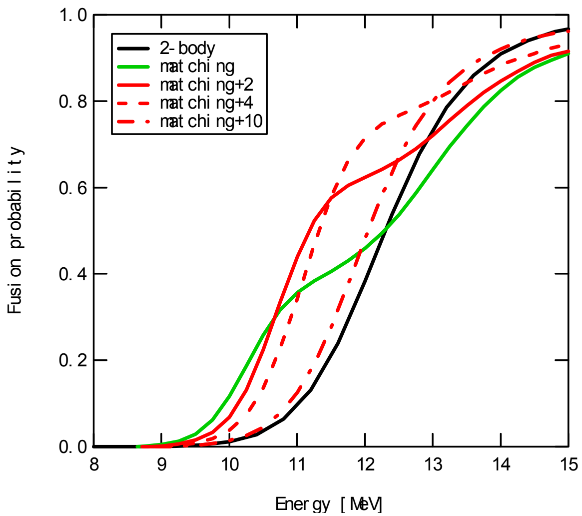


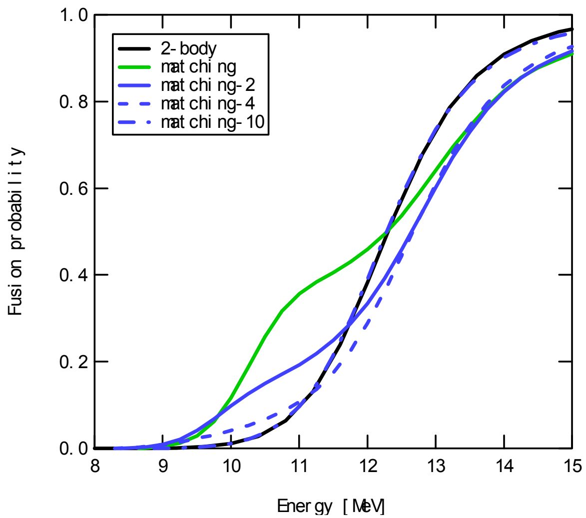
Large subbarrier enhancement

Role of added neutron in fusion process when neutron is tightly bound

Formation of molecular (two-center) orbital is crucial.







$E_P < E_T$
fusion enhancement

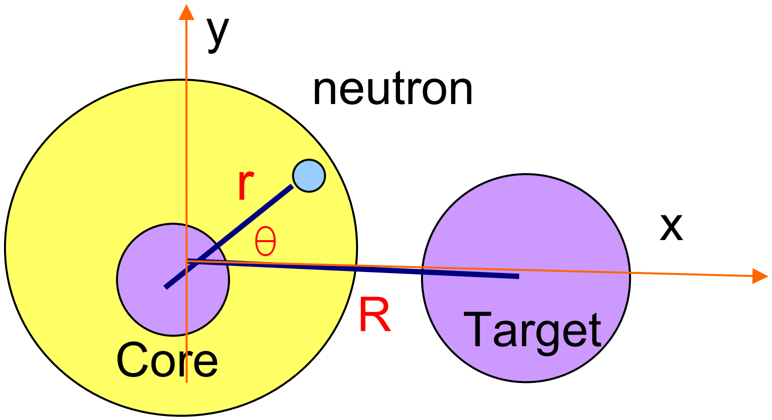
$E_P \approx E_T$
energy-dependent barrier

$E_P > E_T$
fusion suppression

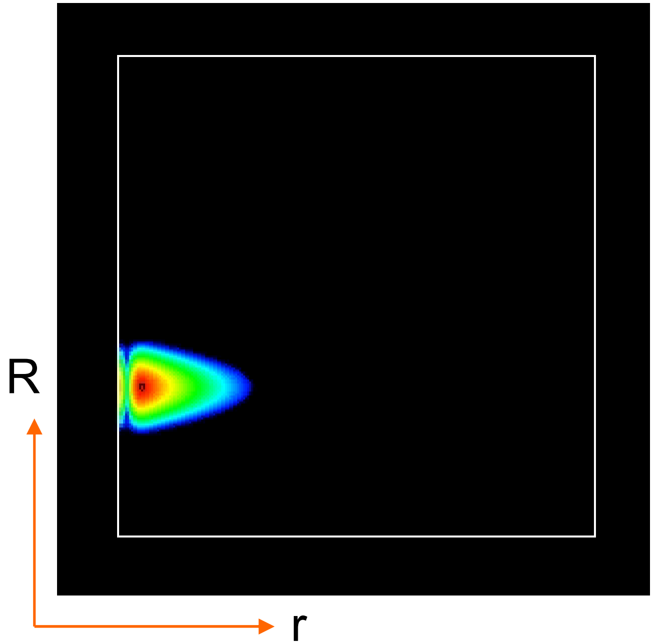
When a neutron is bound weakly in the projectile, Coulomb breakup is significant.

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

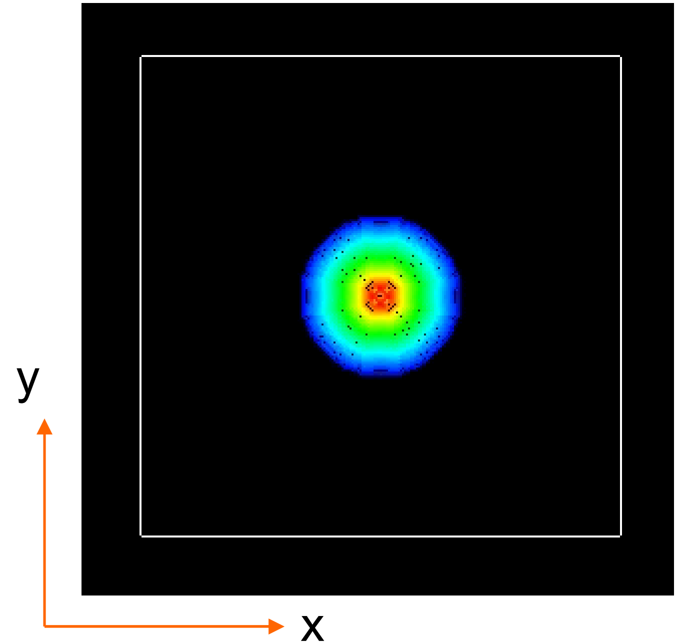
□n-C orbital energy: -0.6 MeV (Halo)



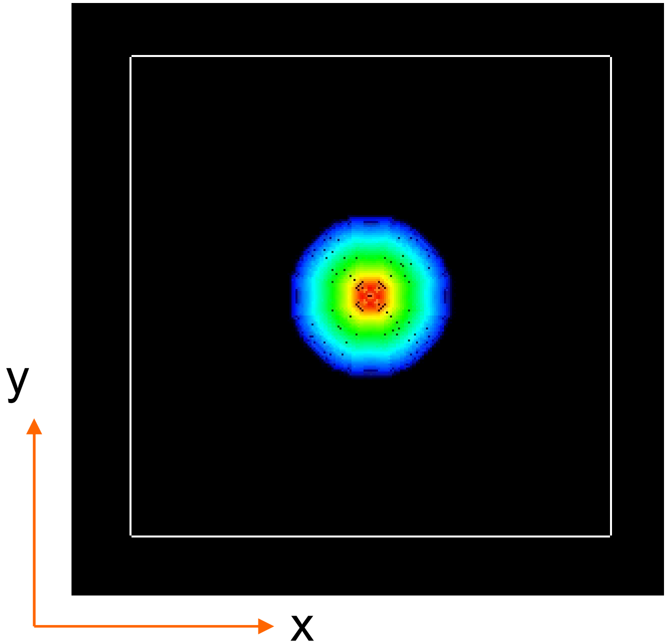
$$\rho(R,r,t)=\int d(\cos\theta)\left|\psi(R,r,\theta,t)\right|^2$$

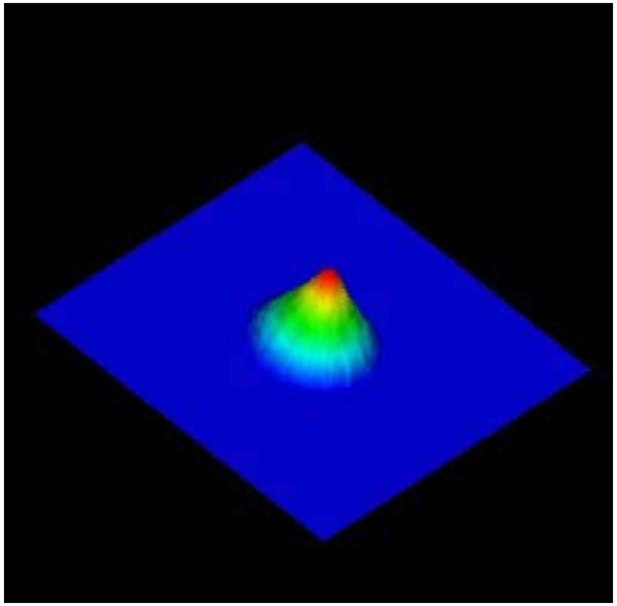


$$\rho(r,\theta,t)=\int dR\left|\psi(R,r,\theta,t)\right|^2$$

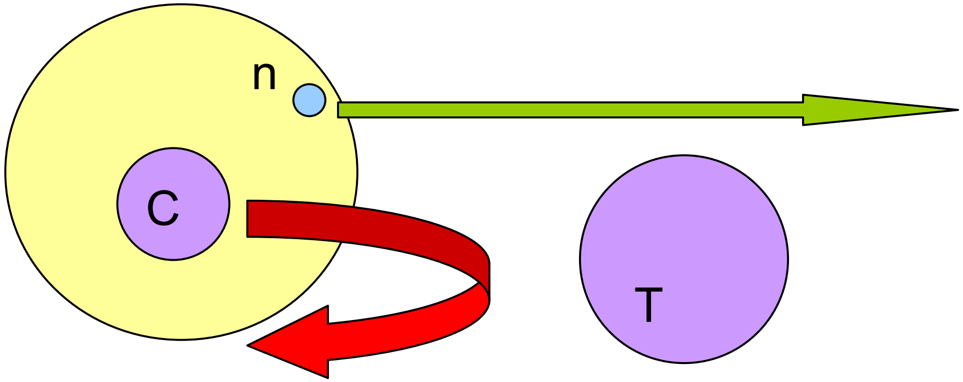


$$\rho(r,\theta,t) = \int dR \left|\psi(R,r,\theta,t)\right|^2$$

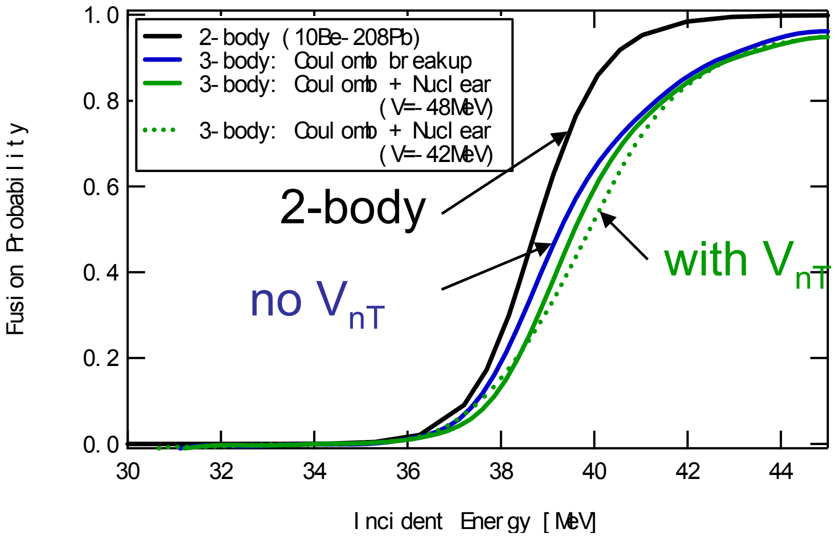




Coulomb breakup of halo neutron



Fusion probability of neutron-halo nuclei is suppressed

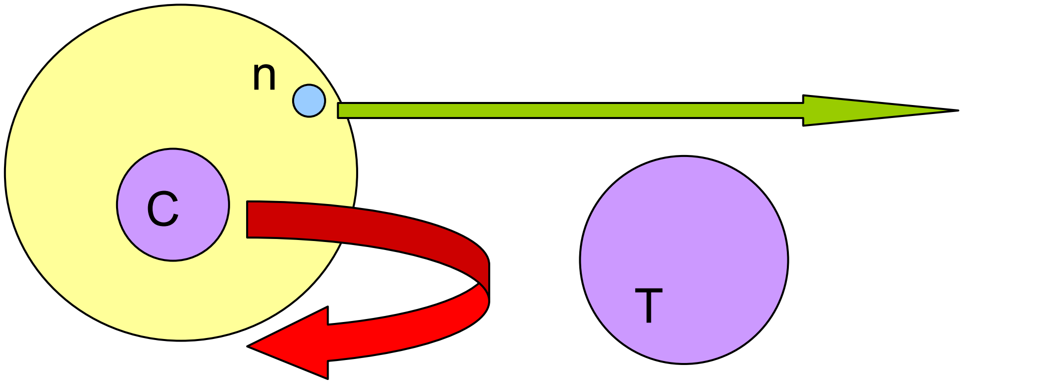


Why fusion probability suppressed by the Coulomb breakup?

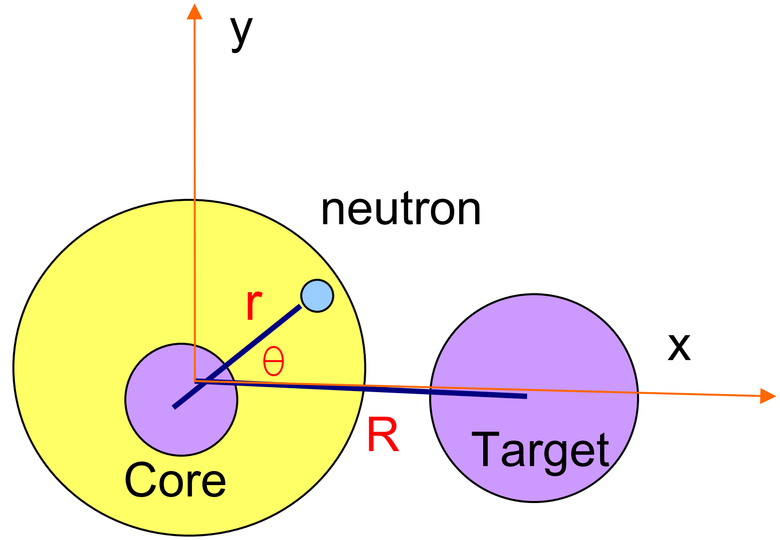
Possible Reason:

Core incident energy decreases effectively by neutron breakup

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



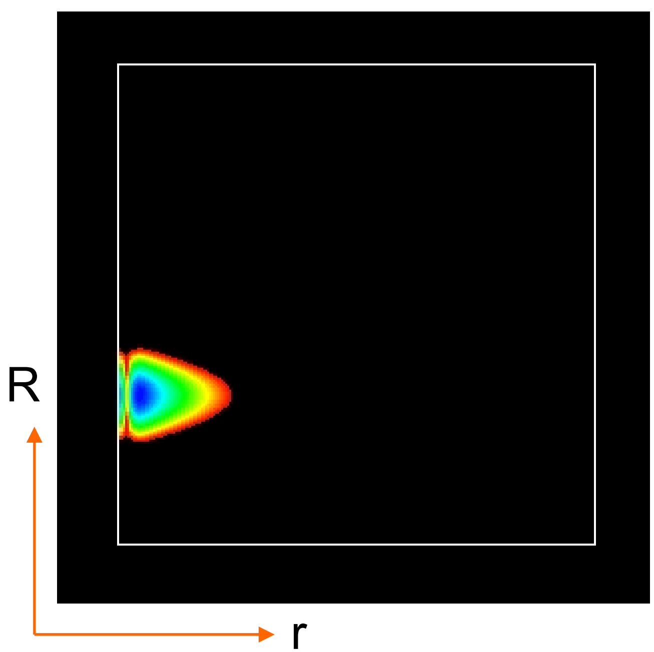
When a proton is bound weakly in the projectile, again Coulomb breakup is significant.



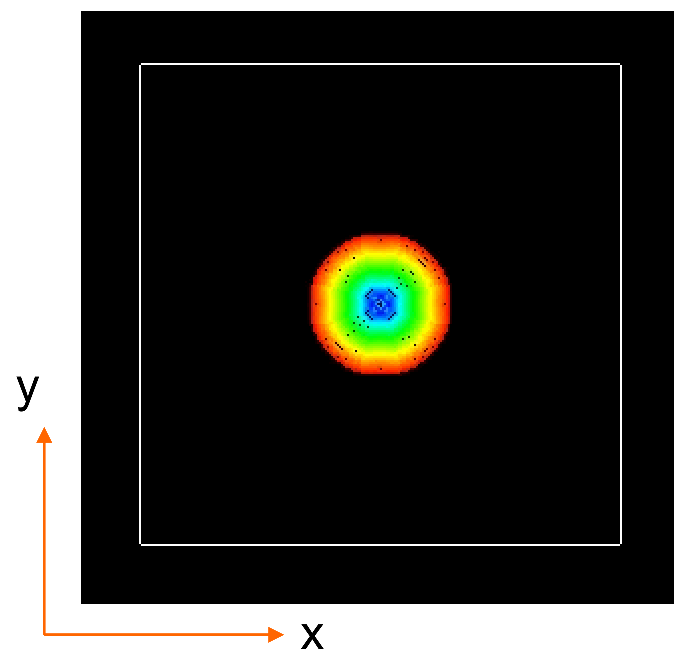
^{11}Be(p+^{10}Li)-^{208}Pb head-on collision (J=0)

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

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

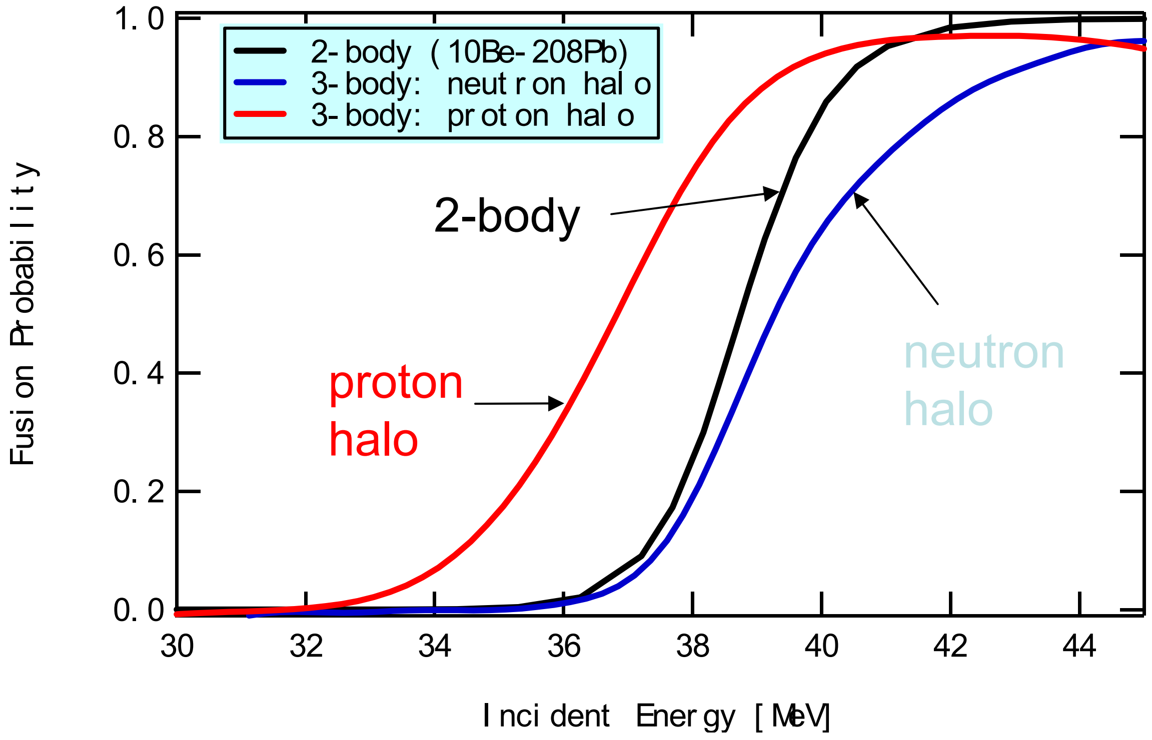


$$\rho(r,\theta,t)=\int dR\left|\psi(R,r,\theta,t)\right|^2$$



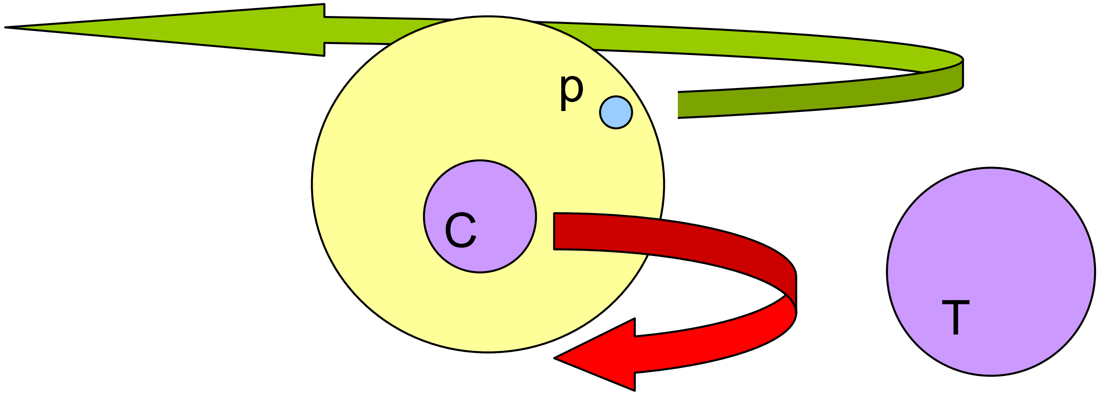
^{11}Be-^{208}Pb fusion probability

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?

Stronger backward acceleration by [charge/mass] ratio



Proton breakup :

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

Cross section calculation:

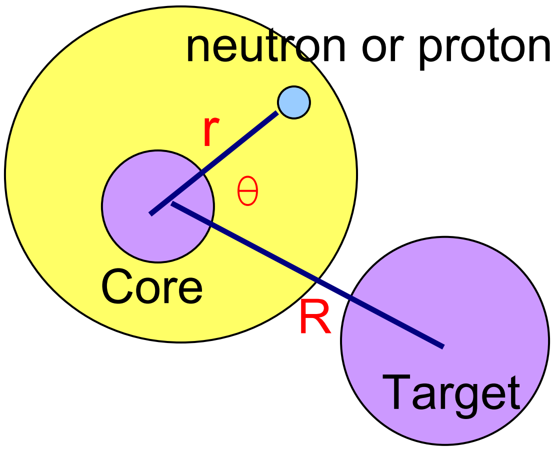
up to $J = 30\hbar, \quad \Omega_{\max} = 0$ (no-Coliolis approx.)

Computational aspects

□Partial wave expansion in body-fixed frame

$$\psi_{JM}\left(\vec{R},\vec{r},t\right) = \sum_{J\Omega l} \frac{u^J_{\Omega l}\left(R,r,t\right)}{Rr} \Theta^{\Omega}{}_{l}\left(\theta\right) D^J_{\Omega M}\left(\alpha\beta\gamma\right)$$

R.T.Pack, J. Chem. Phys. 60(1974)633



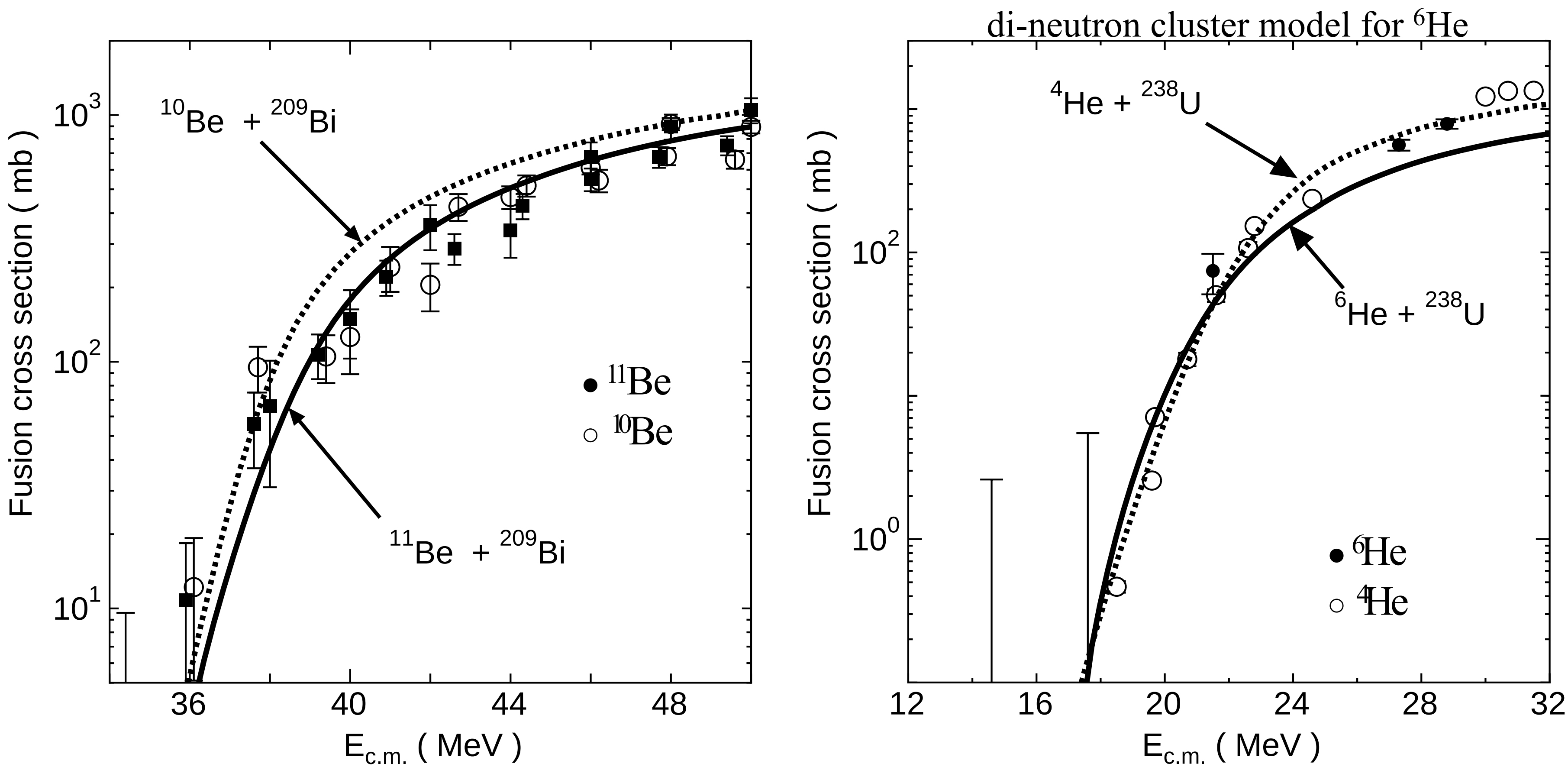
□Uniform grids for R and r

□Large cutoff angular momentum, up to l_{max}=70 (maximum)

□Taylor expansion of time-evolution operator
(as in TDHF calculations)

3-body time-dependent wave packet calculation
Fusion cross section of neutron halo nuclei

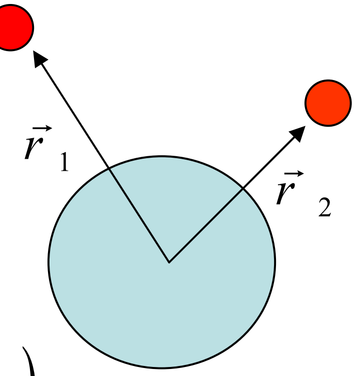
M. Ito, K. Yabana, T. Nakatsukasa, M. Ueda, submitted to Phys. Lett. B



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

Exp. R. Raabe et.al, Nature 431(2004) 823.

Dipole strength of borromean nuclei: real-time calculation



A simple 3-body model for ^{11}Li

$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{r}_1,\vec{r}_2,t\right)=\left(-\frac{\hbar^2}{2m}\nabla_{r_1}{}^2-\frac{\hbar^2}{2m}\nabla_{r_2}{}^2+V_{nC}(r_1)+V_{nC}(r_2)+V_{nn}\left(\left|\vec{r}_1-\vec{r}_2\right|\right)\right)\psi\left(\vec{r}_1,\vec{r}_2,t\right)$$

Simple treatment:

ignore recoil, no spin-orbit, just S=0 channel,...

Real-time propagation

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

$$=\frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty dt\,e^{iEt/\hbar}\sum_m\left\langle\psi_{1m}(0)\middle|\psi_{1m}(t)\right\rangle$$

$$\psi\left(\vec{r}_1,\vec{r}_2,t=0\right)=\left(z_1+z_2\right)\phi_0\left(\vec{r}_1,\vec{r}_2\right)$$

(Dipole operator) x (3-body ground state)

$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{r}_1,\vec{r}_2,t\right)=H\psi\left(\vec{r}_1,\vec{r}_2,t\right)$$

Hamiltonian

Woods-Saxon shape with

V_{nn}: R=1.5fm, a=0.6fm

V_{nC}: R=2.3fm, a=0.6fm

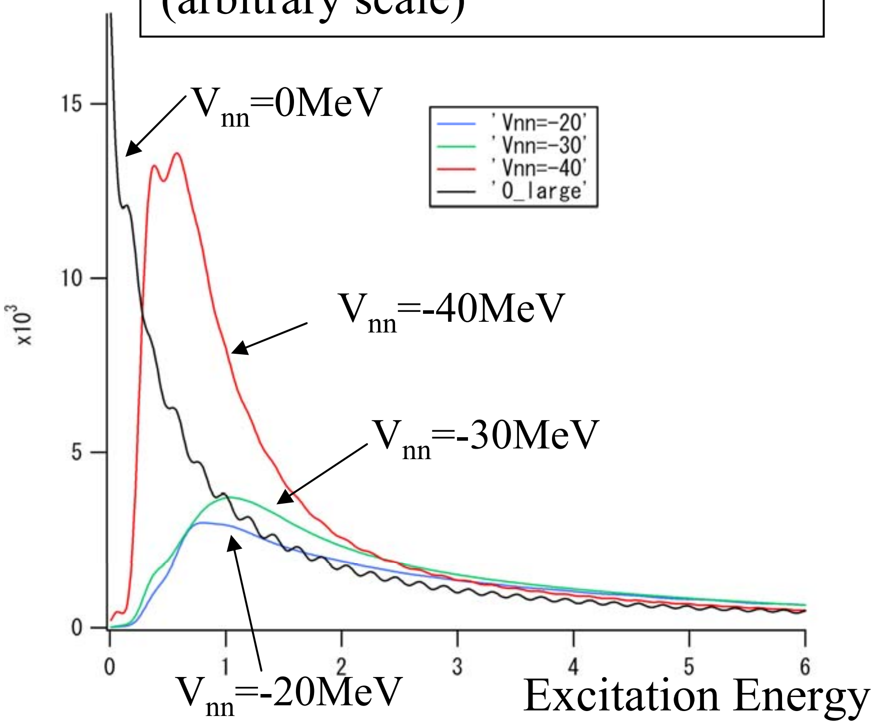
Potentials depth
set to 3-body binding energy at 0.3MeV

V_{nn}	E_{n-n}	V_{nC}	$E_{n-C}(l=1)$
0	No	-42.10	-0.15
-10	No	-40.23	No
-20	No	-37.94	
-30	No	-35.15	
-35	-0.019 MeV	-33.51	
-40	-0.33	-31.60	
-50	-1.78	-23.70	

Δr = 0.6fm, up to 90fm
absorbing potential at 30fm < r < 90fm
l_{max}=10

$$\psi(\vec{r}_1,\vec{r}_2,t)=\sum_{l_1,l_2}\frac{u_{l_1,l_2}(r_1,r_2,t)}{r_1 r_2}\left[Y_{l_1}(\hat{r}_1)Y_{l_2}(\hat{r}_2)\right]_{L=1}$$

Calculated dipole strength of ^{11}Li
(arbitrary scale)



Potentials depth
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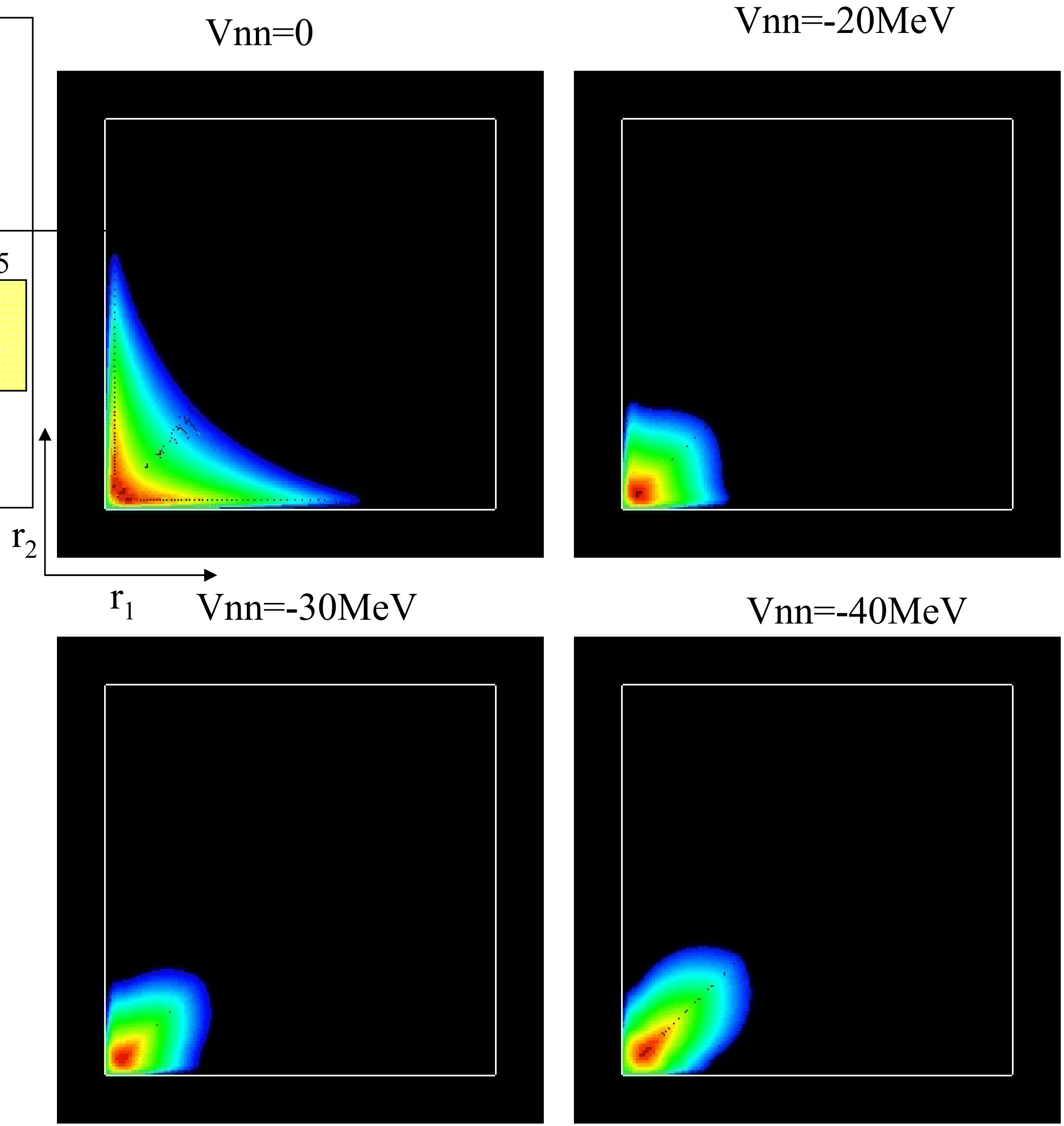
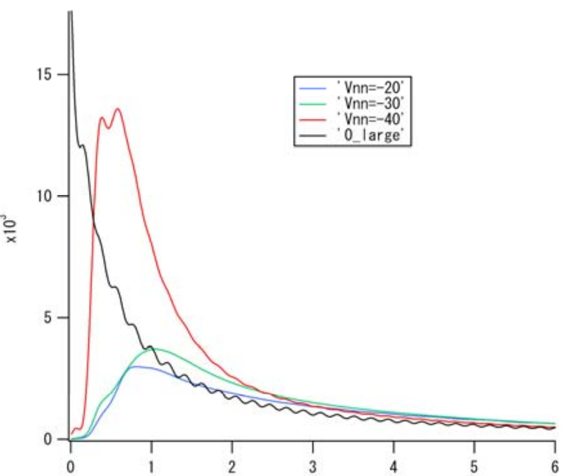
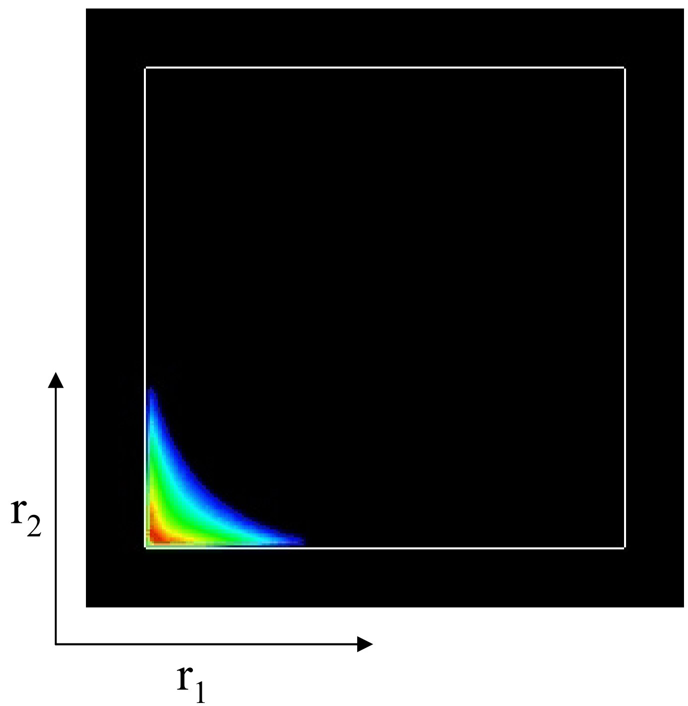




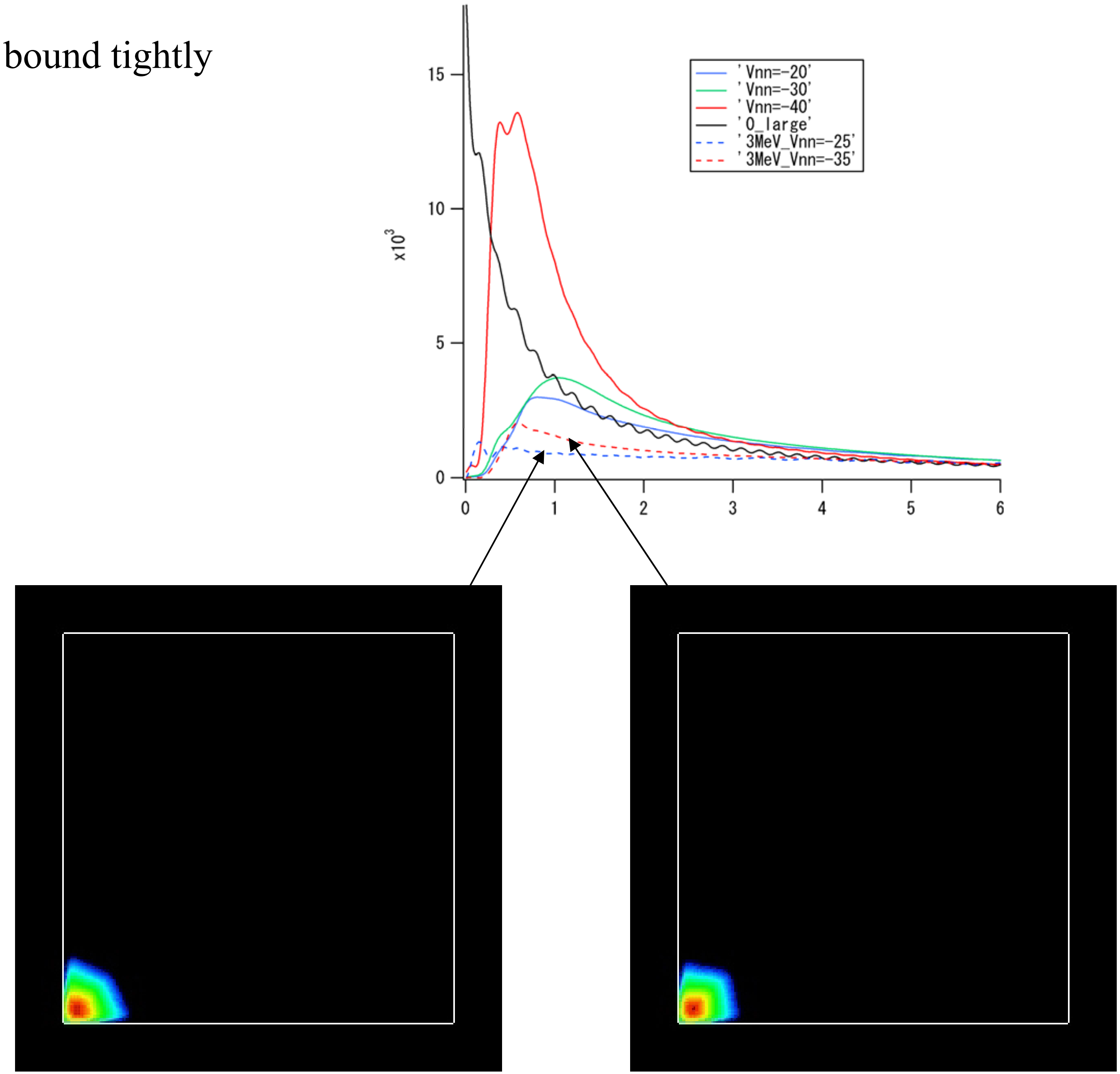
No correlation: single-neutron response x 2

$$(z_1 + z_2)\phi_p(\vec{r}_1)\phi_p(\vec{r}_2) = z_1\phi_p(\vec{r}_1)\cdot\phi_p(\vec{r}_2) + \phi_p(\vec{r}_1)\cdot z_2\phi_p(\vec{r}_2)$$

$$H = \left[-\frac{\hbar^2}{2m}\nabla_{r_1}{}^2 + V_{nC}(r_1)\right] + \left[-\frac{\hbar^2}{2m}\nabla_{r_2}{}^2 + V_{nC}(r_2)\right]$$



When 2n are bound tightly (3MeV)



Vnn=-25MeV

Vnn=-35MeV

Summary

Real-time approach for static problem

Intuitive understanding of the dynamics (movie show)
No need to think about boundary condition
Program is simple but computation is heavy

Future direction

"Few-body reaction simulator"
Connecting model Hamiltonian and reaction observables

$$\frac{dB(E1)}{d\vec{p}_1 d\vec{p}_2}$$

3-body dynamics in time-dependent external field (4-body problem)