Time-dependent approaches to quantum dynamics of many-body systems

Takashi Nakatsukasa
RIKEN Nishina Center

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Contents

- Real-time propagation approaches to many-body quantum dynamics
- Time-dependent Schroedinger equation for nuclear fusion
- Time-dependent density-functional theory
  - Oscillator strength distribution in molecules
  - Dynamics under laser pulse
    - Molecular dissociation
    - Optical breakdown of dielectrics

Time-dependent Schroedinger equation

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

Time-independent treatment

$$\psi(\vec{r},t) = \phi(\vec{r})e^{-iEt/\hbar}$$

$$H\phi(\vec{r}) = E\phi(\vec{r})$$

Solve equation with scattering boundary condition

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

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

Observables: cross section, etc.

Time-dependent approaches

Why time-dependent?

- Wave-packet dynamics provides intuitive picture

- No need for scattering boundary condition

  Advantage for complex systems: non-spherical potential, 3-body reaction, …

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

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

- Full spectral information from single wave-packet dynamics

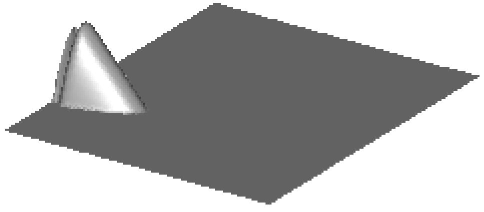
Two topics with time-dependent method

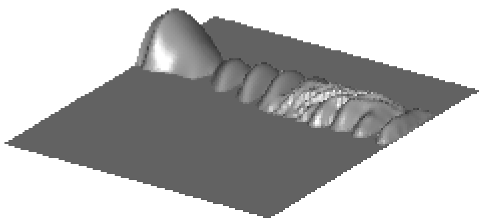
1. Three-body reaction of halo nuclei
2. TDDFT studies

Fusion reaction of halo nuclei

A real-time wave-packet method for three-body tunneling dynamics

Time-dependent approach to quantum dynamics in low-energy reaction

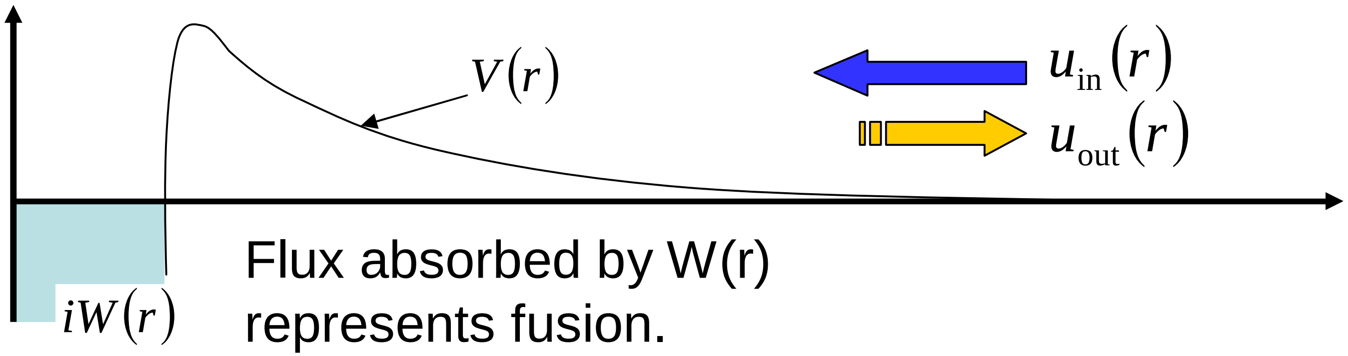




Fusion reaction in terms of flux loss inside a Coulomb barrier

Time-independent (radial) Schroedinger equation for l=0

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



Flux absorbed by W(r) represents fusion.

We need to take account of a boundary condition at r→∞, when solving the differential equation.

Time-dependent (radial) Schroedinger equation for l=0

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

Use of wave packet does not require a boundary condition.

Wave packet dynamics of fusion reaction
potential scattering with absorption inside a Coulomb barrier

Radial Schroedinger equation for l=0

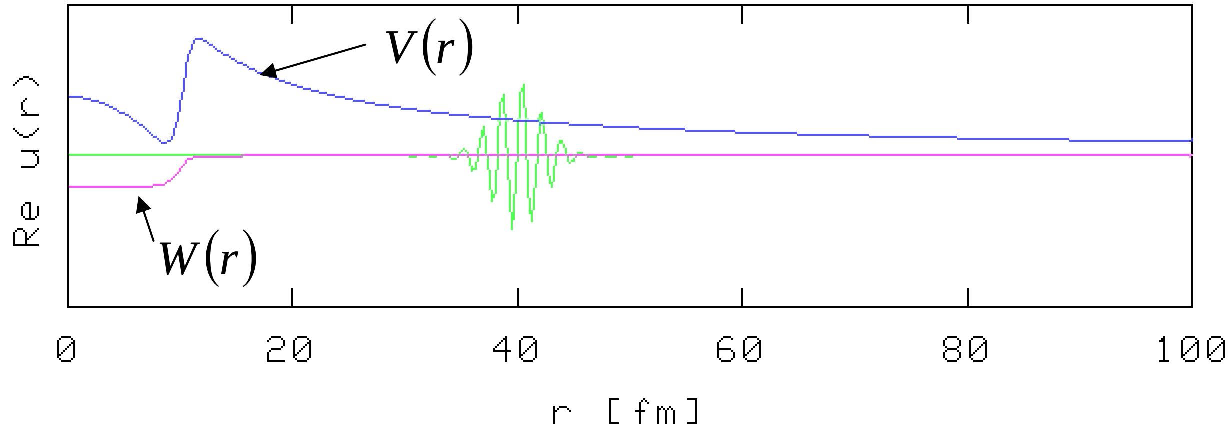
$$i\hbar\frac{\partial}{\partial t}u(r,t)=\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)+iW(r)\right]u(r,t)$$

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

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



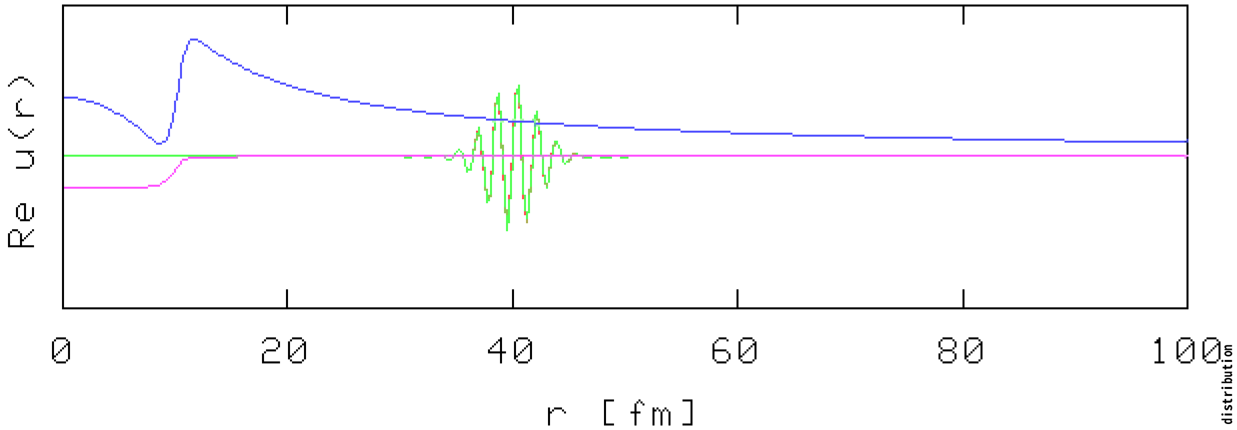
Flux absorbed by W(r) represents fusion.

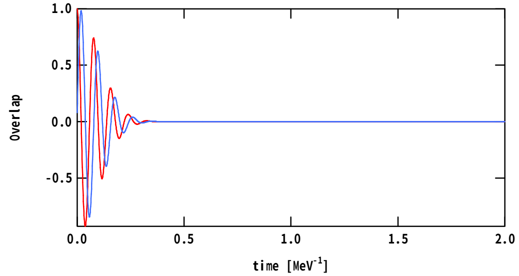
Wave packet dynamics include scattering information for wide energy region.
Then, how to extract reaction information for a fixed energy?

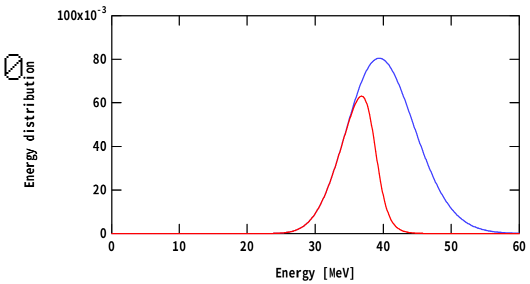
Extract static (fixed-E) information from wave-packet dynamics:

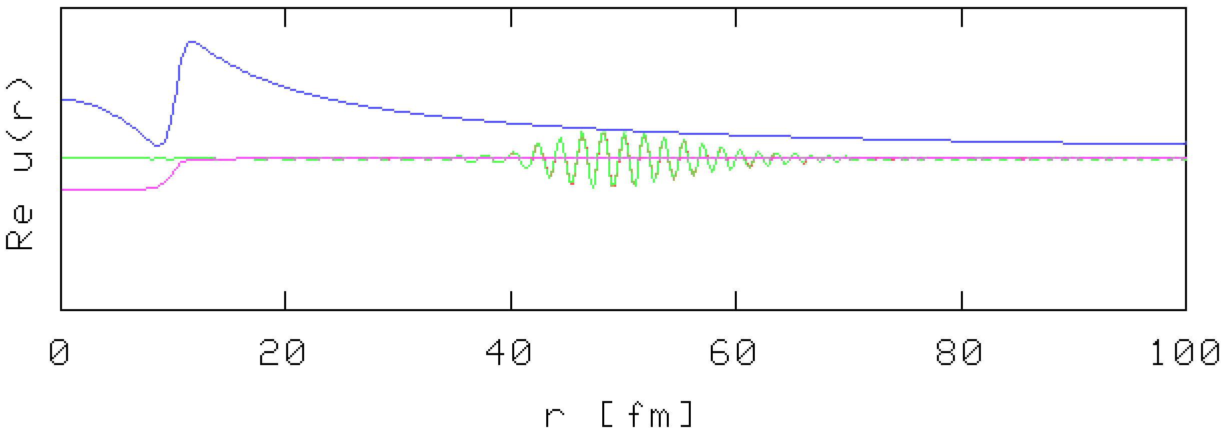
define energy distribution

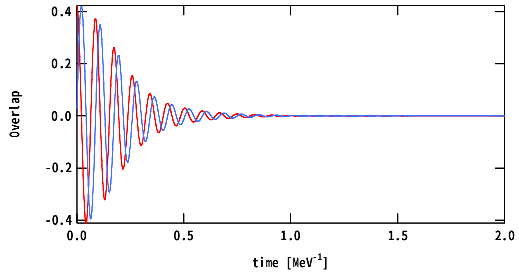
$$P_a(E) = \langle u_a | \delta(E-H) | u_a \rangle = \frac{1}{2\pi\hbar}\int_0^\infty dt\, e^{iEt/\hbar} \left\langle u_a\left(-\frac{t}{2}\right) \middle| u_a\left(\frac{t}{2}\right) \right\rangle$$









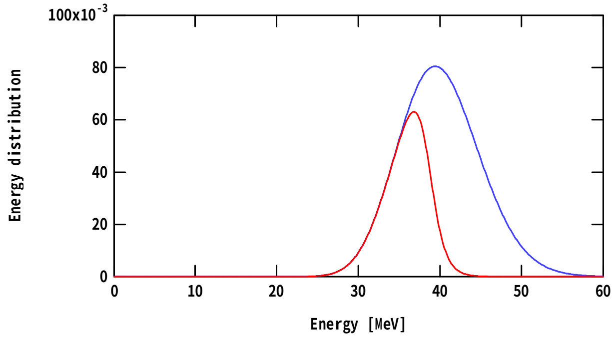


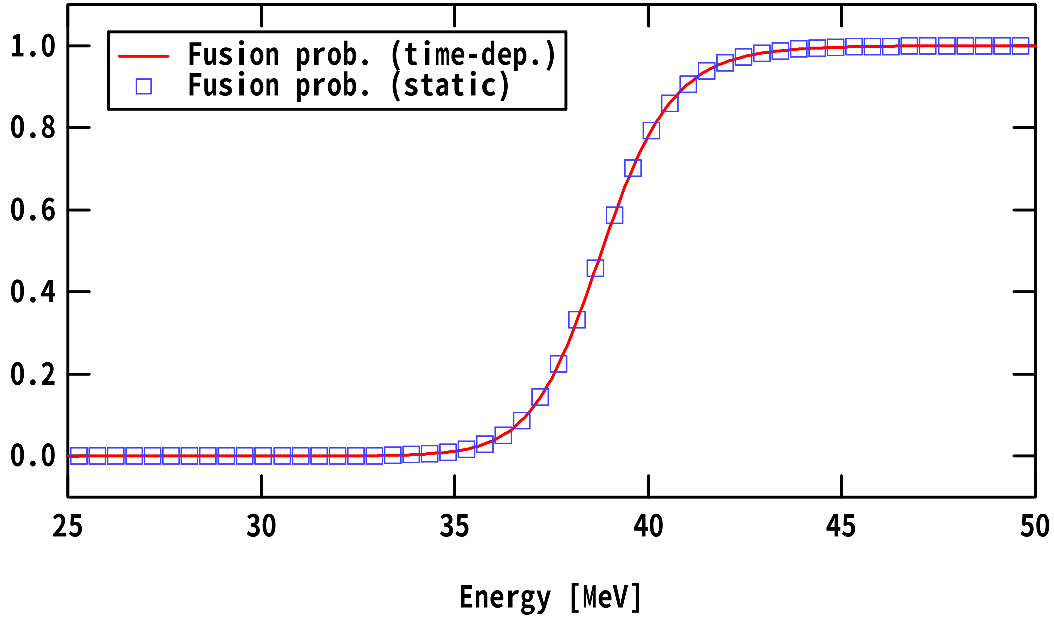
Fusion probability

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

□ differential. eq. (static cal)

—— wave packet method





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

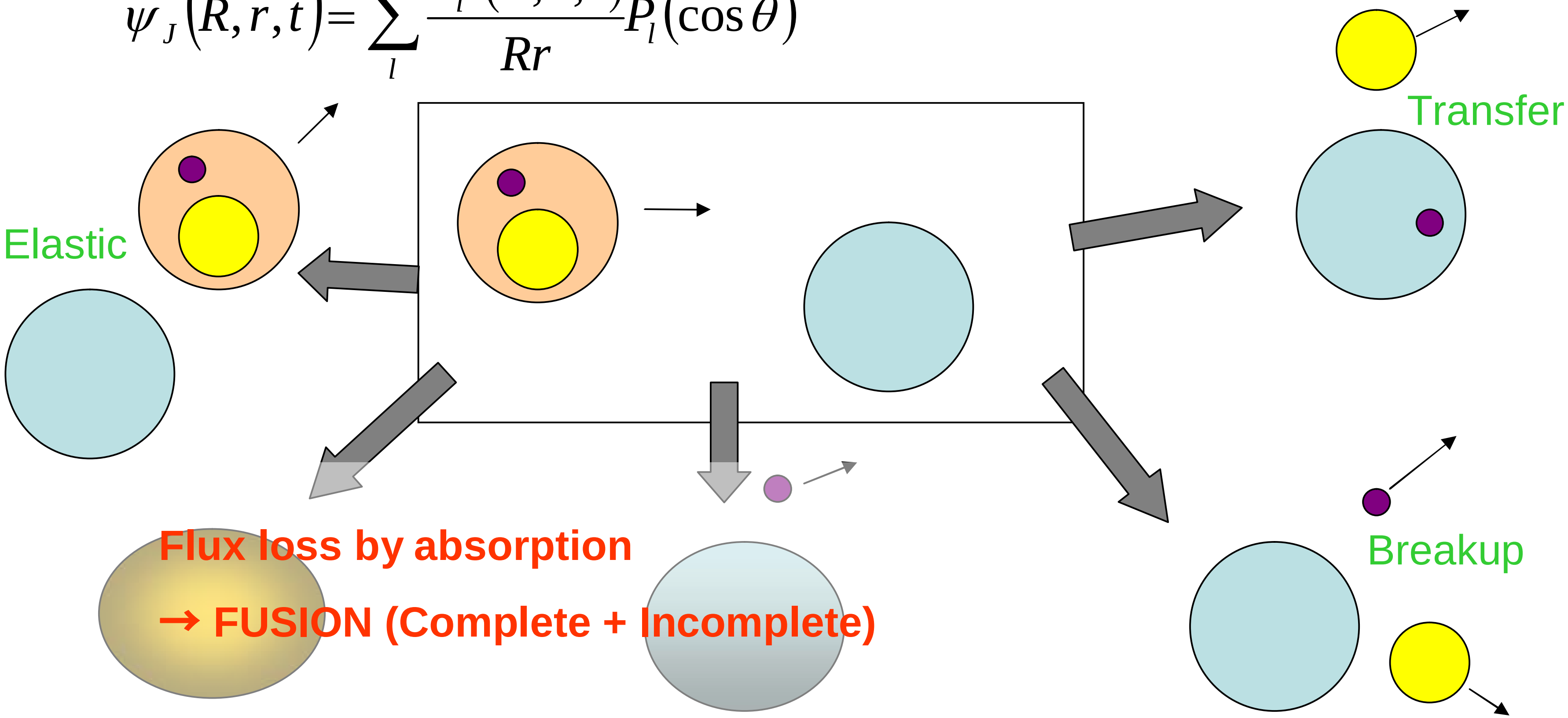
Fusion probability of three-body reaction

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

Coulomb + Nuclear potential
Absorption => C-T fusion

Initial incident wave

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

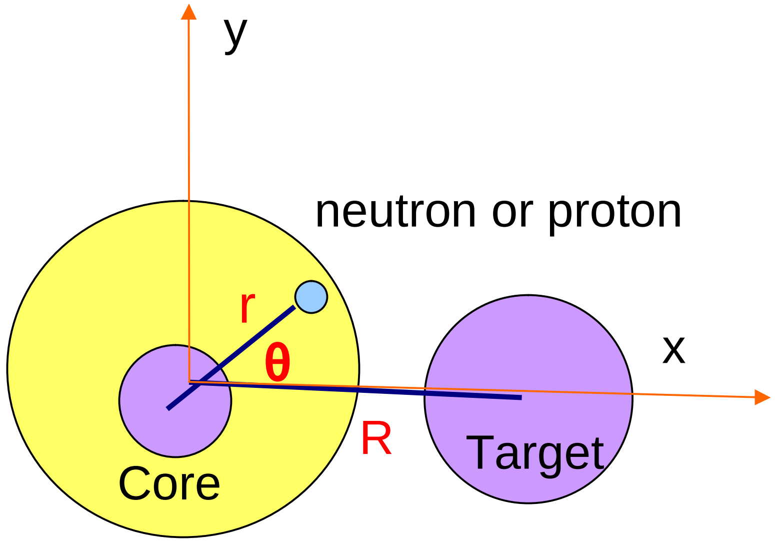


Case (1): Tightly-bound projectile

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

Initial wave packet:

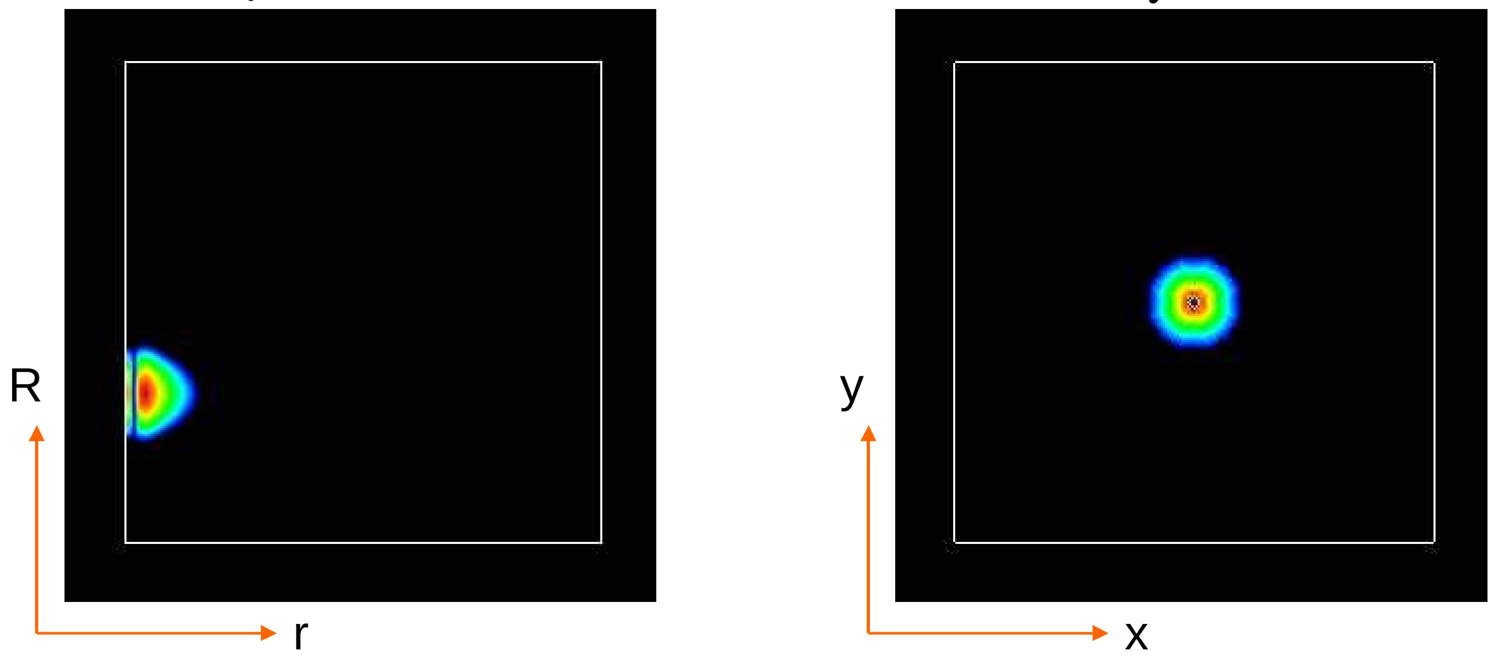
$$u_l(R,r,t_0) = \delta_{l0} \exp\left[-iKR - \gamma(R-R_0)^2\right] u_0(r)$$



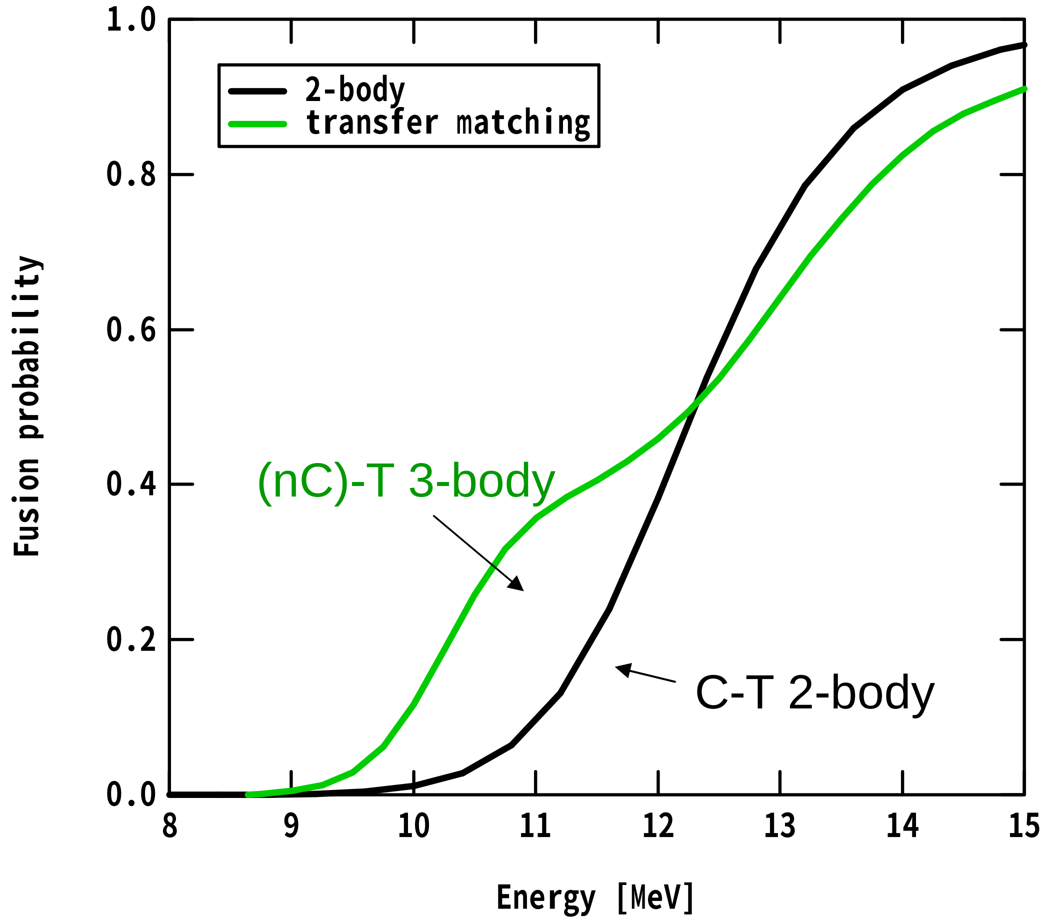
Head-on collision (J=0)

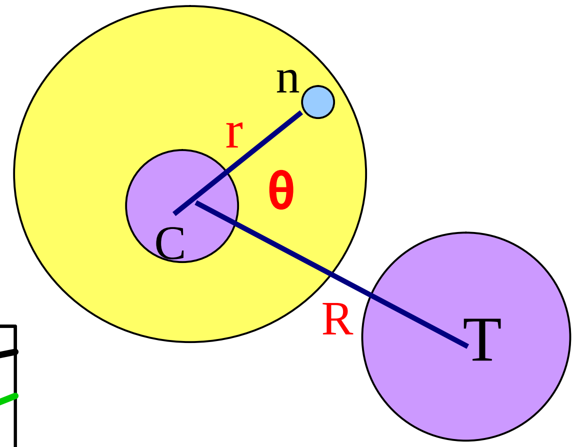
$$\rho(R,r,t) = \int d(\cos\theta) \left|\psi(R,r,\theta,t)\right|^2$$

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



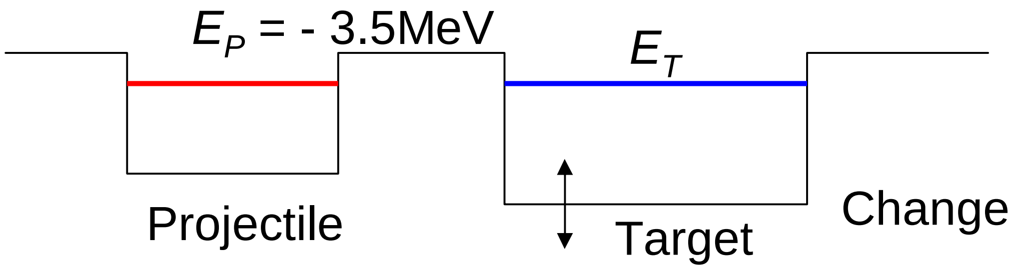
$$P_{fusion}(E) = \frac{P_i(E) - P_f(E)}{P_i(E)}$$





Enhancement of fusion probability at sub-barrier energies

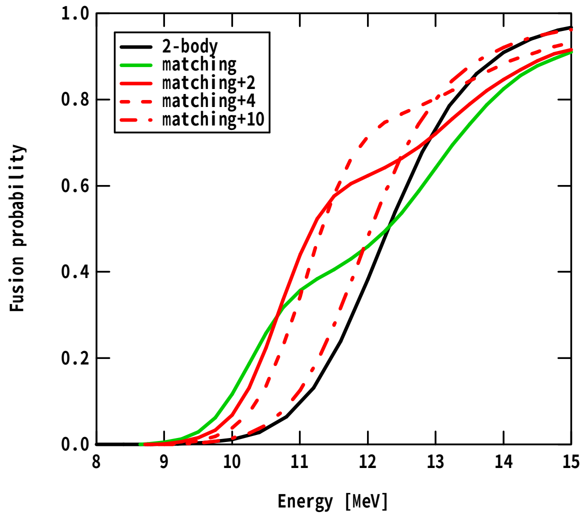
Transfer probability and Q-value matching

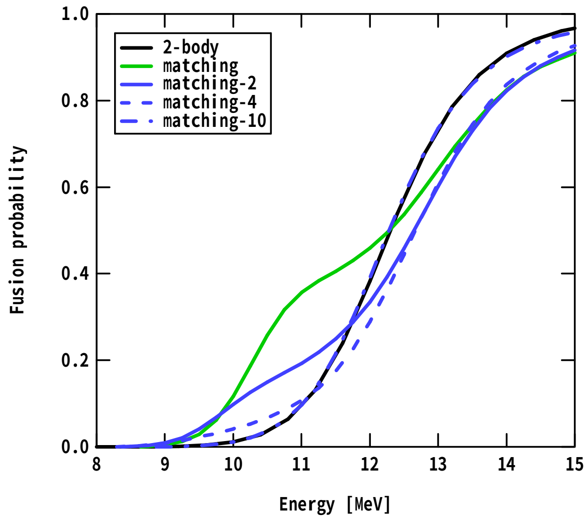


Change n-T potential depth

$$E_P \approx E_T$$

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

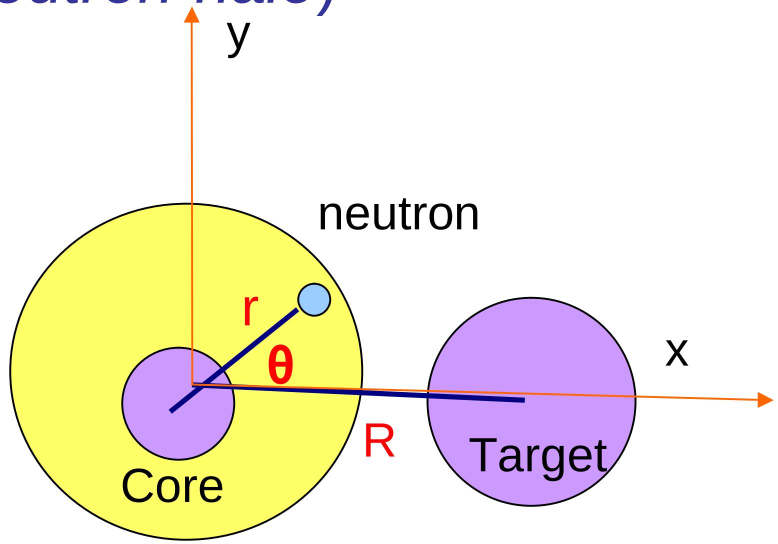
$E_P > E_T$
fusion suppression

Case (2): Weakly-bound projectile (*Neutron-halo*)

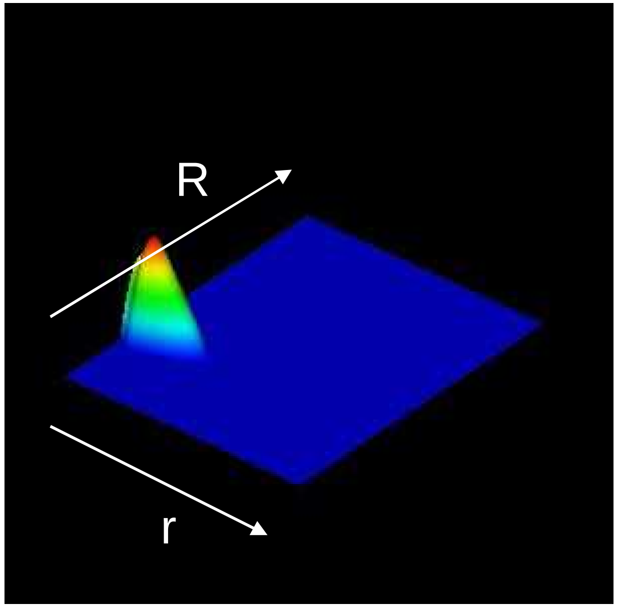
- n-C orbital energy: -0.6 MeV (Halo)

$^{11}Be(n+^{10}Be)-^{208}Pb$

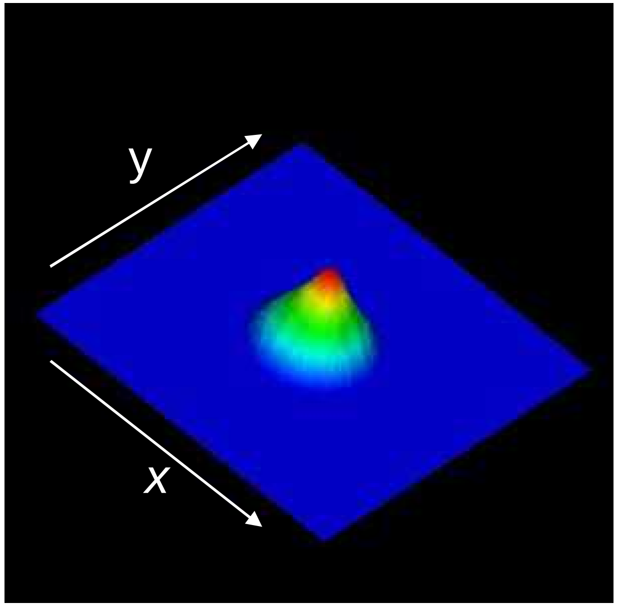
head-on collision (J=0)



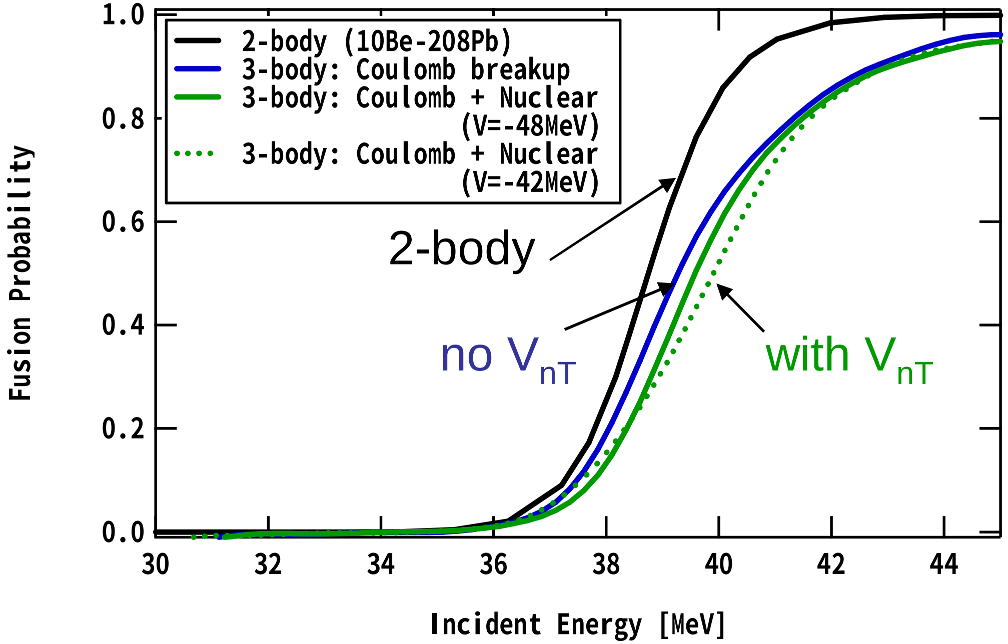
$$\rho(R,r,t)=\int d(\cos\theta)\left|\psi(R,r,\theta,t)\right|^2$$



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

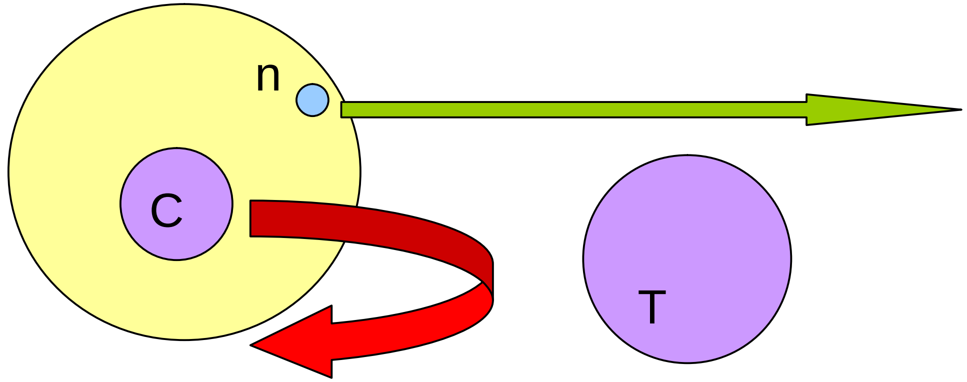


Fusion probability of neutron-halo nuclei is suppressed

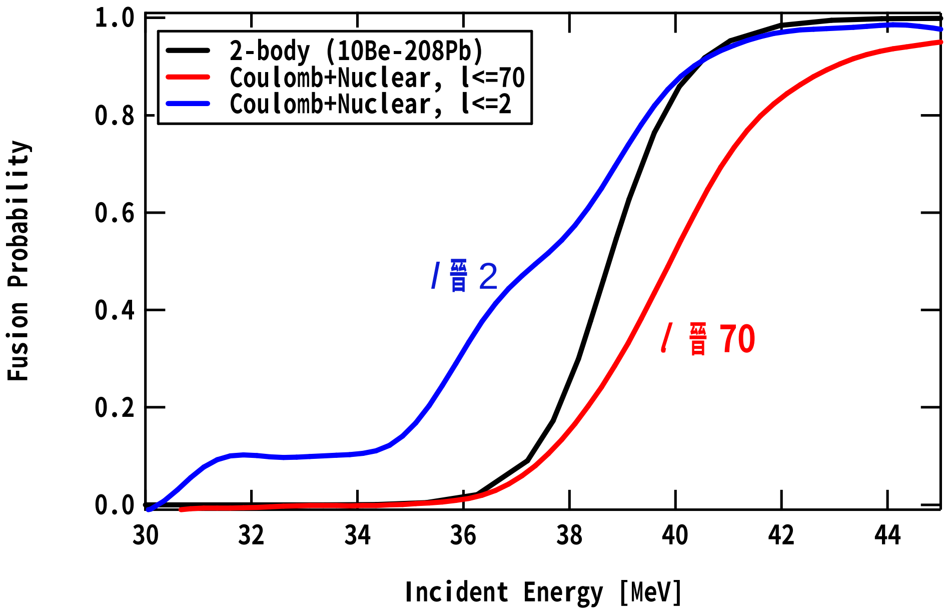


Core incident energy decreases effectively by neutron breakup

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



Why different from other studies?



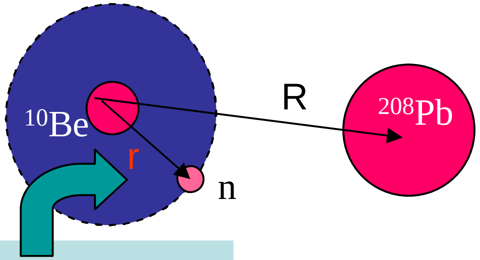
Conclusions of other studies

- Quantum calculations have been done using the discretized continuum channels.

  Hagino et al, PRC61 (2000) 037602

  Diaz-Torres & Thompson, PRC65 (2002) 024606

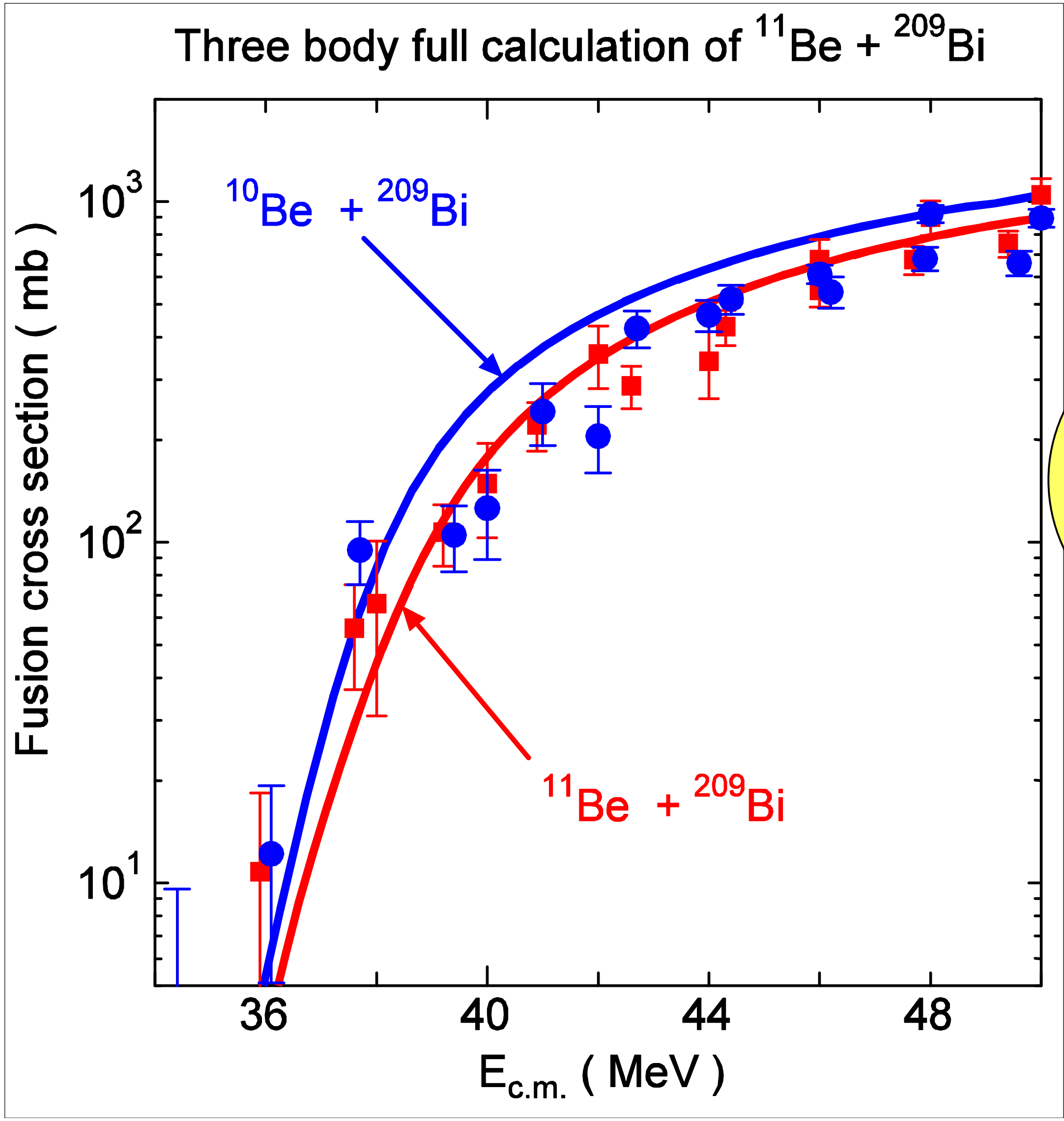
- Fusion was enhanced with a weakly-bound neutron at sub-barrier energies
- Nuclear coupling was important for an the fusion enhancement



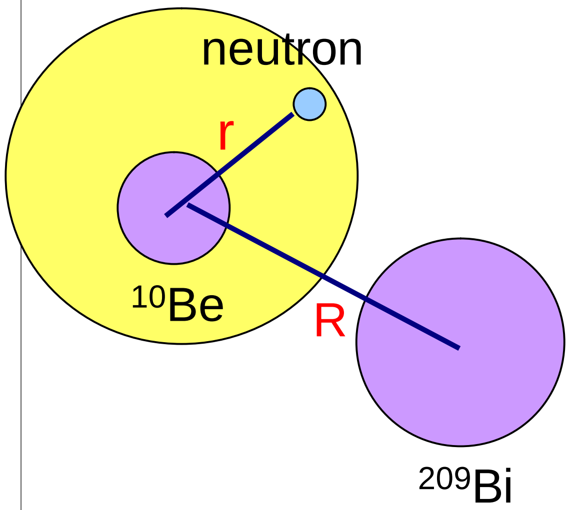
We need to include high-partial waves for n-^{10}Be motions.

The low-partial-wave truncation leads to an opposite conclusion!

Fusion Cross Section of ^{11}Be



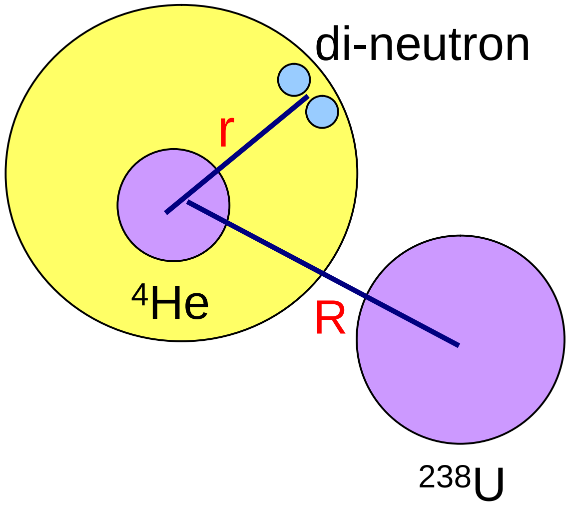
Fusion probability is hindered
by the presence of the halo neutron



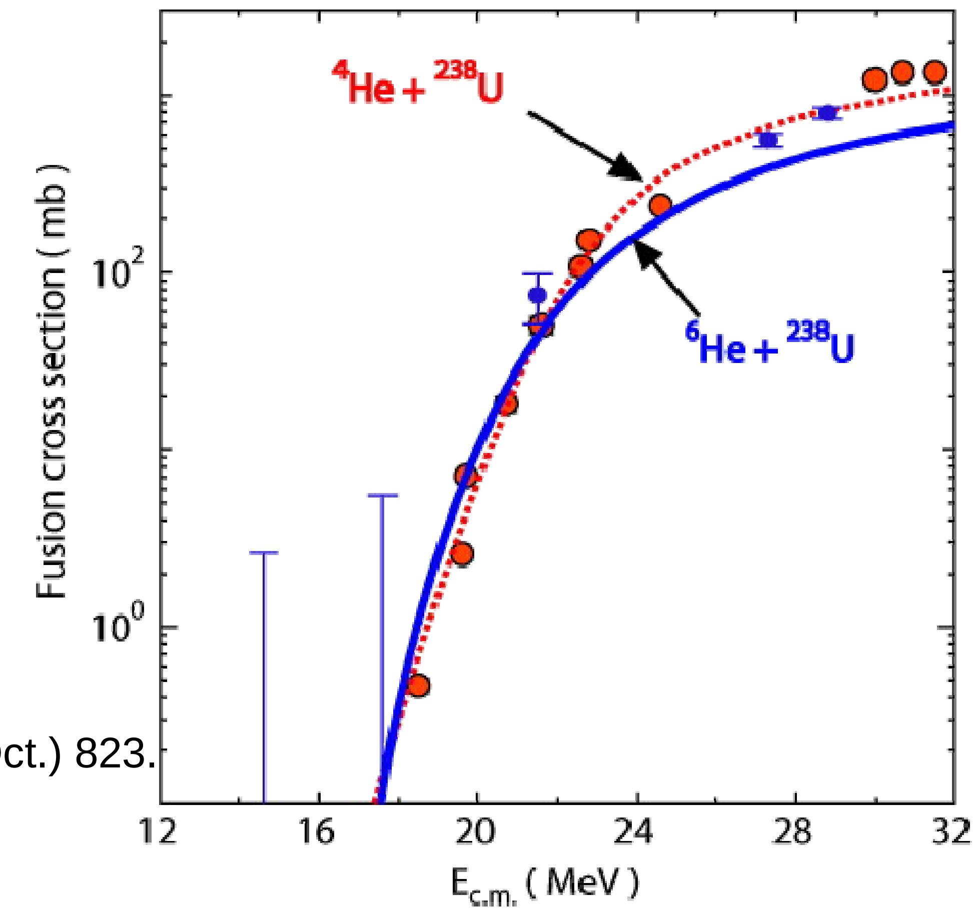
Experiment
C. Signorini et.al, Nucl. Phys. 735 (2004) 329.

Theory
M. Ito, M. Ueda, T. Nakatsukasa, K. Yabana,
Phys. Lett. B 637, 53(2006)

Fusion cross section of $^{6}He+^{238}U$



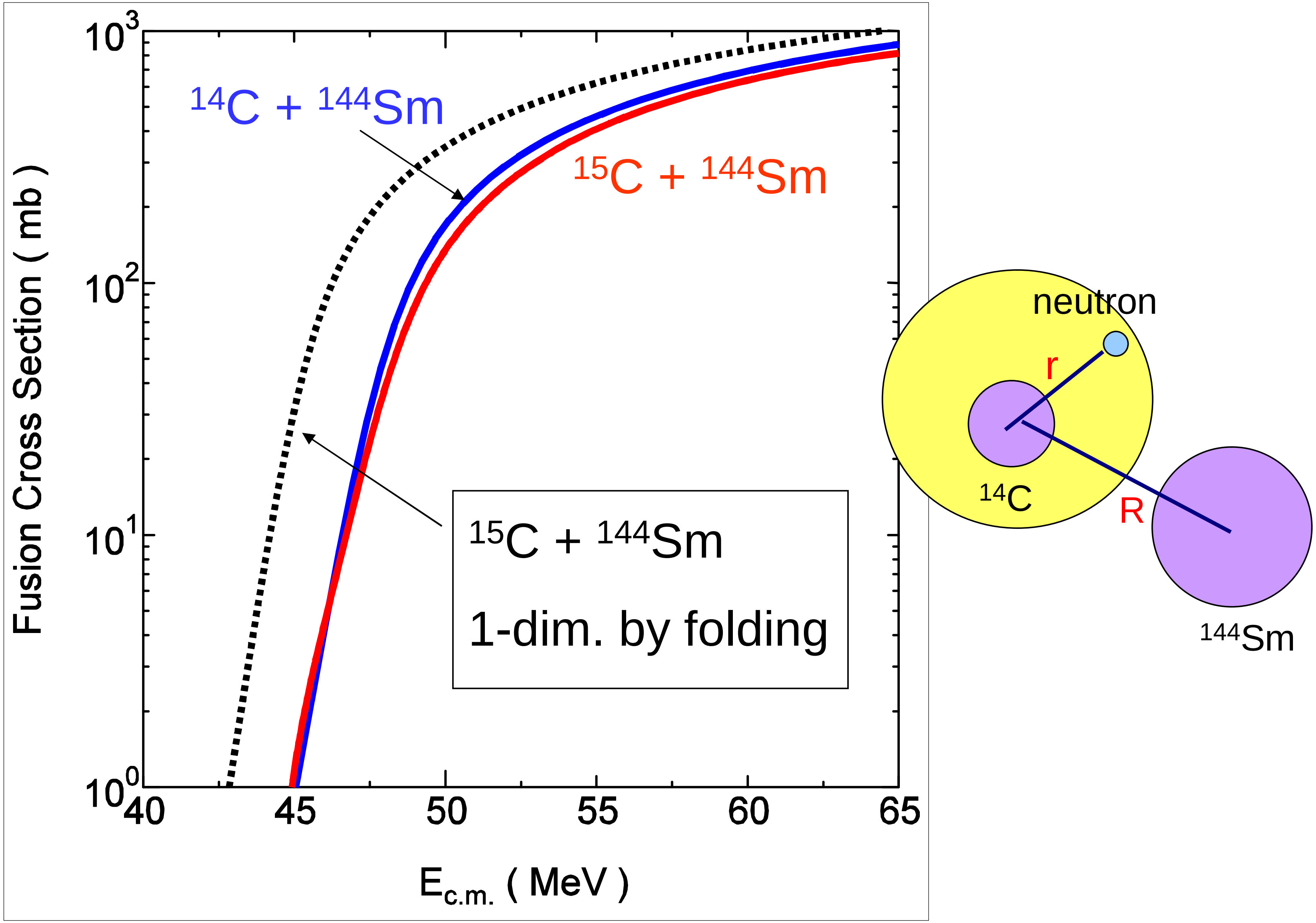
Di-neutron model for $^{6}He=^{4}He+(2n)$



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

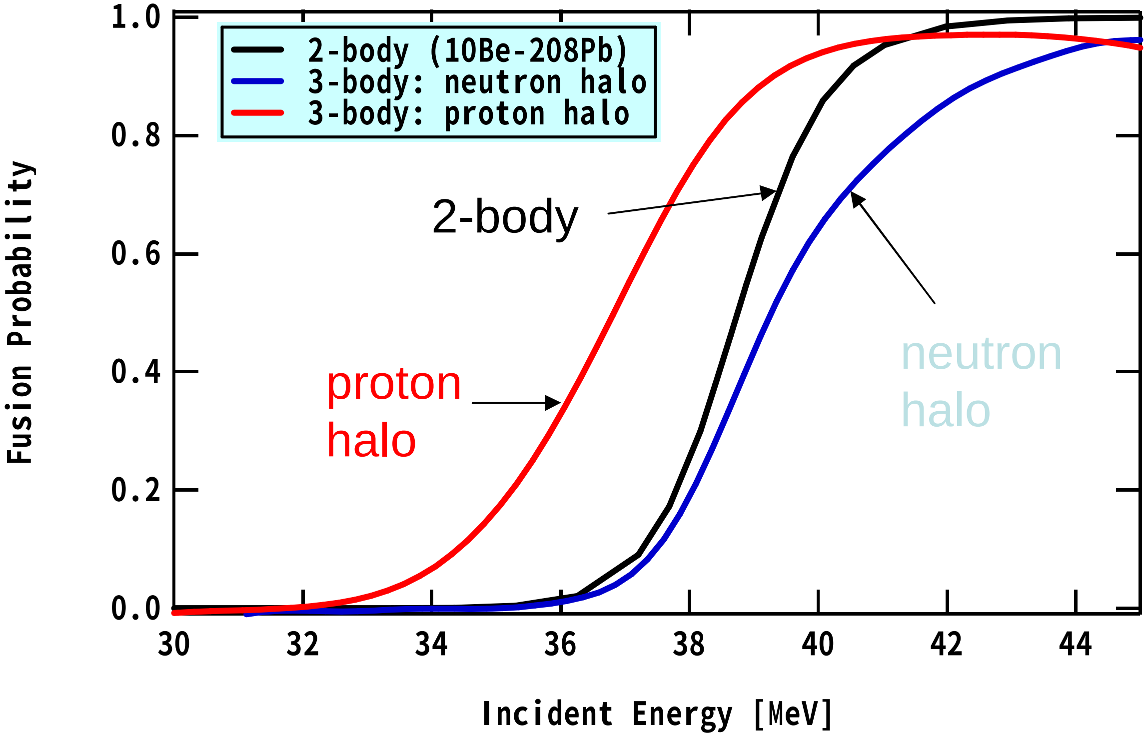
Calculation:
M. Ito, M. Ueda, T. Nakatsukasa, K. Yabana,
Phys. Lett. B 637, 53(2006)

Fusion cross section of $^{15}C + ^{144}Sm$



^{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

Summary

- Time-dependent approaches to quantum mechanical problems
  - Gross properties over a wide energy range
  - Continuum boundary condition
- Three-body nuclear fusion problem
  - Accurate calculation within the 3-body model
- Electronic TDDFT dynamics coupled with classical ionic dynamics
  - Dynamics under strong laser pulses suggest that the energy transfer from electrons to ions strongly depends on the pulse duration