

TDHF計算による核子移行反応の記述

# Description of Nucleon Transfer Reaction by TDHF Method

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# 1. Introduction

## Time-dependent Hartree-Fock method (TDHF)

- **mean-field theory**; based on **microscopic** degree of freedom
- has **no parameter** about reaction mechanism

So far

Fusion cross section, deep inelastic collision, etc. ← averaging quantities

Nucleon transfer reaction

→ We need to extract probabilities of each transfer channel.

Last year, an innovative method was proposed by C. Simenel

We extract nucleon transfer probabilities from TDHF final state wave function and compare the transfer cross section with experimental data.

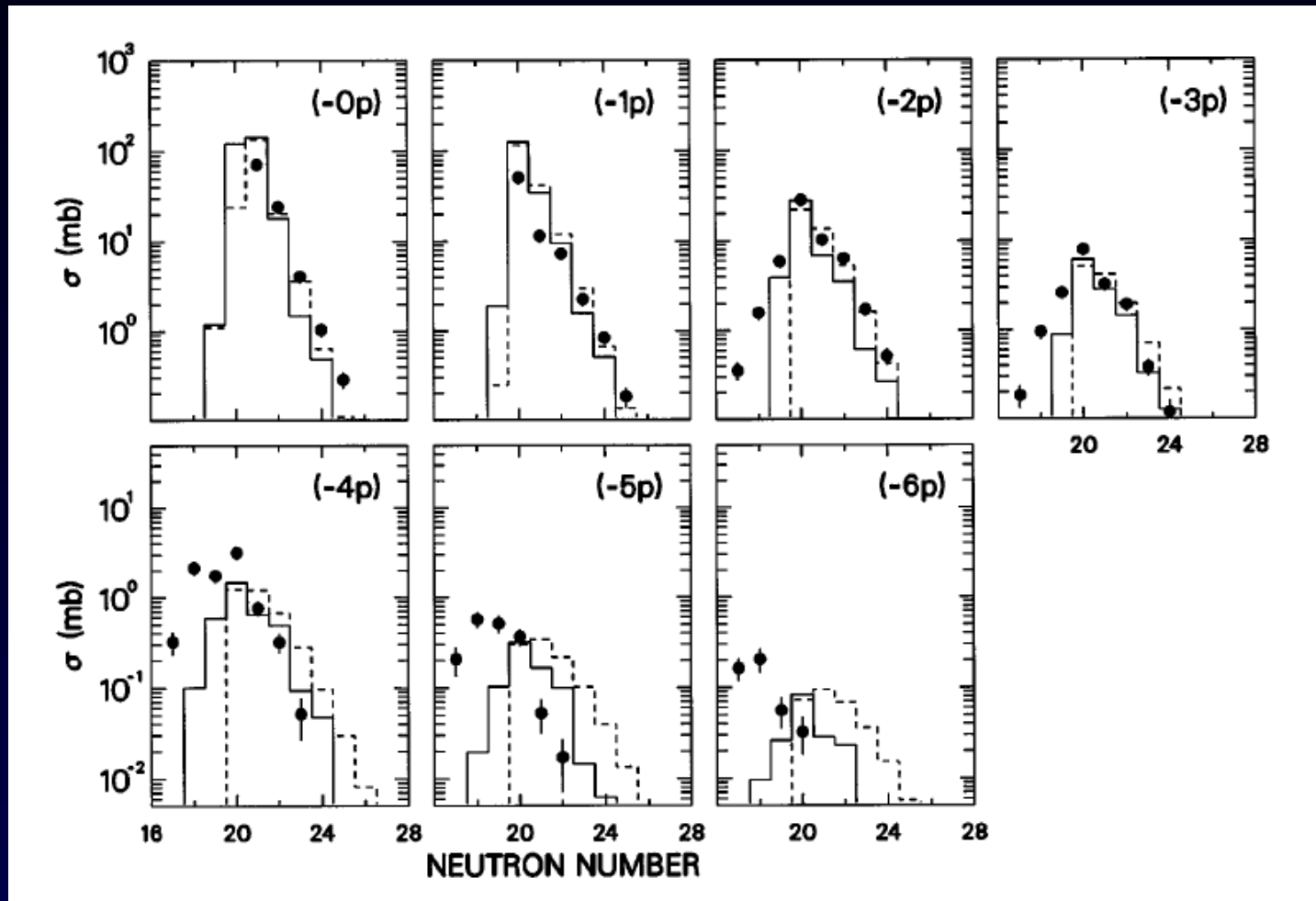
# 1. Introduction

L. Corradi et.al. Phys. Rev. C 54, 201 (1996)

## Nucleon transfer cross section

$^{40}\text{Ca} + ^{124}\text{Sn}$ ,  $E_{\text{lab}} = 170$  [MeV]

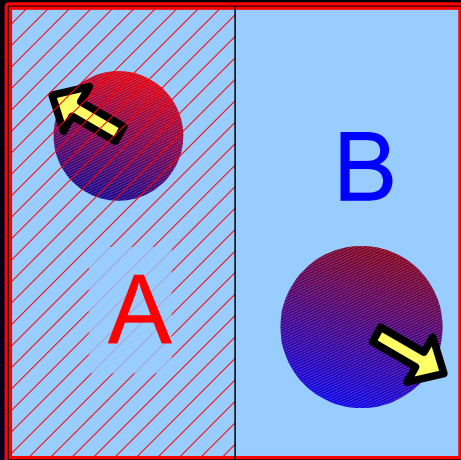
- isotope distribution for a particular proton stripping channel
- full line; GRAZING



# 2. Formulation

Preparation to define  
the nucleon transfer probabilities

Final state



Normalization of many-body wave function

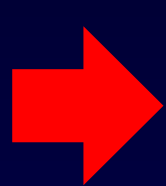
$$\int d\vec{r}_1 \cdots \int d\vec{r}_N |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2 = 1$$

$N$ ; total nucleon number

$$\int d\vec{r} = \int_A d\vec{r} + \int_B d\vec{r}$$

divide spacial integral  
into two parts

$$\left( \int_A d\vec{r}_1 + \int_B d\vec{r}_1 \right) \cdots \left( \int_A d\vec{r}_N + \int_B d\vec{r}_N \right) |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2 = 1$$

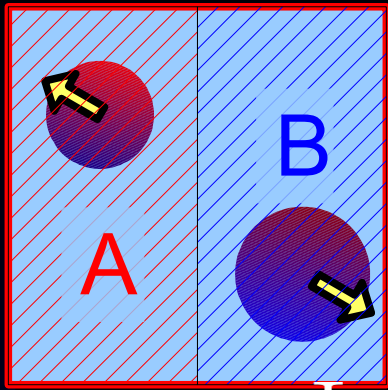


$$\sum_{\tau_1 \cdots \tau_N} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_N} d\vec{r}_N |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2 = 1$$

$\tau_i = A$  or  $B$       Summation over  $2^N$  all patterns of  $\tau_i$

# 2. Formulation

Definition of nucleon transfer probabilities



Final state  $\Phi_f$

Normalization of many-body wave function

$$\sum_{\tau_1 \cdots \tau_N} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_N} d\vec{r}_N |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2 = 1$$



breakdown of the summation

# of terms	${}^N C_0$	${}^N C_1$	$\cdots$	${}^N C_n$	$\cdots$	${}^N C_N$
configurations	$\{BB \cdots B\}$	$\{AB \cdots B\}$ $\{BAB \cdots B\}$ $\vdots$	$\{AA \cdots ABB \cdots B\}$	$\underbrace{\quad\quad\quad}_n$ $\vdots$ $\underbrace{\quad\quad\quad}_{N-n}$	$\{AA \cdots A\}$	

Probability; n nucleons in A and N-n nucleons in B

$$P_A(n) \equiv \sum_{\{\tau_i; A^n B^{N-n}\}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_N} d\vec{r}_N |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2$$

$$\sum_{n=0}^N P_A(n) = 1$$

all combinations; A appears n times and B appears N-n times

## 2. Formulation

Expression of the nucleon transfer probabilities using space division function

Probability;  $n$  nucleons in A and  $N-n$  nucleons in B

$$P_A(n) \equiv \sum_{\{\tau_i; A^n B^{N-n}\}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_N} d\vec{r}_N |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2$$

Space division function

$$\Theta_\tau(\vec{r}) \equiv \begin{cases} 1 & \vec{r} \in \tau \\ 0 & \vec{r} \notin \tau \end{cases} \quad \tau_i = A \text{ or } B$$

$$\int_\tau d\vec{r} = \int d\vec{r} \Theta_\tau(\vec{r})$$

Then, we can write  $P_A(n)$  as

$$P_A(n) = \int d\vec{r}_1 \cdots \int d\vec{r}_N \sum_{\{\tau_i; A^n B^{N-n}\}} \Theta_{\tau_1}(\vec{r}_1) \cdots \Theta_{\tau_N}(\vec{r}_N) |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2$$

We can extract nucleon transfer probabilities applying this formula to the final-state wave function.

➔ We apply this to the final-state of TDHF, i.e., single Slater determinant

# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ①

Final state of TDHF; single Slater determinant

Slater determinant

$$\begin{aligned}\Phi_f(\vec{r}_1, \dots, \vec{r}_N) &= \frac{1}{N!} \begin{vmatrix} \phi_1(\vec{r}_1) & \cdots & \phi_1(\vec{r}_N) \\ \vdots & & \vdots \\ \phi_N(\vec{r}_1) & \cdots & \phi_N(\vec{r}_N) \end{vmatrix} = \frac{1}{N!} \det \{ \phi_i(\vec{r}_j) \} \\ &= \frac{1}{N!} \sum_{\sigma} \text{sgn}(\sigma) \phi_{\sigma_1}(\vec{r}_1) \cdots \phi_{\sigma_N}(\vec{r}_N)\end{aligned}$$

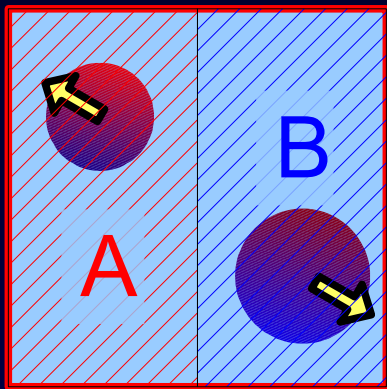
$\phi_i(\vec{r})$  ; single particle wave function

$i = 1, \dots, N$  ( $N = N_1 + N_2$ )

each orbitals exist in whole space

$$\phi_i(\vec{r}) = \phi_i^A(\vec{r}) + \phi_i^B(\vec{r}) \quad \phi_i^{\tau}(\vec{r}) = \phi_i(\vec{r}) \Theta_{\tau}(\vec{r})$$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij} \quad ; \text{ orthonormalization}$$



Final state

# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ①

Probability; n nucleons in A and N-n nucleons in B

$$P_A(n) = \int d\vec{r}_1 \cdots \int d\vec{r}_N \sum_{\{\tau_i; A^n B^{N-n}\}} \Theta_{\tau_1}(\vec{r}_1) \cdots \Theta_{\tau_N}(\vec{r}_N) |\Phi_f(\vec{r}_1, \cdots, \vec{r}_N)|^2$$

invariant under exchange  $r_i$  and  $r_j$

$$= \int d\vec{r}_1 \cdots \int d\vec{r}_N \sum_{\{\tau_i; A^n B^{N-n}\}} \Theta_{\tau_1}(\vec{r}_1) \cdots \Theta_{\tau_N}(\vec{r}_N) \frac{1}{N!} \sum_{\sigma} \text{sgn}(\sigma) \phi_{\sigma_1}^*(\vec{r}_1) \cdots \phi_{\sigma_N}^*(\vec{r}_N) \det \{\phi_i(\vec{r}_j)\}$$

all permutation gives same contribution

cancel  
1/N!

$$= \int d\vec{r}_1 \cdots \int d\vec{r}_N \sum_{\{\tau_i; A^n B^{N-n}\}} \Theta_{\tau_1}(\vec{r}_1) \cdots \Theta_{\tau_N}(\vec{r}_N) \phi_1^*(\vec{r}_1) \cdots \phi_N^*(\vec{r}_N) \det \{\phi_i(\vec{r}_j)\}$$

$$= \sum_{\{\tau_i; A^n B^{N-n}\}} \sum_{\sigma} \text{sgn}(\sigma) \int d\vec{r}_1 \Theta_{\tau_1}(\vec{r}_1) \phi_1^*(\vec{r}_1) \phi_{\sigma_1}(\vec{r}_1) \cdots \int d\vec{r}_N \Theta_{\tau_N}(\vec{r}_N) \phi_N^*(\vec{r}_N) \phi_{\sigma_N}(\vec{r}_N)$$

We obtain probability  $P_A(n)$  for single Slater determinant



# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ①

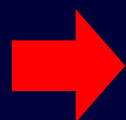
Probability; n nucleons in A and N-n nucleons in B for Slater det. [1], [2]

$$P_A(n) = \sum_{\{\tau_i; A^n B^{N-n}\}} \begin{vmatrix} \langle \phi_1 | \phi_1 \rangle_{\tau_1} & \cdots & \langle \phi_N | \phi_1 \rangle_{\tau_N} \\ \vdots & & \vdots \\ \langle \phi_1 | \phi_N \rangle_{\tau_1} & \cdots & \langle \phi_N | \phi_N \rangle_{\tau_N} \end{vmatrix}$$

all combinations; A appears n times and B appears N-n times

$$\langle \phi_i | \phi_j \rangle = \langle \phi_i | \phi_j \rangle_A + \langle \phi_i | \phi_j \rangle_B = \delta_{ij}$$

$$\langle \phi_i | \phi_j \rangle_{\tau} \equiv \int d\vec{r} \phi_i^*(\vec{r}) \phi_j(\vec{r}) \Theta_{\tau}(\vec{r}) \quad \text{inner product in the region } \tau$$



$2^N$  times calculation of determinant are required to obtain all (n=0, 1, ..., N) probabilities.

N;	order of $2^N$
10;	$10^3$
20;	$10^6$
50;	$10^{15}$
100;	$10^{30}$

[1] H J Lüdde and R M Dreizler, J. Phys. B 16, 3973 (1983)

[2] R. Nagano, K. Yabana, T. Tazawa, and Y. Abe, Phys. Rev. A, 62, 062721 (2000)

# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ②

Last year, an innovative method was proposed by C. Simenel [3]

[3] C. Simenel, Phys. Rev. Lett. **105**, 192701 (2010)

$$P_A(n) = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \det \left\{ \langle \phi_i | \phi_j \rangle_B + e^{-i\theta} \langle \phi_i | \phi_j \rangle_A \right\}$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \sum_{\sigma} \text{sgn}(\sigma) \left( \langle \phi_{\sigma_1} | \phi_1 \rangle_B + e^{-i\theta} \langle \phi_{\sigma_1} | \phi_1 \rangle_A \right) \cdots \left( \langle \phi_{\sigma_N} | \phi_N \rangle_B + e^{-i\theta} \langle \phi_{\sigma_N} | \phi_N \rangle_A \right)$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \sum_{\sigma} \text{sgn}(\sigma) \sum_{n'=0}^N e^{-in'\theta} \sum_{\{\tau_i; A^{n'} B^{N-n'}\}} \langle \phi_{\sigma_1} | \phi_1 \rangle_{\tau_1} \cdots \langle \phi_{\sigma_N} | \phi_N \rangle_{\tau_N}$$

$$= \sum_{\{\tau_i; A^n B^{N-n}\}} \sum_{\sigma} \text{sgn}(\sigma) \langle \phi_{\sigma_1} | \phi_1 \rangle_{\tau_1} \cdots \langle \phi_{\sigma_N} | \phi_N \rangle_{\tau_N}$$

These two expressions are equivalent exactly.

# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ②

Interpretation by particle number projection operator

particle number projection operator

$$\delta(n - \hat{N}_A) = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{i(n - \hat{N}_A)\theta}$$

$$\hat{N}_A = \sum_{i=1}^N \Theta_A(\vec{r}_i) \quad \text{number operator in the region A}$$

$$P_A(n) = \langle \Phi_f | \delta(n - \hat{N}_A) | \Phi_f \rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \langle \Phi_f | e^{-i\Theta_A(\vec{r}_1)\theta} \dots e^{-i\Theta_A(\vec{r}_N)\theta} | \Phi_f \rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \sum_{\sigma} \text{sgn}(\sigma) \int d\vec{r}_1 \phi_1^*(\vec{r}_1) e^{-i\Theta_A(\vec{r}_1)\theta} \phi_{\sigma_1}(\vec{r}_1) \dots \int d\vec{r}_N \phi_N^*(\vec{r}_N) e^{-i\Theta_A(\vec{r}_N)\theta} \phi_{\sigma_N}(\vec{r}_N)$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \det \{ \langle \phi_i | \phi_j \rangle_B + e^{-i\theta} \langle \phi_i | \phi_j \rangle_A \}$$

[3] C. Simenel, Phys. Rev. Lett. **105**, 192701 (2010)

# 2. Formulation

Nucleon transfer probabilities;  
for single Slater determinant ②

Comparison of these two expressions

$$P_A(n) = \sum_{\{\tau_i; A^n B^{N-n}\}} \begin{vmatrix} \langle \phi_1 | \phi_1 \rangle_{\tau_1} & \cdots & \langle \phi_N | \phi_1 \rangle_{\tau_N} \\ \vdots & & \vdots \\ \langle \phi_1 | \phi_N \rangle_{\tau_1} & \cdots & \langle \phi_N | \phi_N \rangle_{\tau_N} \end{vmatrix}$$

all combinations; A appears n times and B appears N-n times

→  $\sum_{n=0}^N {}_N C_n = 2^N$  times calculations of the determinant

N order of  $2^N$   
10;  $10^3$   
100;  $10^{30}$

$$P_A(n) = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{in\theta} \det \left\{ \langle \phi_i | \phi_j \rangle_B + e^{-i\theta} \langle \phi_i | \phi_j \rangle_A \right\}$$

This expression contains all of permutations

discretization of  $\theta$

→ ~100 times calculations of the determinant

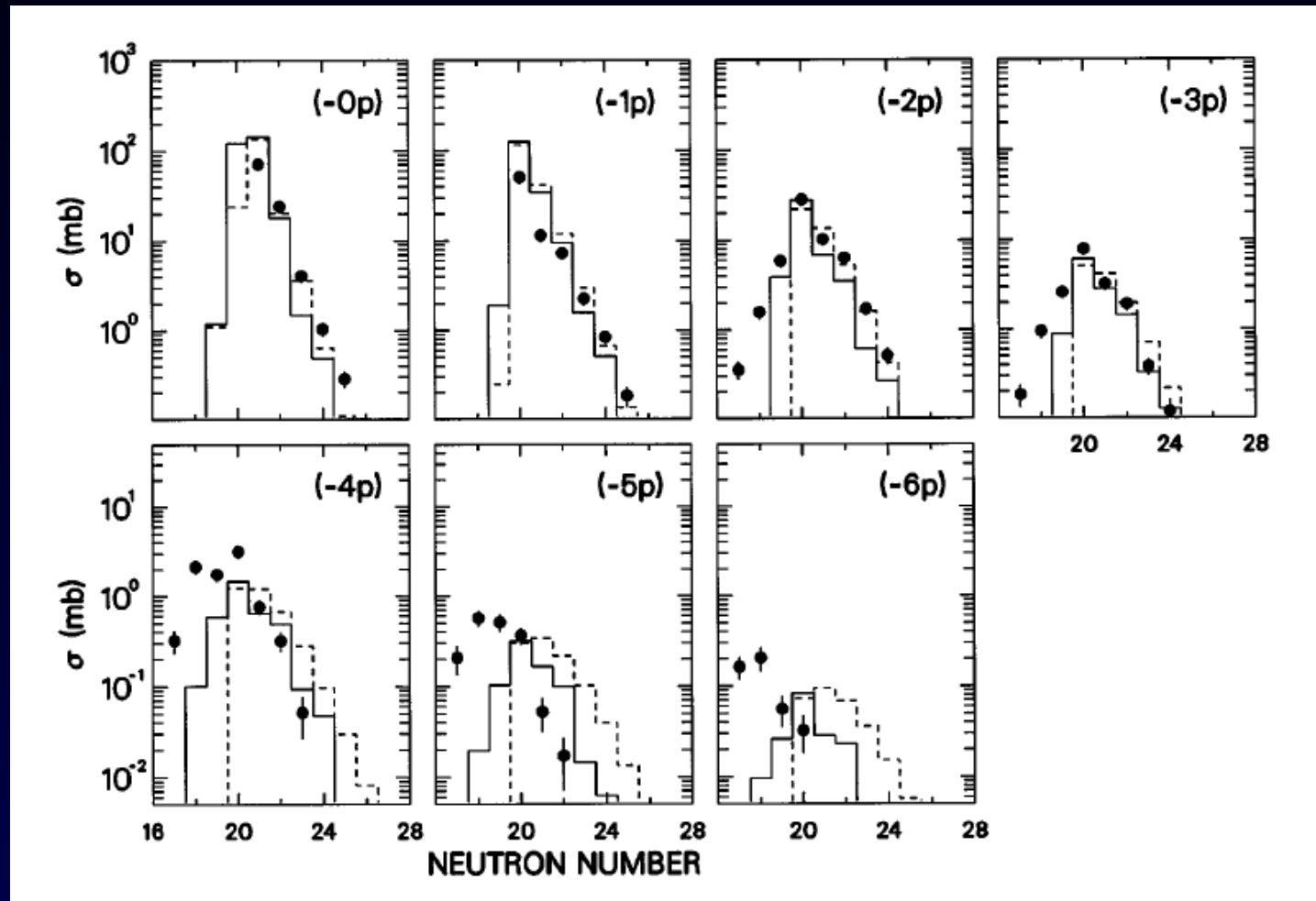
**We can apply this to the heavy ion reaction with realistic computational cost.**

# 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

## Nucleon transfer cross section

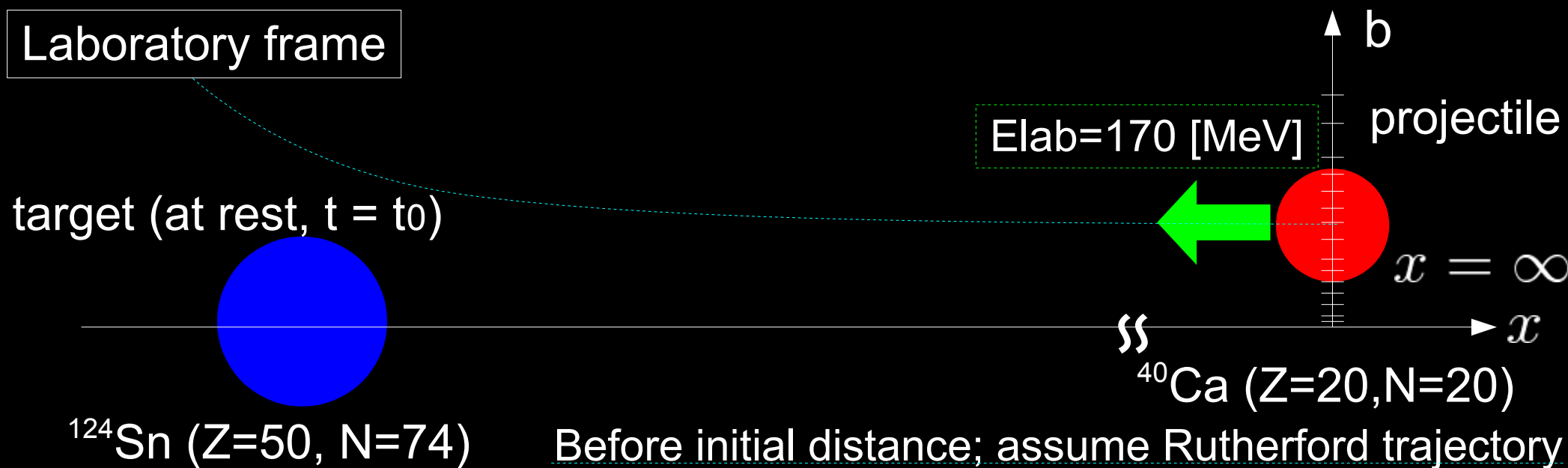
$^{40}\text{Ca}+^{124}\text{Sn}$ ,  $E_{\text{lab}}=170$  [MeV]

- isotope distribution for a particular proton stripping channel
- full line; GRAZING



# 3. Results; $^{40}\text{Ca} + ^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

- ◆ Skyrme interaction; SLy5
  - ◆ 3D Cartesian coordinate; discretized into a uniform mesh
  - ◆ grid size;  $60 \times 60 \times 26$  ( $x \times y \times z$ )
  - ◆ mesh spacing; 0.8 [fm]
  - ◆ time step; 0.2 [fm/c]
  - ◆ impact parameter; 3.7-10.0 [fm]
- Numerical space  
48 [fm] × 48 [fm] × 20.8 [fm]

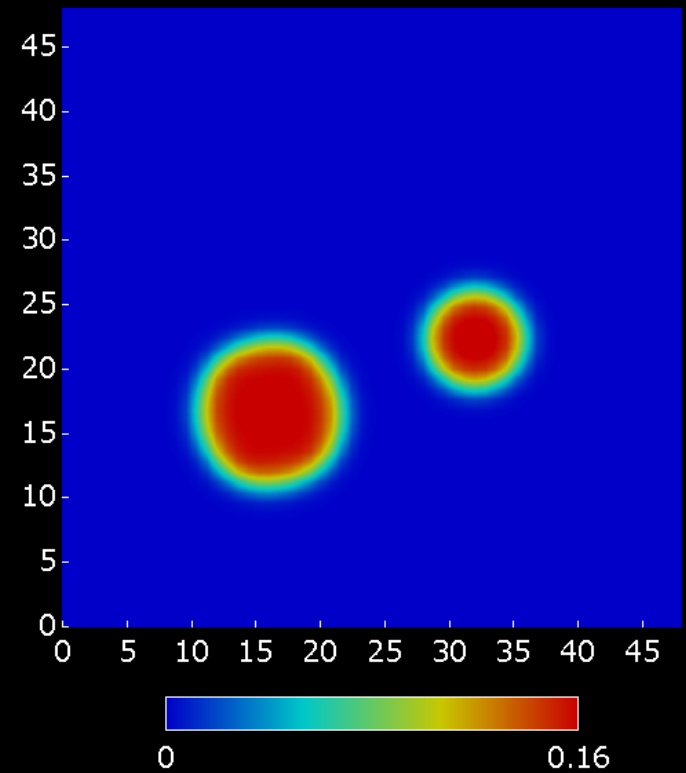
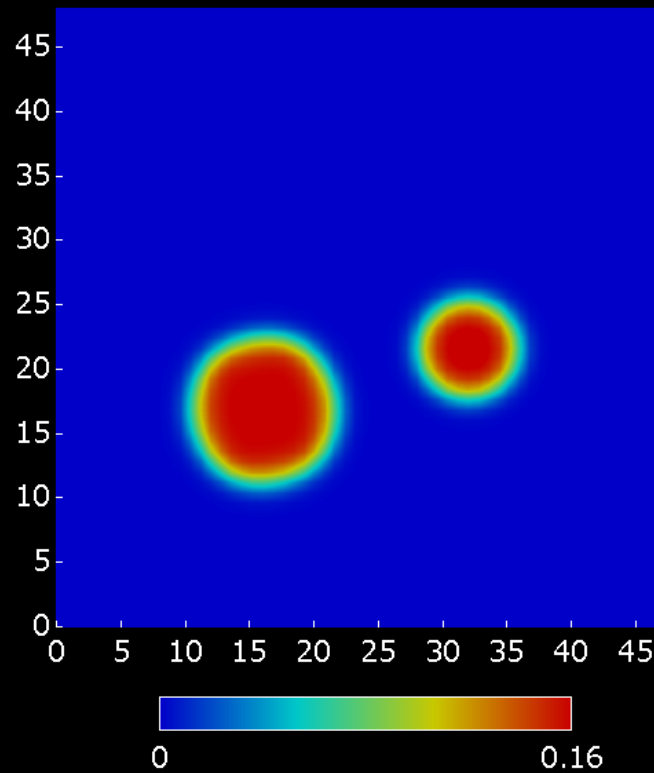
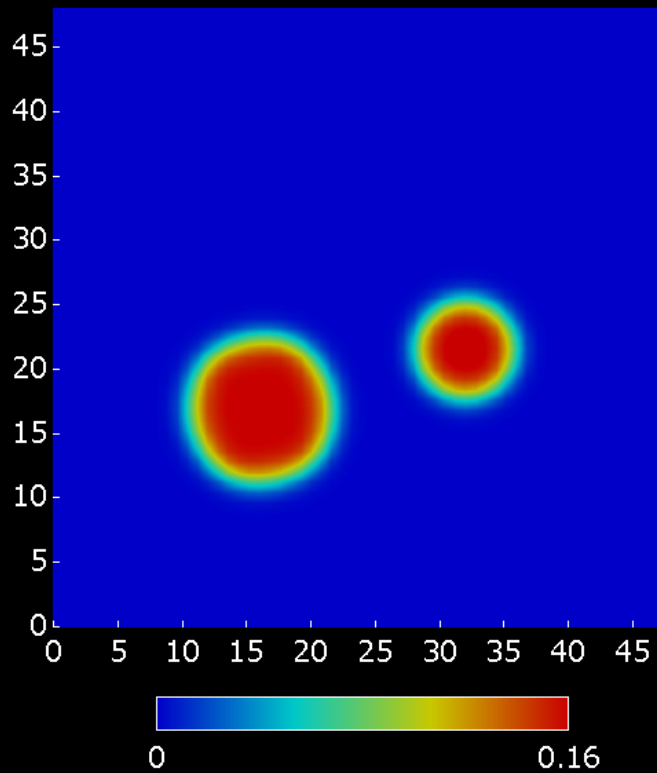


# 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

$b=3.65$  [fm]

$b=3.70$  [fm]

$b=4.50$  [fm]

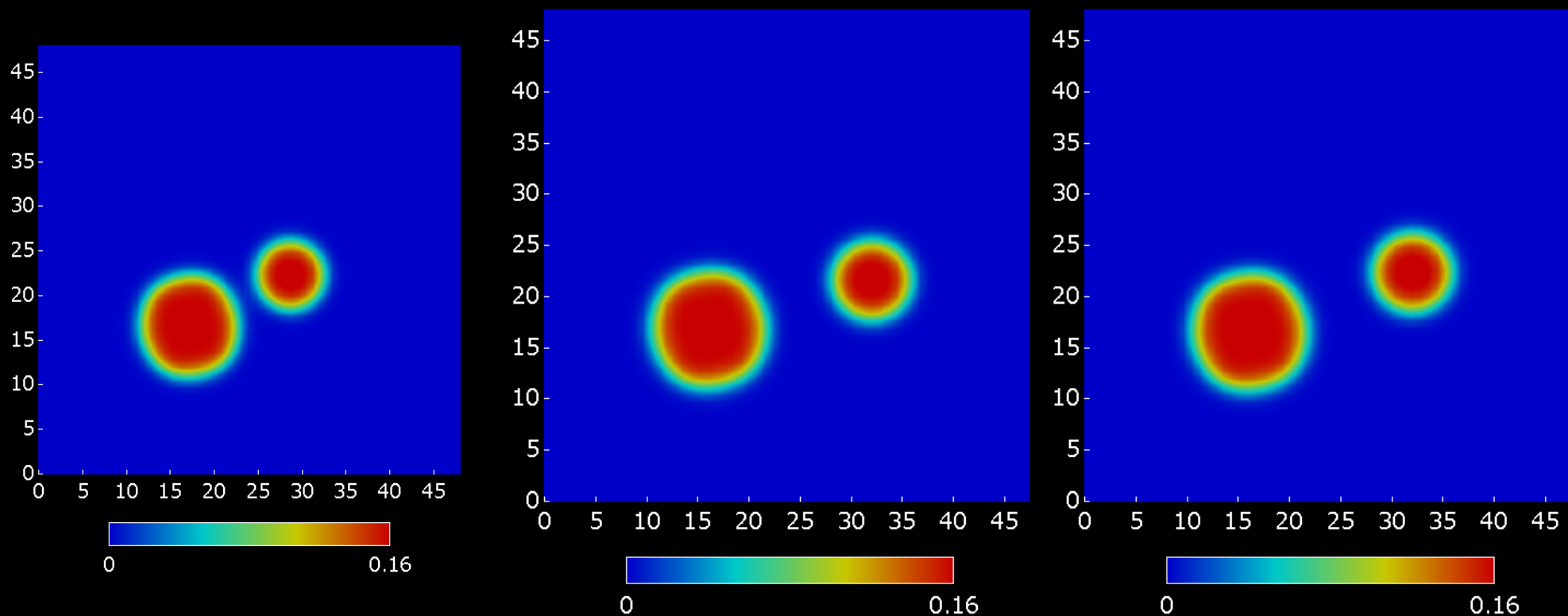


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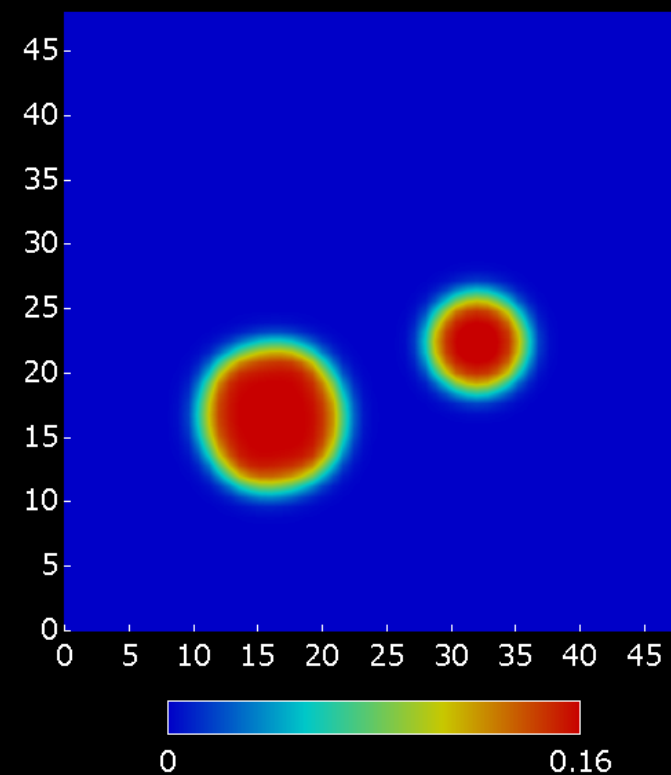
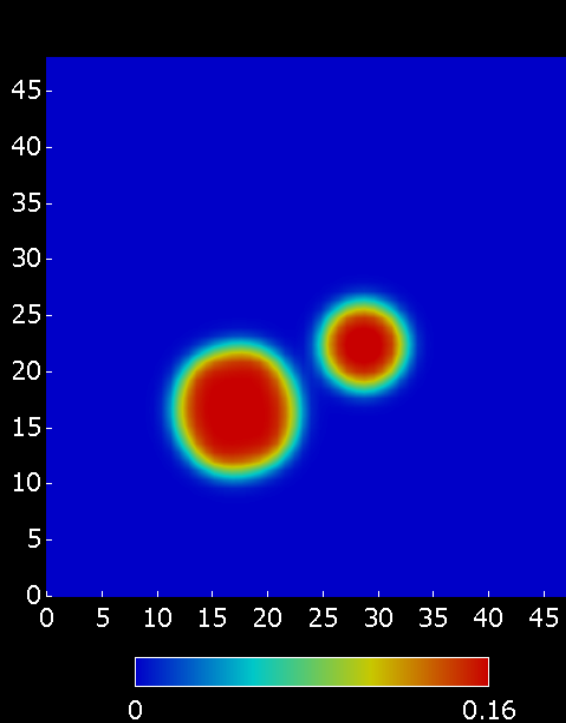
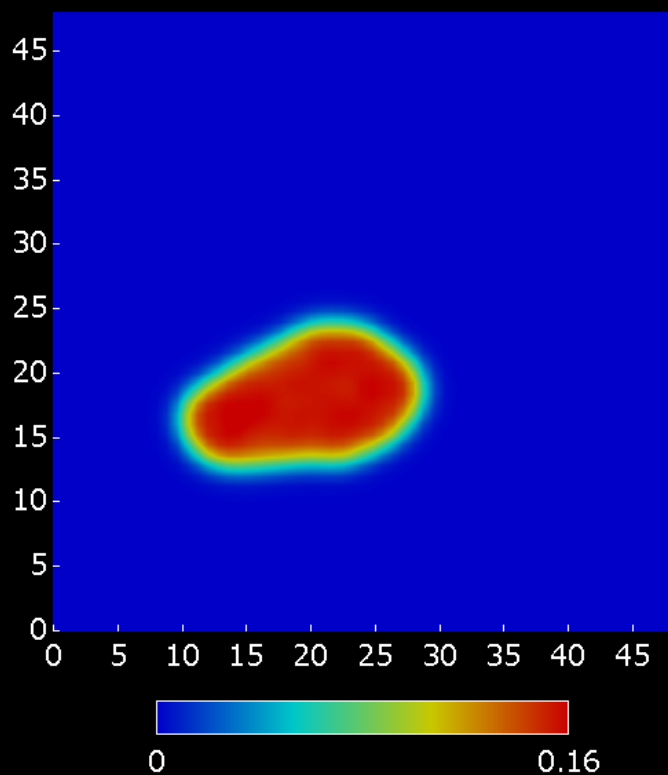


# 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

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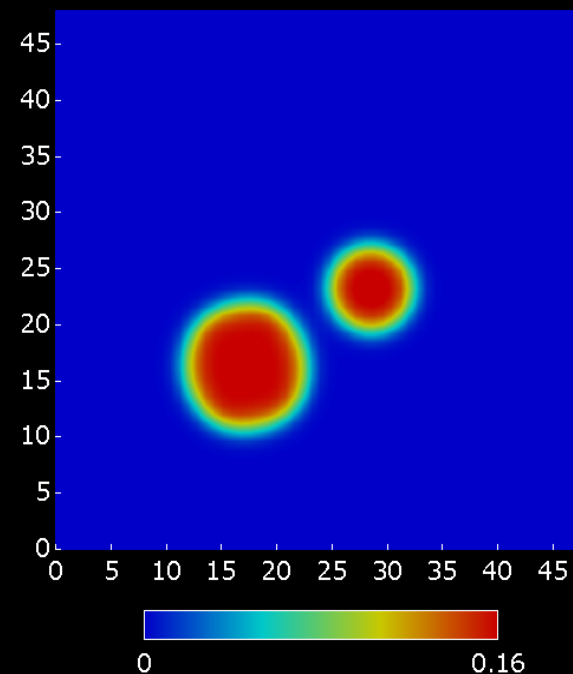
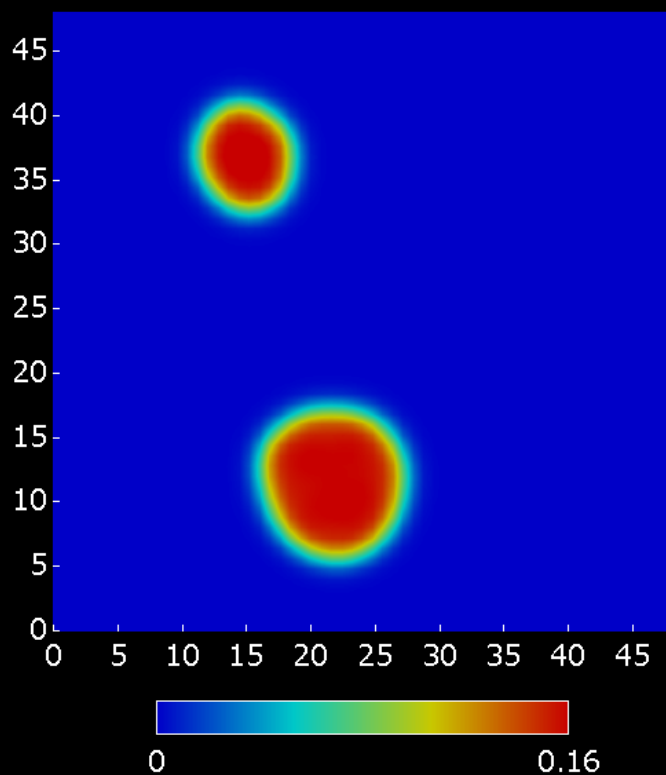
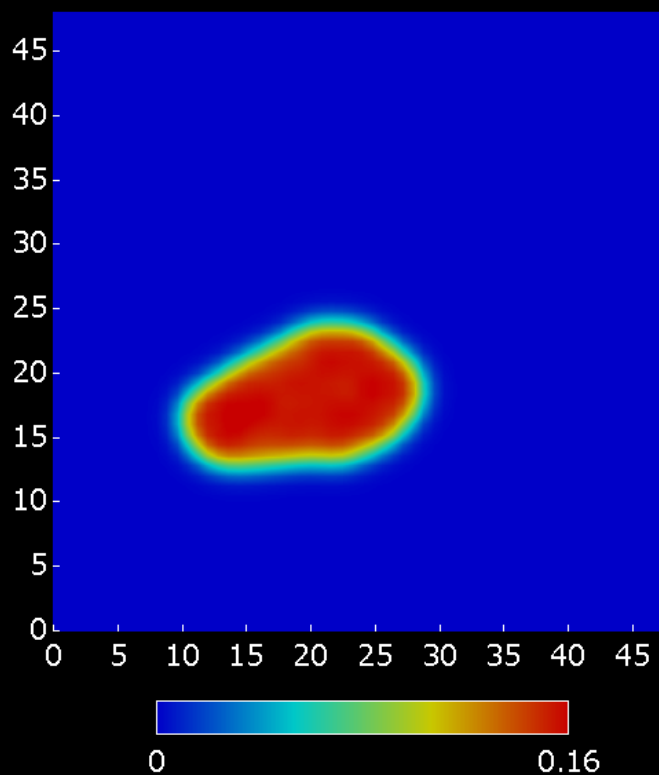


# 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

$b=3.65$  [fm]

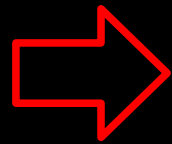
$b=3.70$  [fm]

$b=4.50$  [fm]



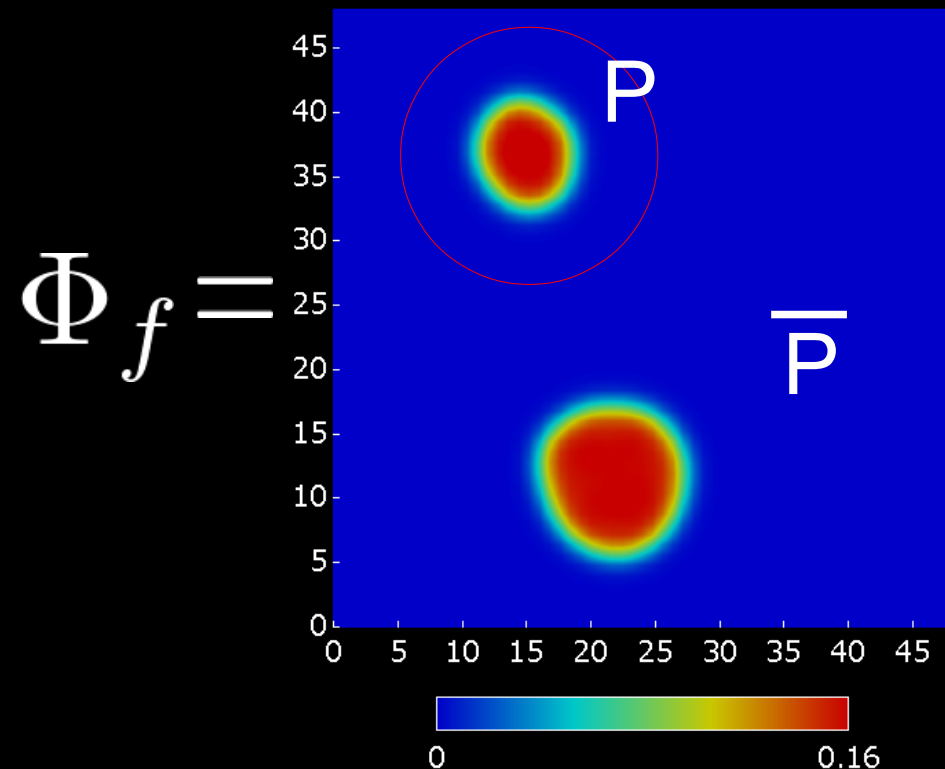
### 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

In the experiment **light ejectiles** have been detected



We define the region “P” around the C. M. of light ejectile which is a sphere with radius 10 [fm].

Ex.)  $b=3.70$  [fm]



And then, we calculate

- ◆ Average nucleon number in the region P

$$\langle \Phi_f | \hat{N}_P | \Phi_f \rangle$$

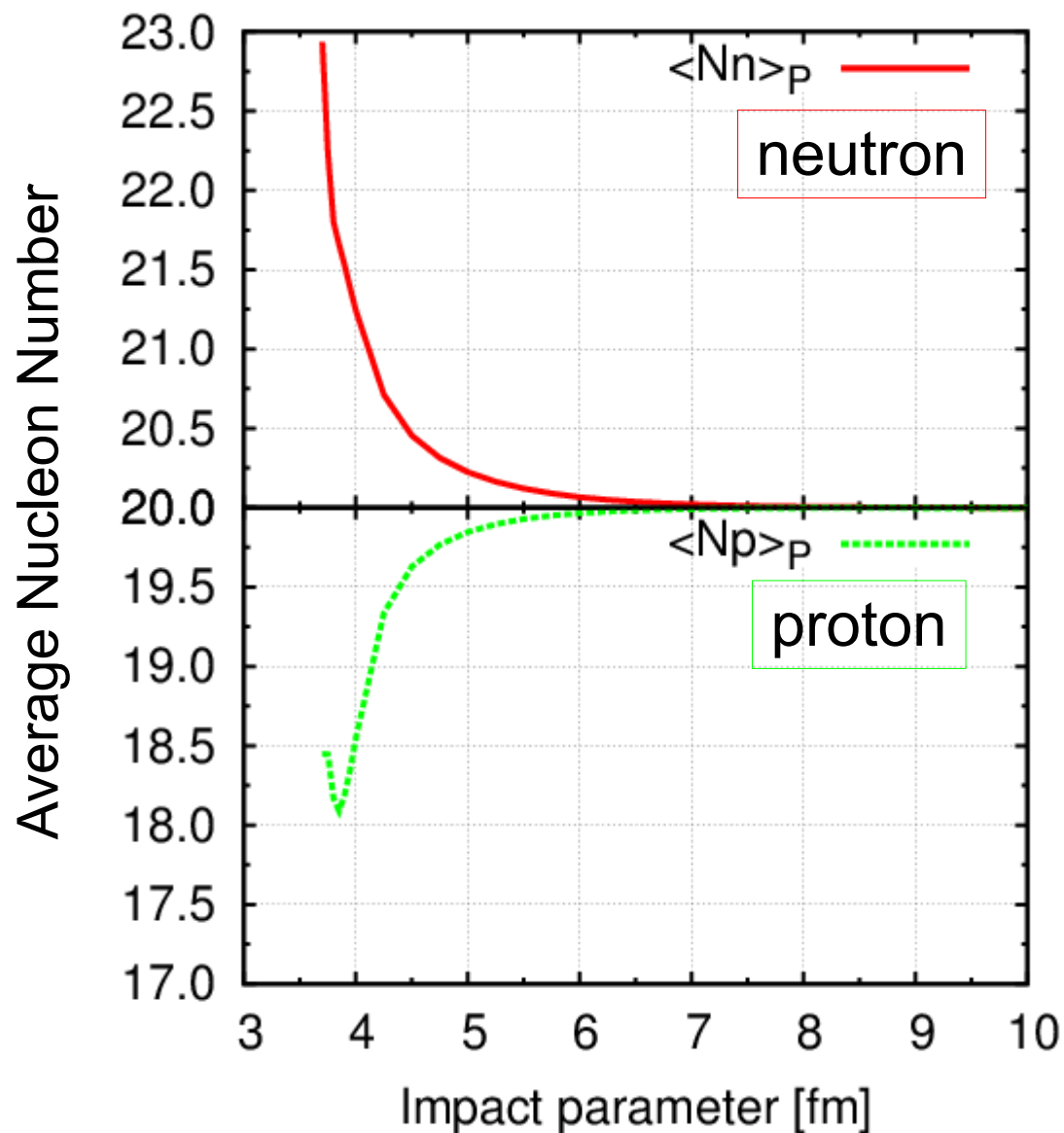
- ◆ Nucleon transfer probabilities

$$P_P(n) = \langle \Phi_f | \delta(n - \hat{N}_P) | \Phi_f \rangle$$

- ◆ Nucleon transfer cross section

$$\sigma_{\text{tr}}(n) = \int_{b_{\text{min}}}^{b_{\text{max}}} 2\pi b P_P(n) db$$

# 3. Results; $^{40}\text{Ca} + ^{124}\text{Sn}$ , $E_{\text{lab}} = 170$ [MeV]



Average nucleon number in the region P

$$\langle \Phi_f | \hat{N}_P | \Phi_f \rangle$$

Number operator

$$\hat{N}_P = \int d\vec{r} \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i) \Theta_P(\vec{r})$$

Projectile;  $^{40}\text{Ca}$  (Z=20, N=20)

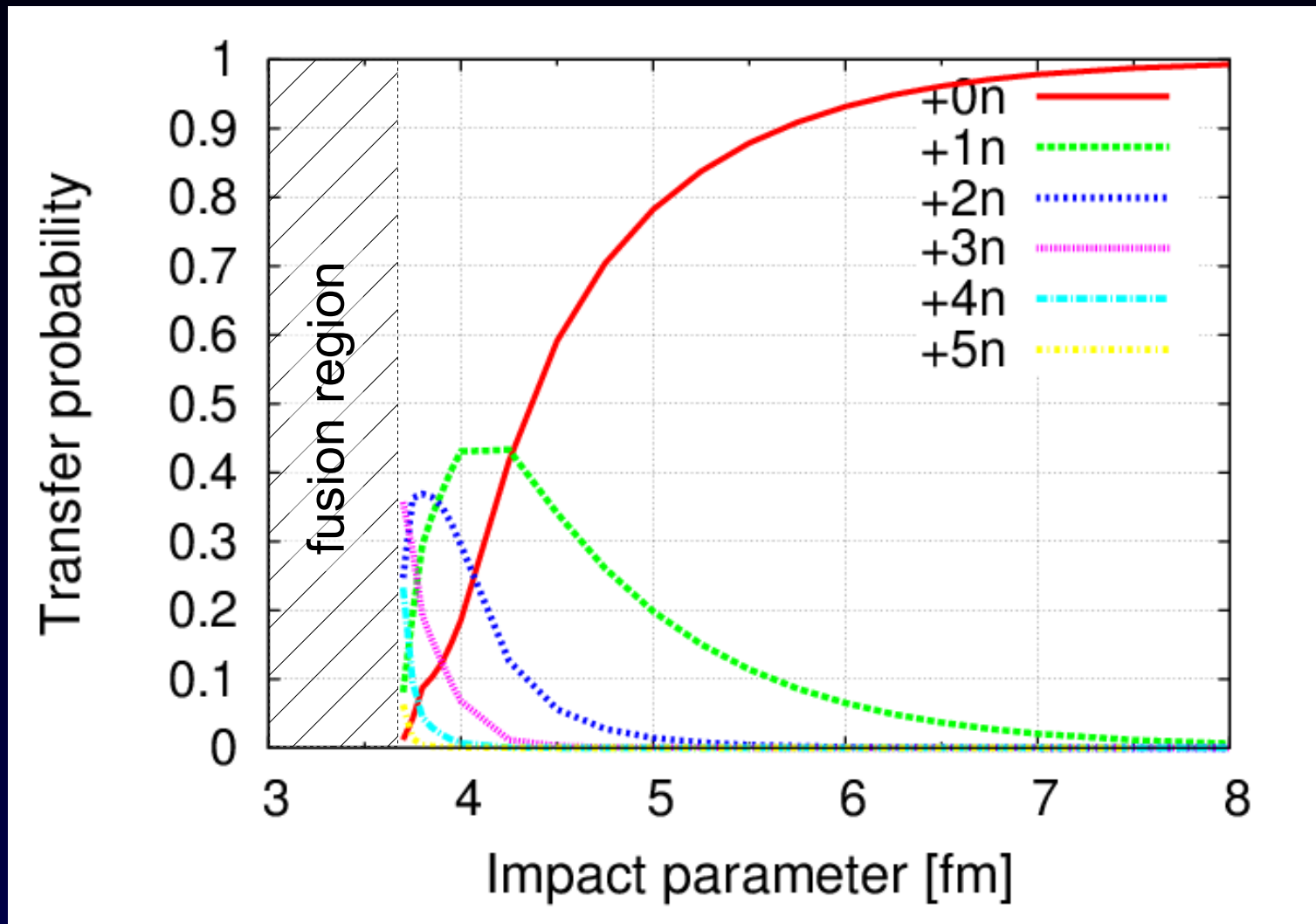
Target;  $^{124}\text{Sn}$  (Z=50, N=74)

neutron;  $^{40}\text{Ca}$  ←  $^{124}\text{Sn}$   
 proton;  $^{40}\text{Ca}$  →  $^{124}\text{Sn}$

### 3. Results; $^{40}\text{Ca} + ^{124}\text{Sn}$ , $E_{\text{lab}} = 170$ [MeV]

Neutron transfer probabilities

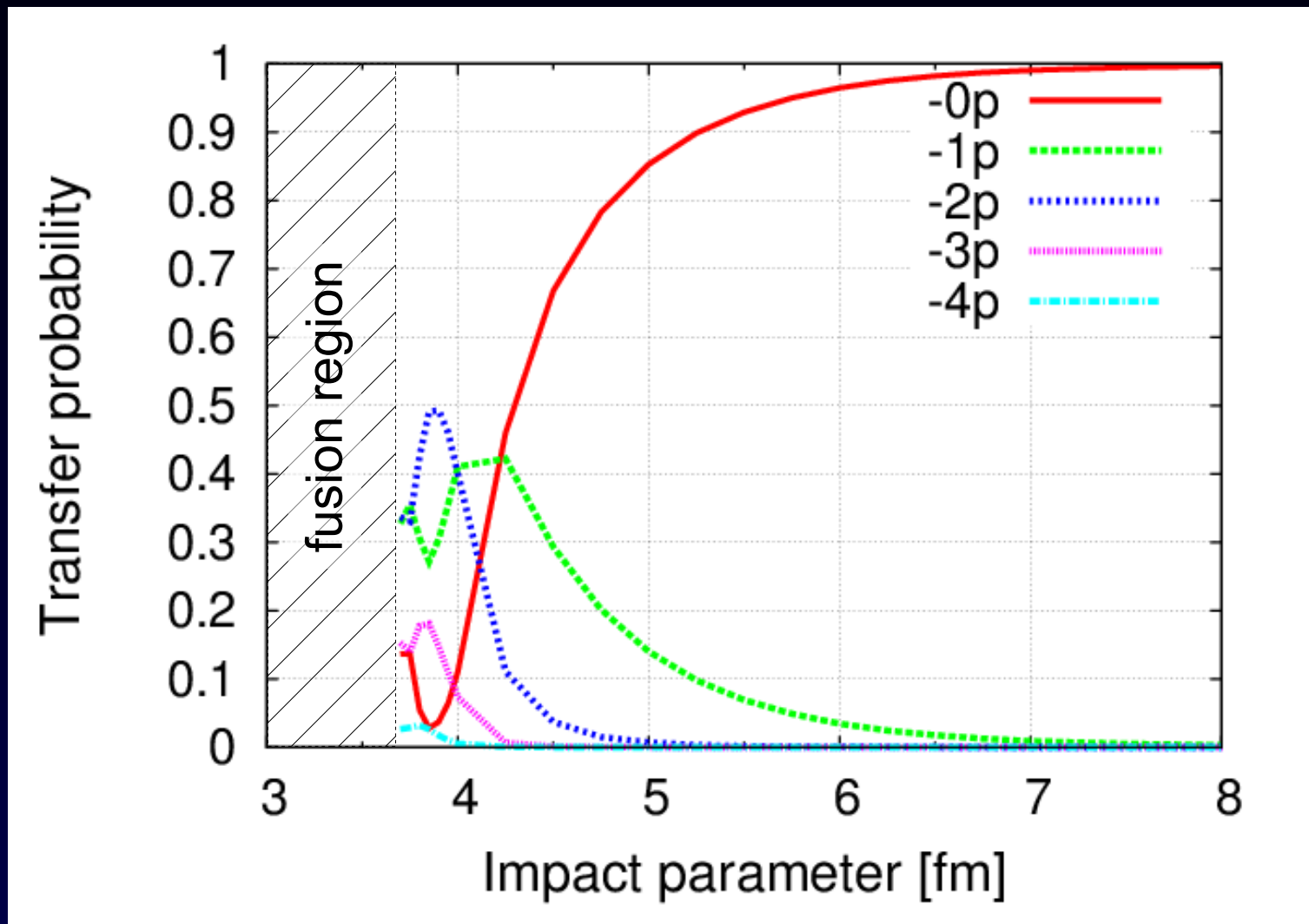
$$P_{\text{P}}(n) = \langle \Phi_f | \delta(n - \hat{N}_{\text{P}}) | \Phi_f \rangle$$



# 3. Results; $^{40}\text{Ca} + ^{124}\text{Sn}$ , $E_{\text{lab}} = 170$ [MeV]

Proton transfer probabilities

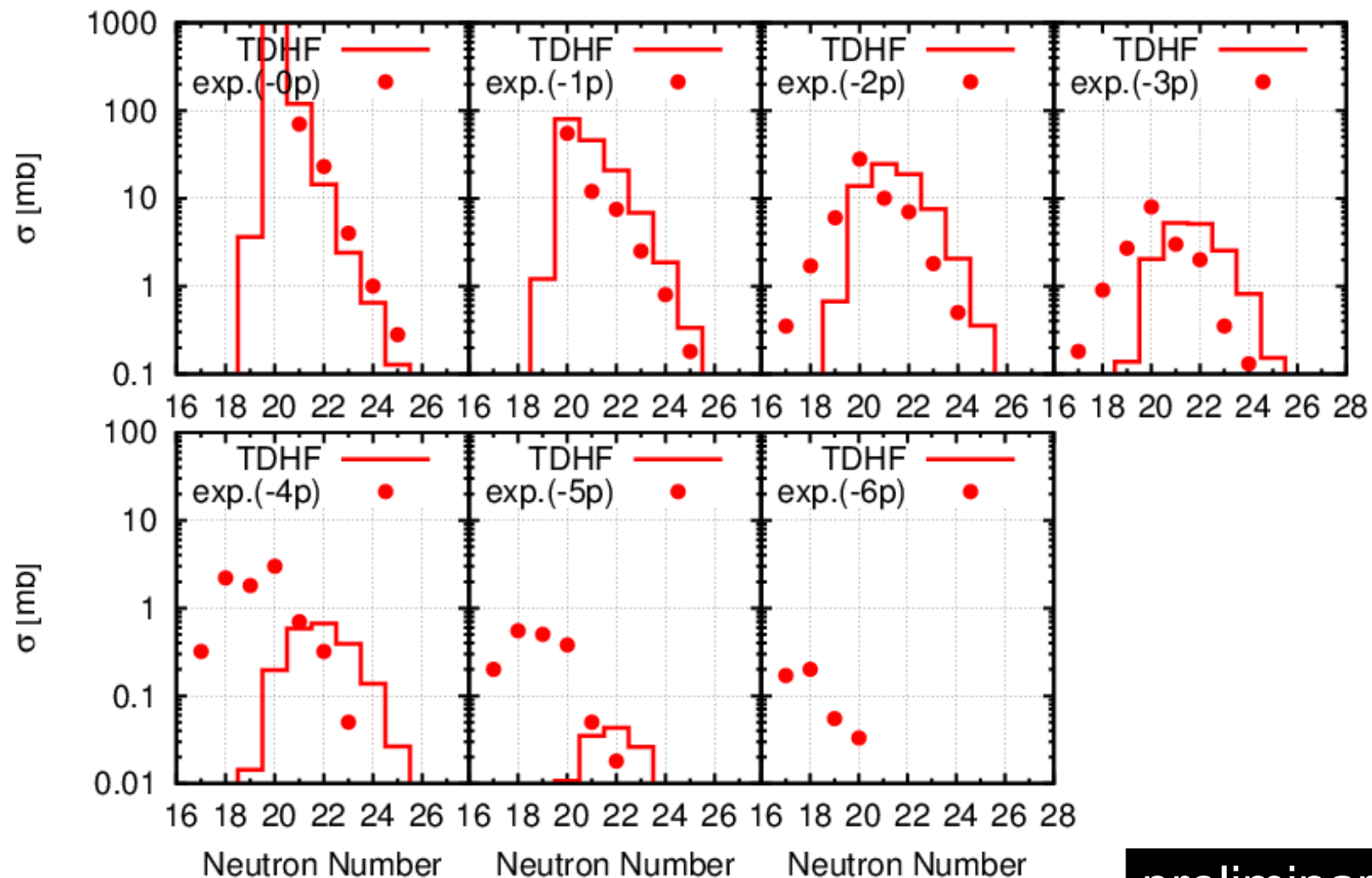
$$P_{\text{P}}(n) = \langle \Phi_f | \delta(n - \hat{N}_{\text{P}}) | \Phi_f \rangle$$



# 3. Results; $^{40}\text{Ca} + ^{124}\text{Sn}$ , $E_{\text{lab}} = 170$ [MeV]

Nucleon transfer cross section

$$\sigma_{\text{tr}}(n) = \int_{b_{\text{min}}}^{b_{\text{max}}} 2\pi b P_{\text{P}}(n) db$$

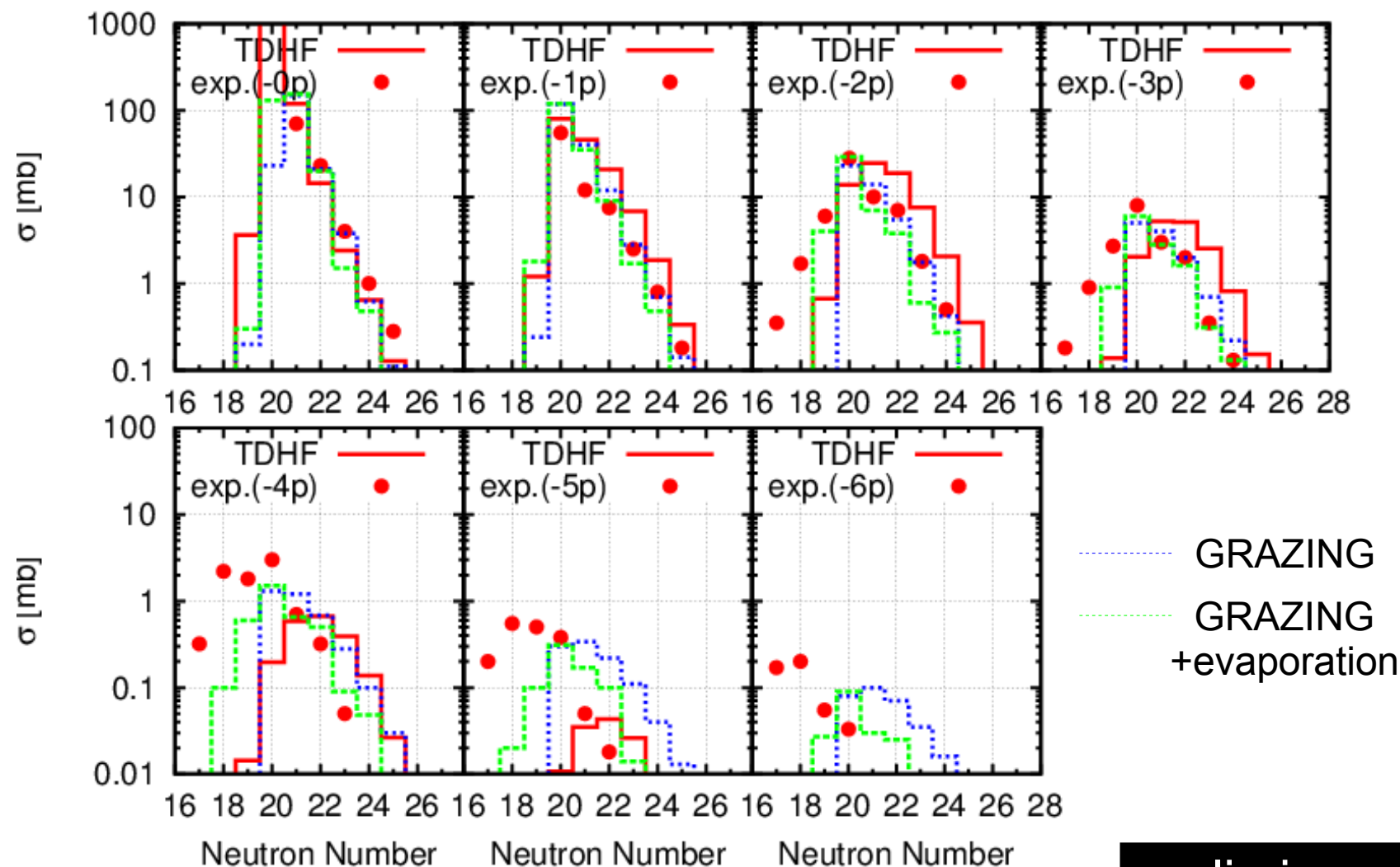


preliminary

# 3. Results; $^{40}\text{Ca}+^{124}\text{Sn}$ , $E_{\text{lab}}=170$ [MeV]

## Nucleon transfer cross section

L. Corradi et.al. Phys. Rev. C 54, 201 (1996)



preliminary



# 4. Summary and Outlook

## Summary

- ✓ The method to calculate nucleon transfer probabilities from final state wave function are presented.
- ✓  $^{40}\text{Ca}+^{124}\text{Sn}$  TDHF calculations have been carried out and yields the nucleon transfer cross sections.
- ✓ Overall agreement is good when 0-2 proton transfer occurred.
- ✓ Neutron-proton correlation is not described in our calculation.

## Outlook

- Calculate the other collision and compare the result with experiment quantitatively.
- Inclusion of the evaporation's effect.