計算核データ構築に向けて

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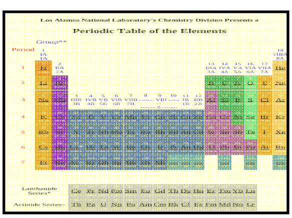
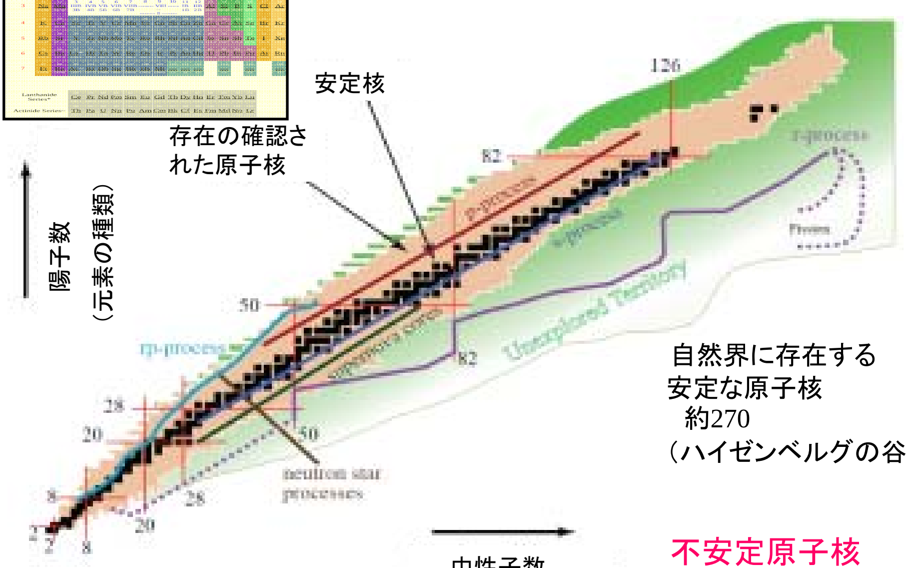
- Real-space, real-time approaches
  - → DFT, TDDFT　((Q)RPAと相補的)
  - Few-body model　(CDCCと相補的)

2009.3.25-26 Mini-WS:核データと核理論

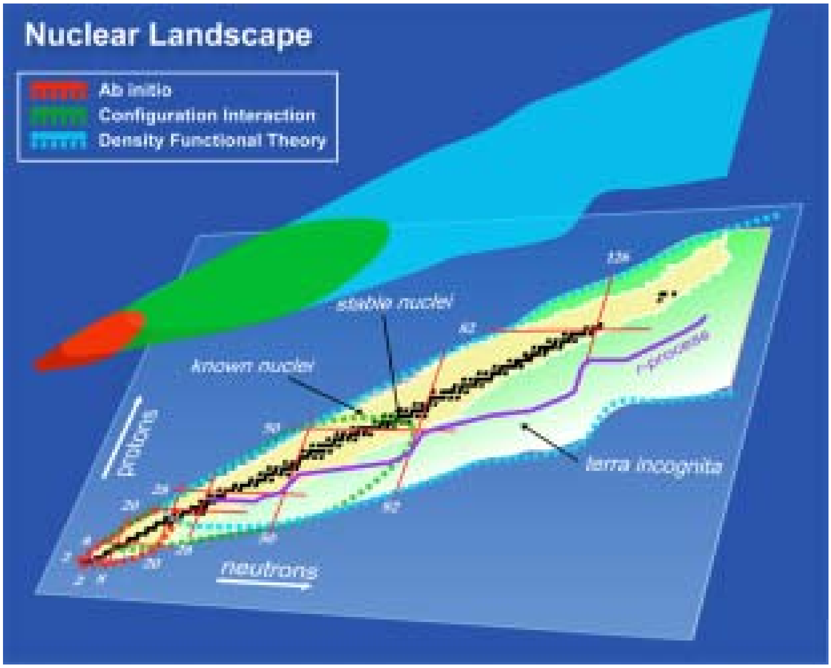


核図表（Nuclear Chart）



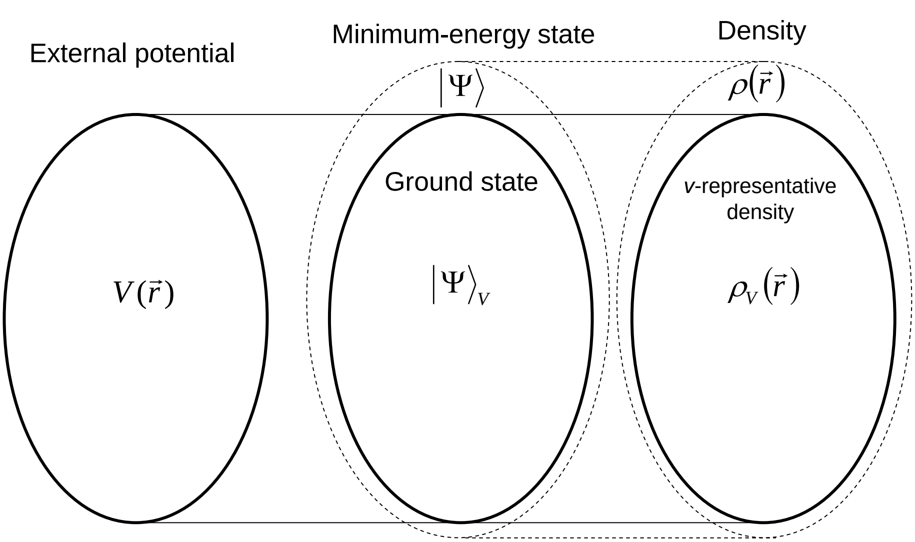
自然界に存在する
安定な原子核
約270
（ハイゼンベルグの谷）

不安定原子核
約1万（？）



High-performance computing ~ DFT to cover all

One-to-one Correspondence



The following variation leads to all the ground-state properties.

$$\delta\left\{ F[\rho] + \int \rho(\vec{r})v(\vec{r})d\vec{r} - \mu\left(\int \rho(\vec{r})d\vec{r} - N \right) \right\} = 0$$

In principle, any physical quantity of the ground state should be a functional of density.

Variation with respect to many-body wave functions $\Psi(\vec{r}_1, \cdots, \vec{r}_N)$

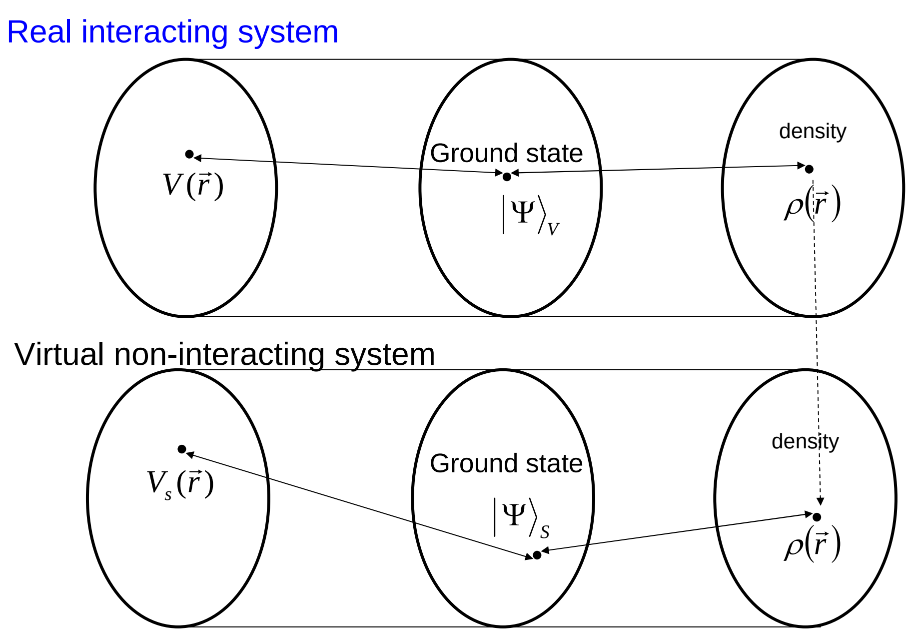
↓

Variation with respect to one-body density $\rho(\vec{r})$

↓

Physical quantity $A[\rho(\vec{r})] = \left\langle \Psi[\rho] \middle| \hat{A} \middle| \Psi[\rho] \right\rangle$

Kohn-Sham Scheme



Kohn-Sham scheme

$$\rho(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2 \qquad |\Psi\rangle_S = \det\{\phi_i(\vec{r}_j)\}$$

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i + v_S[\rho]\phi_i = \varepsilon_i\phi_i$$

KS canonical equation

Density functional

$$F[\rho(\vec{r})] = T_S[\rho(\vec{r})] + (F[\rho(\vec{r})] - T_S[\rho(\vec{r})]) \Longrightarrow V_{\text{eff}}[\rho(\vec{r})]$$

$$= \sum_i \langle \phi_i | \frac{\vec{p}^2}{2m} | \phi_i \rangle + V_{\text{eff}}[\rho(\vec{r})]$$

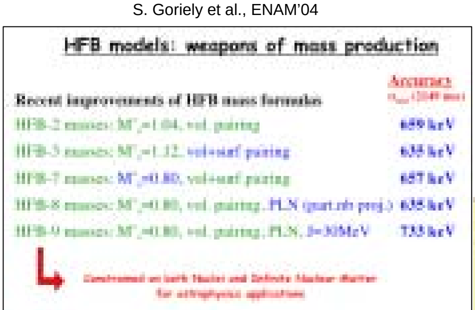
Minimization of this density functional leads to

$$v_S[\rho](\vec{r}) = \frac{\delta V_{\text{eff}}}{\delta\rho(\vec{r})}$$

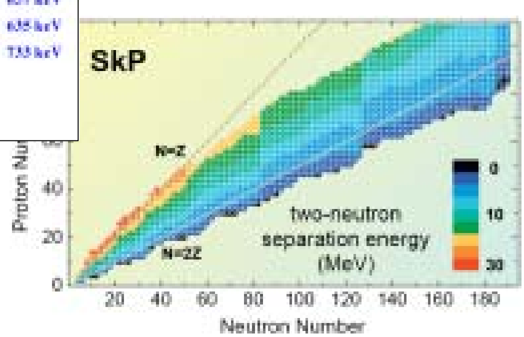
Nuclear DFT

Global properties, global calculations

S. Goriely et al., ENAM'04

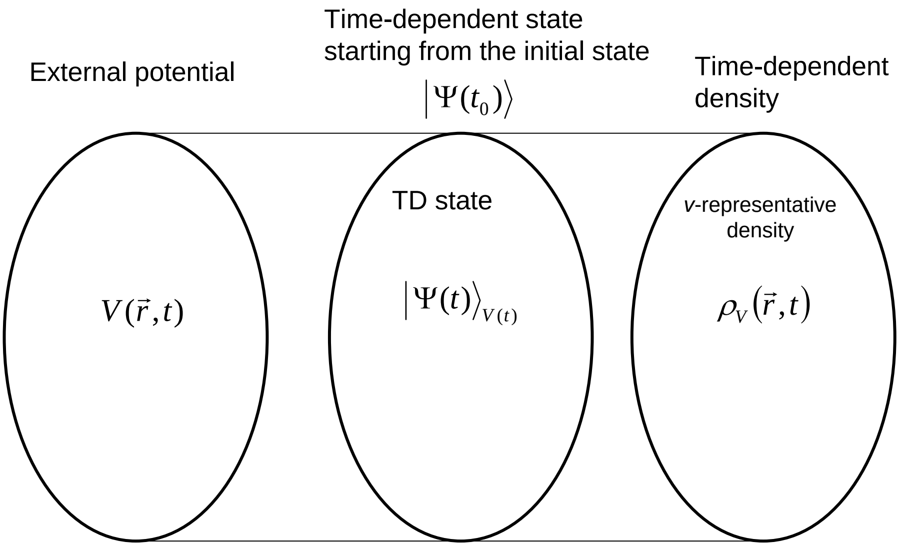


M. Stoitsov et al.



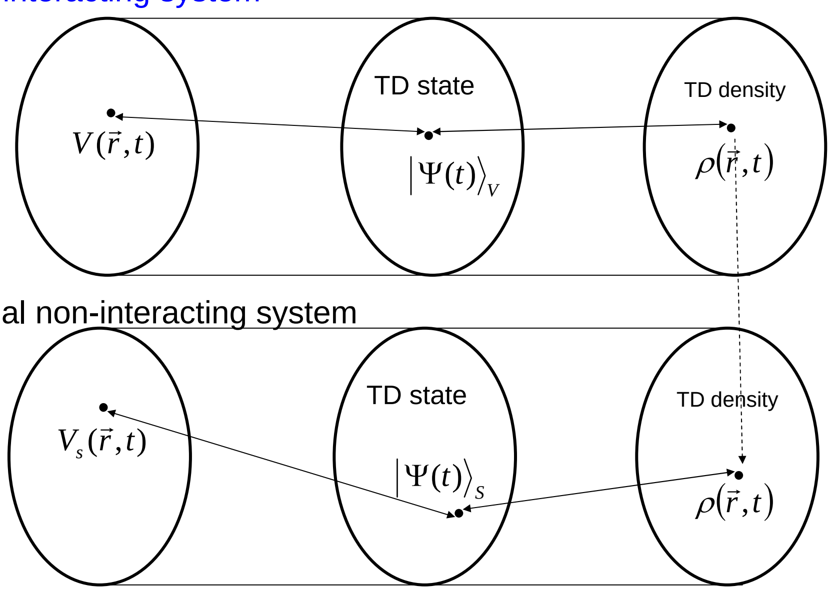
* Global DFT mass calculations: HFB mass formula: Δm~700keV
• Taking advantage of high-performance computers

One-to-one Correspondence



TD Kohn-Sham Scheme

Real interacting system



Skyrme TDDFT in real space

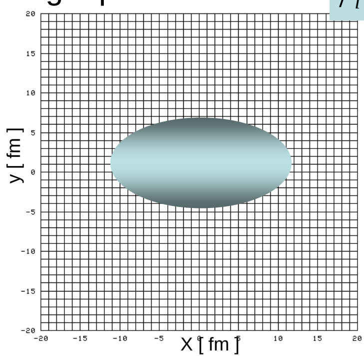
Time-dependent Kohn-Sham equation

$$i\frac{\partial}{\partial t}\psi_i(\mathbf{r}\sigma\tau,t)=\left(h_{\mathrm{HF}}[\rho,\tau,\mathbf{j},\mathbf{s},\vec{\mathbf{J}}](t)+V_{\mathrm{ext}}(t)\right)\psi_i(\mathbf{r}\sigma\tau,t)$$

$$-i\tilde{\eta}(r)$$

3D space is discretized in lattice

Single-particle orbital: $\varphi_i(\mathbf{r},t)=\{\varphi_i(\mathbf{r}_k,t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt},\quad i=1,\cdots,N$



N: Number of particles

Mr: Number of mesh points

Mt: Number of time slices

Spatial mesh size is about 1 fm.

Time step is about 0.2 fm/c

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

Real-time calculation of response functions

1. Weak instantaneous external perturbation

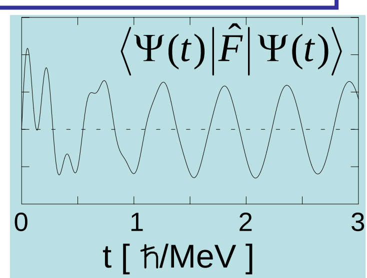
$$V_{\mathrm{ext}}(t)=\hat{F}\delta(t)$$

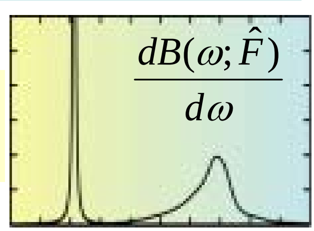
2. Calculate time evolution of

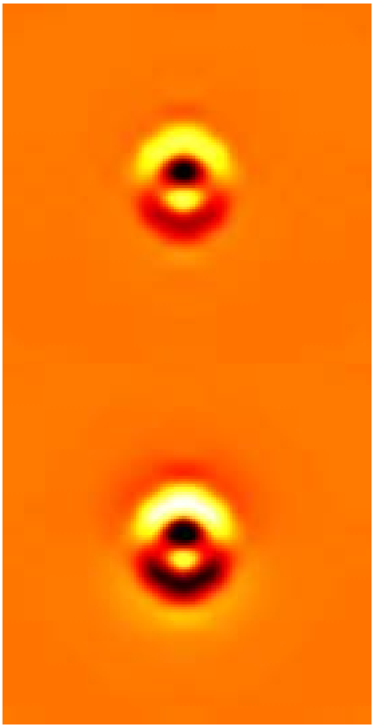
$$\langle\Psi(t)|\hat{F}|\Psi(t)\rangle$$

3. Fourier transform to energy domain

$$\frac{dB(\omega;\hat{F})}{d\omega}=-\frac{1}{\pi}\mathrm{Im}\int\langle\Psi(t)|\hat{F}|\Psi(t)\rangle e^{i\omega t}dt$$







Neutrons

^{16}O

$$\delta\rho_n(t) = \rho_n(t) - (\rho_0)_n$$

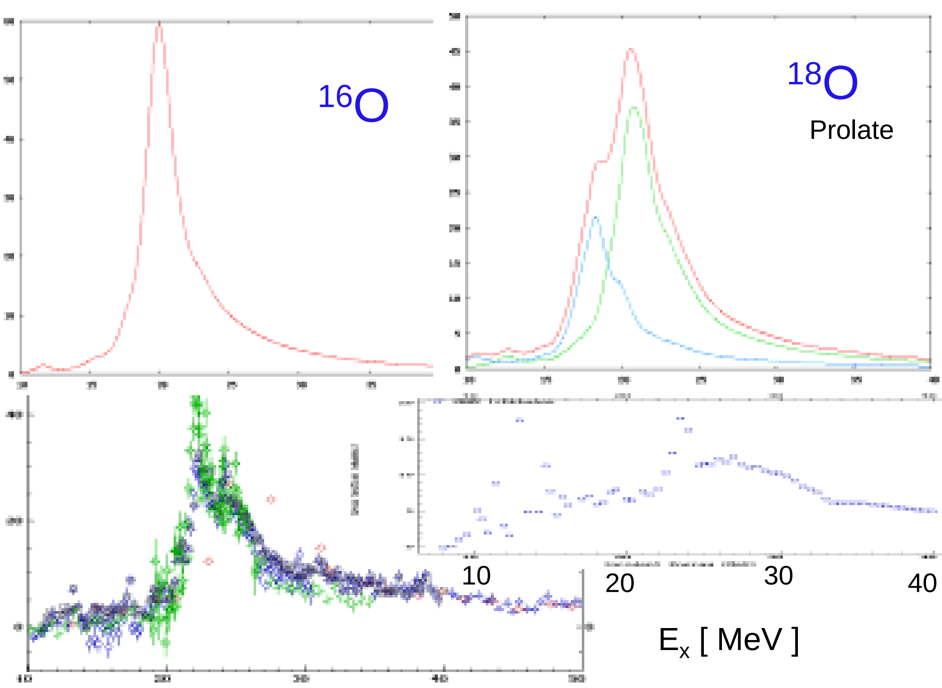
Time-dep. transition density

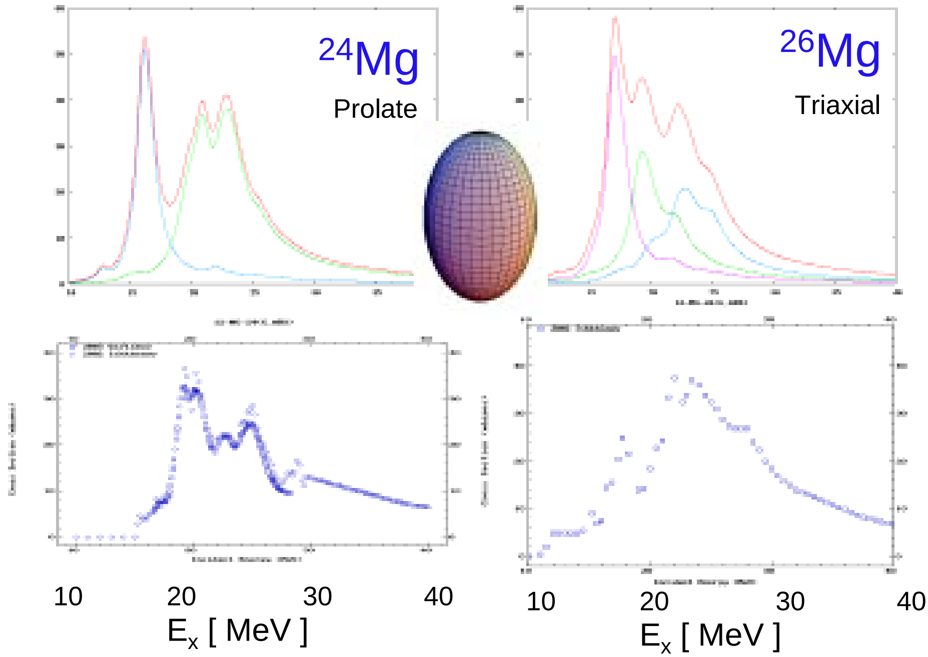
$\delta\rho > 0$

$\delta\rho < 0$

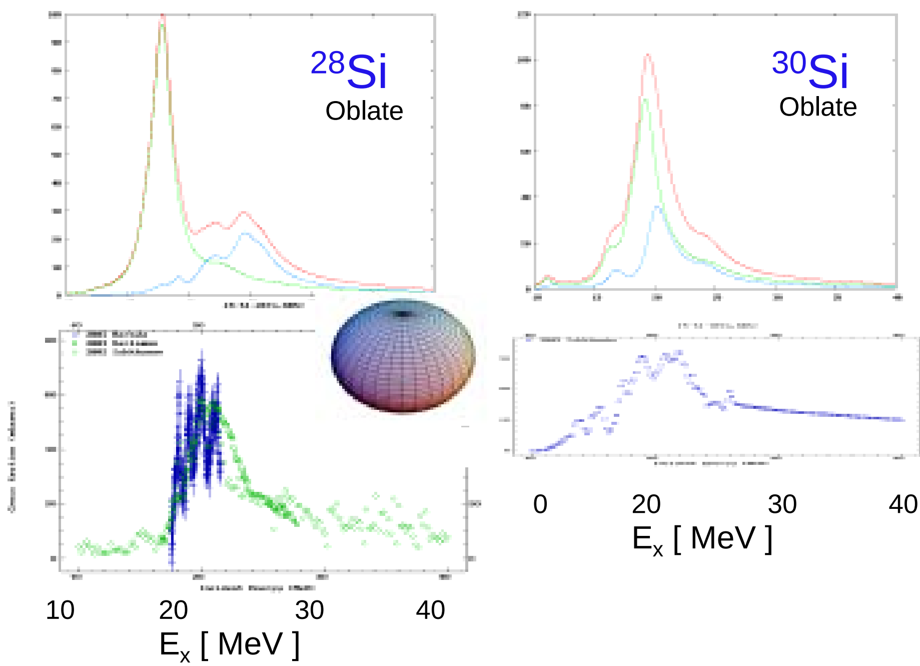
$$\delta\rho_p(t) = \rho_p(t) - (\rho_0)_p$$

Protons

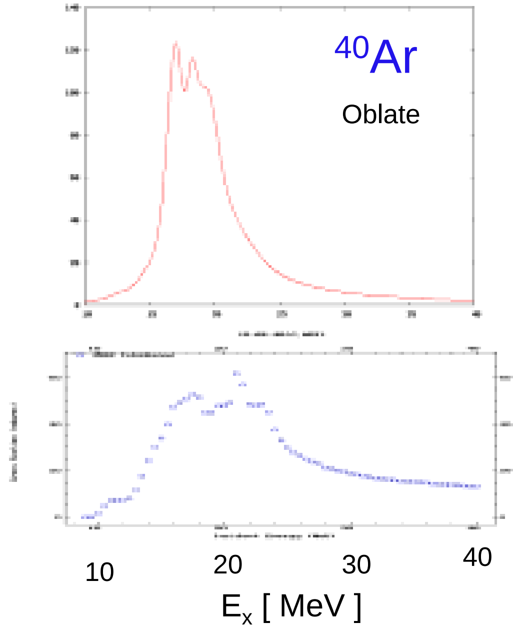




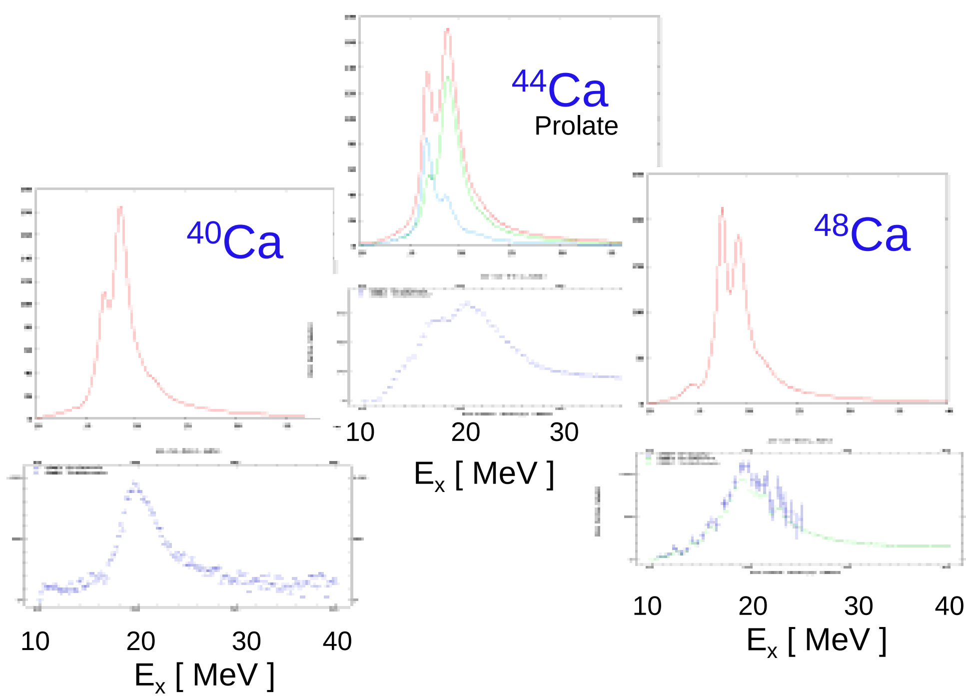
24Mg
Prolate
26Mg
Triaxial
10
20
30
40
Ex [MeV]
10
20
30
40
Ex [MeV]



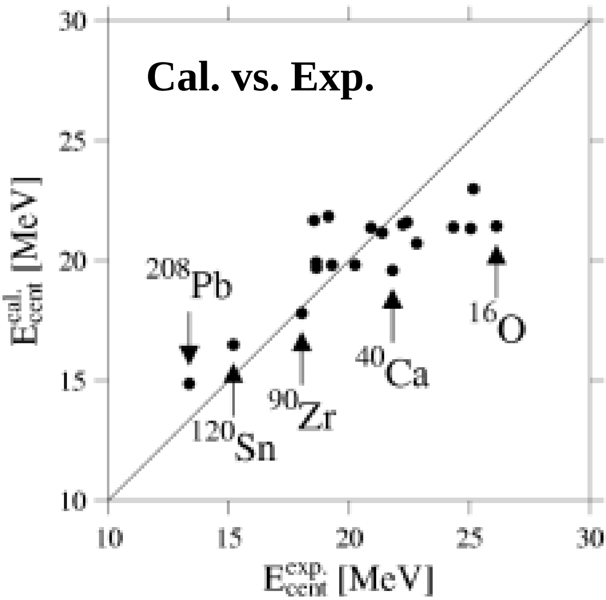
28Si
Oblate
30Si
Oblate
10
20
30
40
Ex [MeV]
0
20
30
40
Ex [MeV]



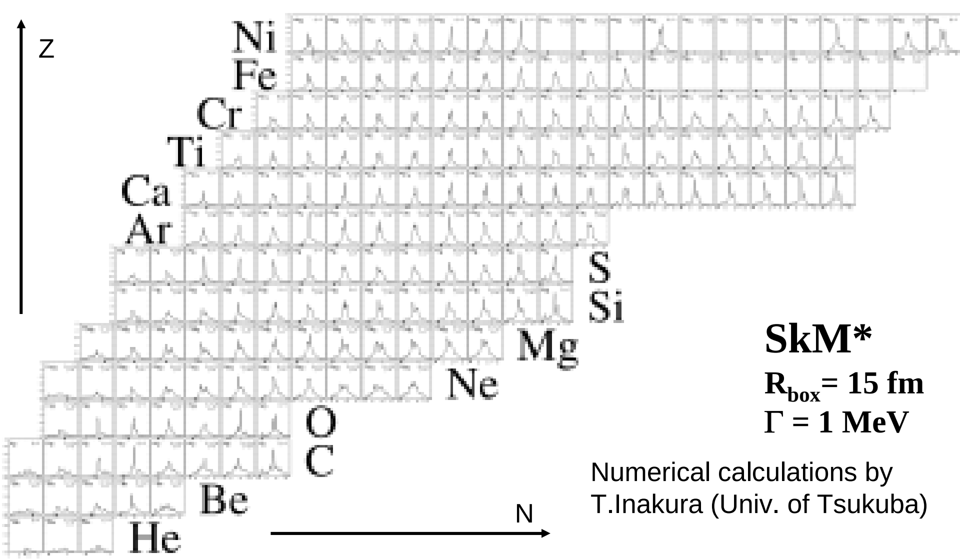
^{40}Ar
Oblate
10
20
30
40
E_x [MeV]



^{44}Ca
Prolate
10
20
30
E_x [MeV]
^{40}Ca
10
20
30
40
E_x [MeV]
^{48}Ca
10
20
30
40
E_x [MeV]



Electric dipole strengths



SkM*

R_{box}= 15 fm

Γ = 1 MeV

Numerical calculations by
T.Inakura (Univ. of Tsukuba)

Few-body-model calculation of fusion cross section

- Real-time, real-space approach
- No need for scattering boundary condition
- Alternative method to the CDCC

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

Radial Schroedinger equation for l=0

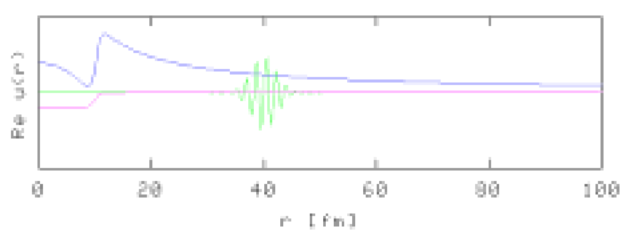
$$i\hbar \frac{\partial}{\partial t} u(r,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + iW(r) \right] u(r,t)$$

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

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

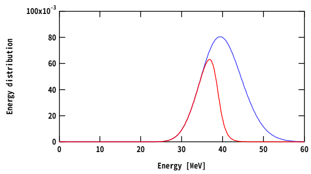


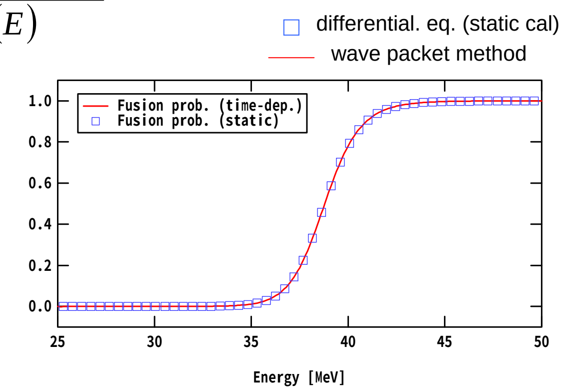
Flux absorbed by W(r) represents fusion.

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

Fusion probability

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





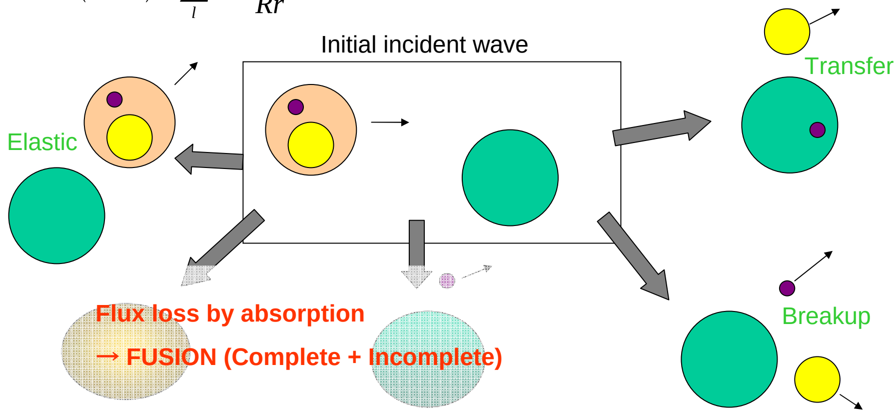
Fusion probability for whole barrier region from single wave-packet calculation.
No boundary condition required in the wave packet calculation.

Fusion probability of three-body reaction

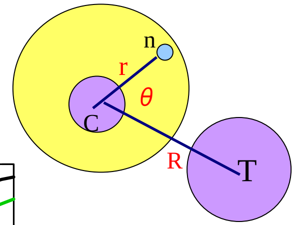
$$i\hbar\frac{\partial}{\partial t}\psi\left(\vec{R},\vec{r},t\right) = \left(-\frac{\hbar^2}{2\mu}\nabla_R^{\ 2} - \frac{\hbar^2}{2m}\nabla_r^{\ 2} + V_{nC}(r_{nC}) + V_{CT}(r_{CT}) + V_{nT}(r_{nT})\right)\psi\left(\vec{R},\vec{r},t\right)$$

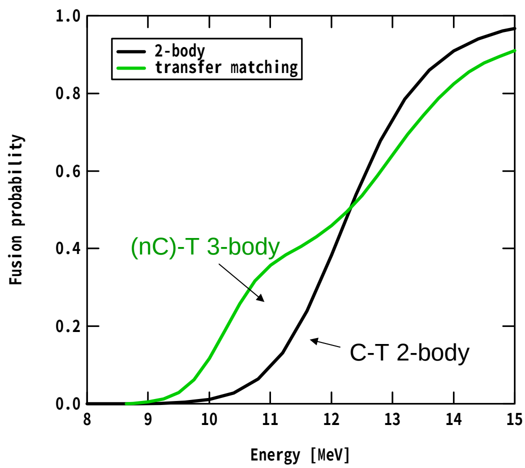
Coulomb + Nuclear potential
Absorption => C-T fusion

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



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

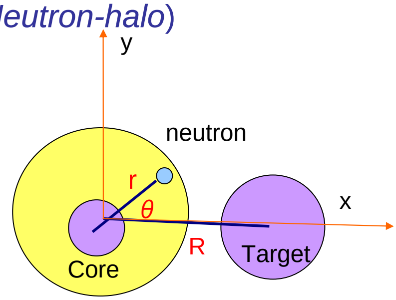




Enhancement of fusion probability at sub-barrier energies

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

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

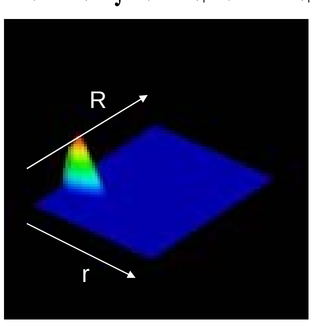


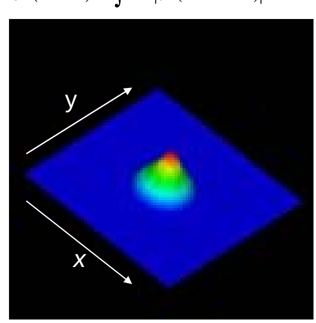
$^{11}Be(n+^{10}Be)$-^{208}Pb

head-on collision (J=0)

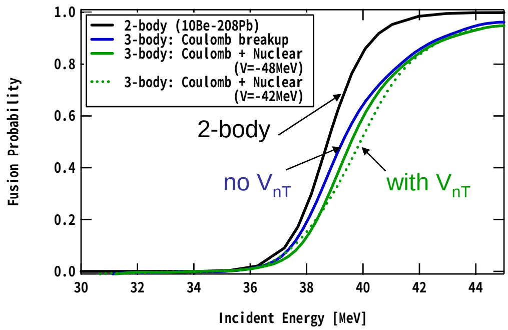
$$\rho(R,r,t) = \int d(\cos\theta) |\psi(R,r,\theta,t)|^2$$

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



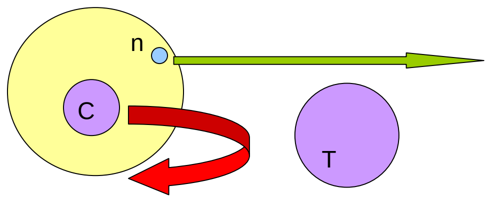


Fusion probability of neutron-halo nuclei is suppressed

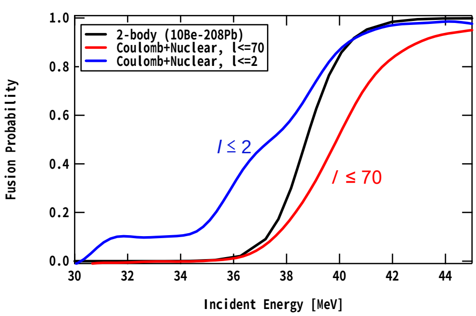


Core incident energy decreases effectively by neutron breakup

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



Why different from other studies?



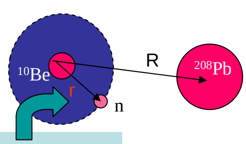
Conclusions of other studies

- 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

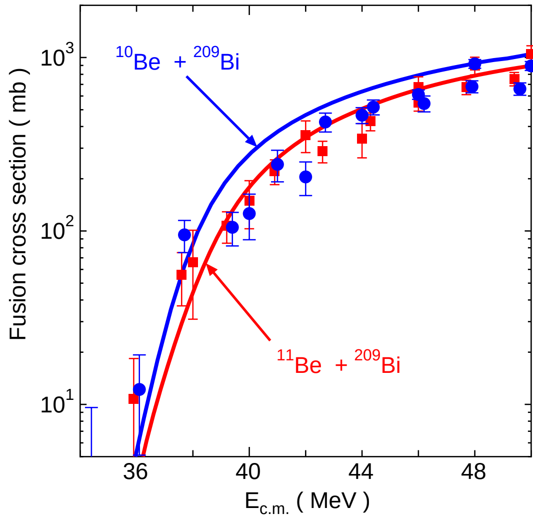


We need to include high-partial waves for n-^{10}Be motions.

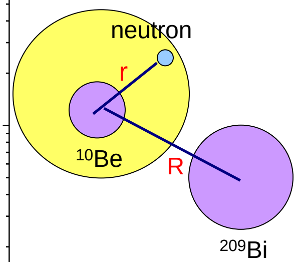
The low-partial-wave truncation leads to an opposite conclusion!

Fusion Cross Section of ^{11}Be

Three body full calculation of $^{11}Be + ^{209}Bi$



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)

Summary

- DFT/TDDFT
  - Systematic calculations for all nuclei including those far from the stability line
  - Description of large amplitude dynamics, such as fission
- Real-time, real-space approach to few-body models
  - Accurate few-body scattering dynamics
  - An alternative approach to CDCC