YIPQS Long-term workshop
Dynamics and Correlations in Exotic Nuclei (DCEN2011)
One-day workshop 4: Transfer reactions
Oct. 24, 2011

Time-Dependent Hartree-Fock Calculation for Multi-Nucleon Transfer Reactions

K. Yabana
Center for Computational Sciences, Univ. Tsukuba

in collaboration with
K. Sekizawa (U. Tsukuba)

Background and motivation

Produce neutron-rich nucleus by multi-nucleon transfer（KISS Project)

Task for theoretists :

What is the best reaction condition?

projectile-target pair, collision energy, …

Existing theoretical approach for multi-nucleon transfer reactions

- GRAZING (A. Winther, 1994)

  Based on direct reaction picture

  To some extent, empirical

How about TDHF? Fully microscopic framework

Applied to fusion, deep inelastic collision, elastic scattering potential,…

Not so much efforts for transfer reaction

1. Examine how TDHF works for multi-nucleon transfer reaction.
2. Investigate preferable condition for production of N-rich nuclei
   by multi-nucleon transfer reaction

Contents
Time-dependent mean-field theory for ‘Transfer’ reaction

- Time-dependent mean-field theory for reactions
  - Nucear reaction : fusion, deep inelastic collision
  - Atomic collision : multi-electron transfer

- How to calculate transfer probability?
  - Method developed in atomic collision
  - Projection operator technique to define transfer probability

- Calculation for ^{40,48}Ca – ^{124}Sn multi-nucleon transfer reaction

Success and failure of TDHF for deep inelastic collision

J.W. Negele, The mean-field theory of nuclear structure and dynamics
Rev. Mod. Phys. 54, 913 (1982)

Good for average (one-body) quantities:

Average number of nucleon transfer
Average loss of kinetic energy

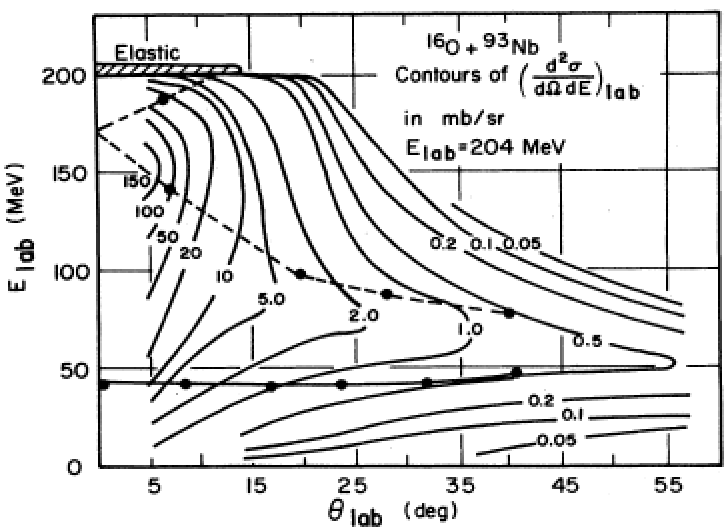


FIG. 46. Comparison of mean-field predictions with the experiemental Wilczyński plot for $^{16}O + ^{93}Nb$ at $E_{lab} = 204$ MeV. Calculated points, denoted by solid points, are connected by dashed lines above the fusion region and solid points below the fusion region to guide the eye.

Elab(204MeV) ∼ 3*Coulomb barrier

Limitation for correlation

ments. To define the number of particles in a final-state fragment, it is convenient to define a number operator which counts particles in an appropriate region of space. For simplicity, consider a binary final state with fragments receding in the positive and negative z directions in the cm frame, so that the particles in the right-hand half space may be counted by the right-hand number operator

$$\hat{N}^R = \sum_{\alpha\beta} N^R_{\alpha\beta}\, a^\dagger_\alpha a_\beta \ , \qquad (3.49)$$

where, in coordinate representation,

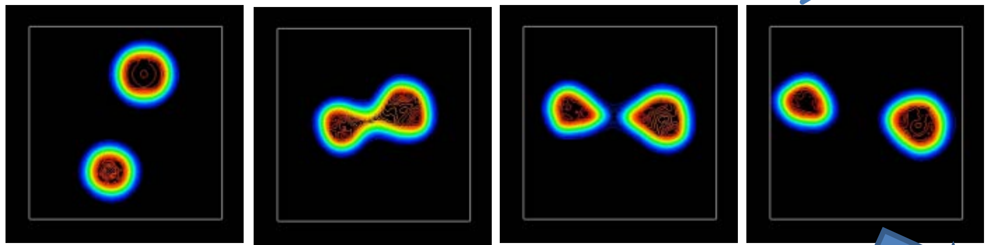
$$N^R(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\theta(z) \ . \qquad (3.50)$$

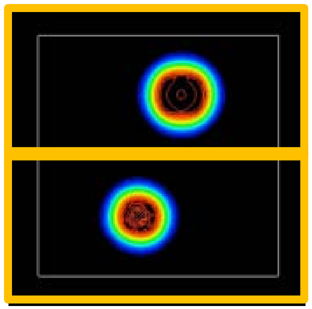
Following Bonche, Koonin, and Negle (1976), from the fact that N^R in Eq. (3.50) is a projector one is enabled to write the determinantal expectation value of the dispersion in particle number as

$$\langle (\hat{N}^R - \langle N^R \rangle)^2 \rangle^{1/2} = \left| \sum_\nu N^R_{\nu\nu} - \sum_{\nu\mu} N^R_{\nu\mu} N^R_{\mu\nu} \right|^{1/2} ,$$

where, as usual, ν and μ denote occupied single-particle wave functions. As observed by Dasso, Døssing, and Pauli (1979), the eigenvalues of the matrix $N^R_{\mu\nu}$ are ≤ 1, so that the dispersion is necessarily less than or equal to $(A/4)^{1/2}$. At the formal level, the observation that the dispersion in fragment particle number is bounded by $(A/4)^{1/2}$ is analogous to the bound on the dispersion in momentum in Eq. (3.47). Physically, it is a much more significant bound, since the experimentally observed dispersion tends to grossly exceed $(A/4)^{1/2}$.

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$$

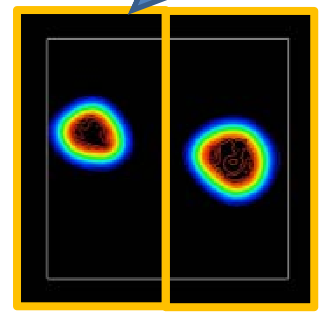




B : Target region

A : Projectile region

A : Projectile region



B : Target region

Initial wave function

$$\Psi_{\text{init}}\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A_P+A_T}\right)$$

$$\hat{N}_A\Psi_{\text{init}} = A_P\Psi_{\text{init}}$$

$$\hat{N}_B\Psi_{\text{init}} = A_T\Psi_{\text{init}}$$

$$\hat{N}_A = \int_A d\vec{r}\psi^+(\vec{r})\psi(\vec{r})$$

$$\hat{N}_B = \int_B d\vec{r}\psi^+(\vec{r})\psi(\vec{r})$$

Final wave function

$$\Psi_{\text{final}}\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A_P+A_T}\right)$$

$$\hat{N}_A\Psi_{\text{final}} \neq A_P\Psi_{\text{final}}$$

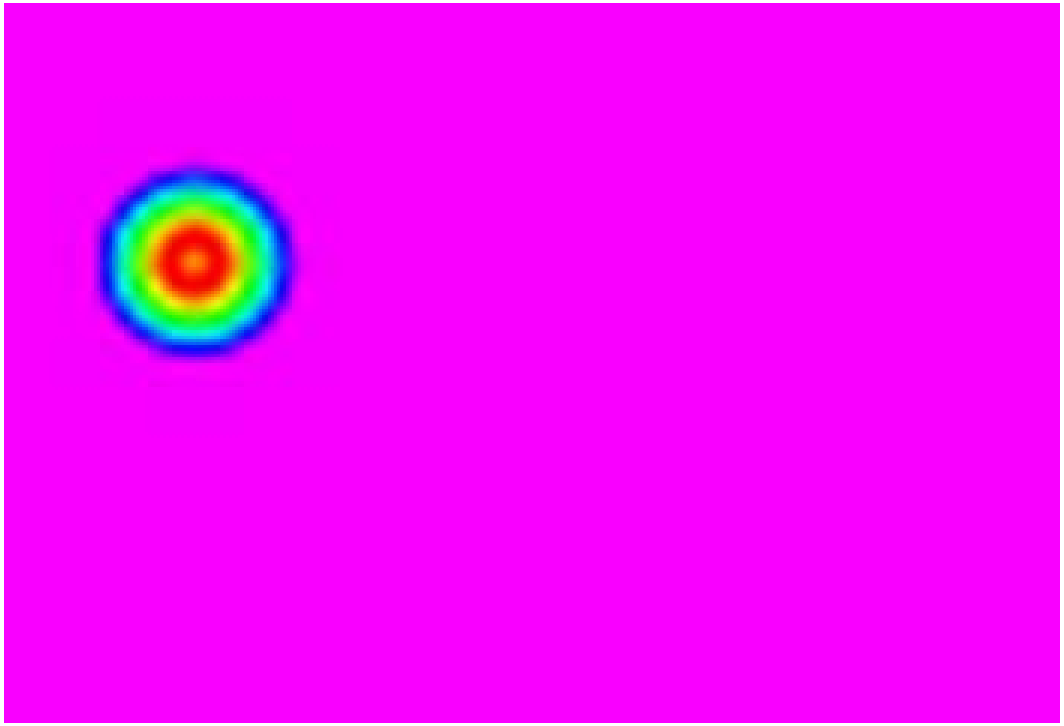
$$\hat{N}_B\Psi_{\text{final}} \neq A_T\Psi_{\text{final}}$$

Final state is a superposition of various nucleon number.

$$\left\langle\hat{N}_A\right\rangle = \left\langle\Psi_{\text{final}}\middle|\hat{N}_A\middle|\Psi_{\text{final}}\right\rangle \qquad \sigma^2 = \left\langle\left(\hat{N}_A - \left\langle\hat{N}_A\right\rangle\right)^2\right\rangle$$

Multi-electron transfer in ion-atom collision

Atom-Ion collision   Ar-Ar^{8+} 18keV



R.Nagano, K. Yabana,
T. Tazawa, Y. Abe
J. Phys. B32(1999)L65
Phys. Rev. A62(2000)062721

Formation of ‘hollow’ atom in collision of highly charged ion

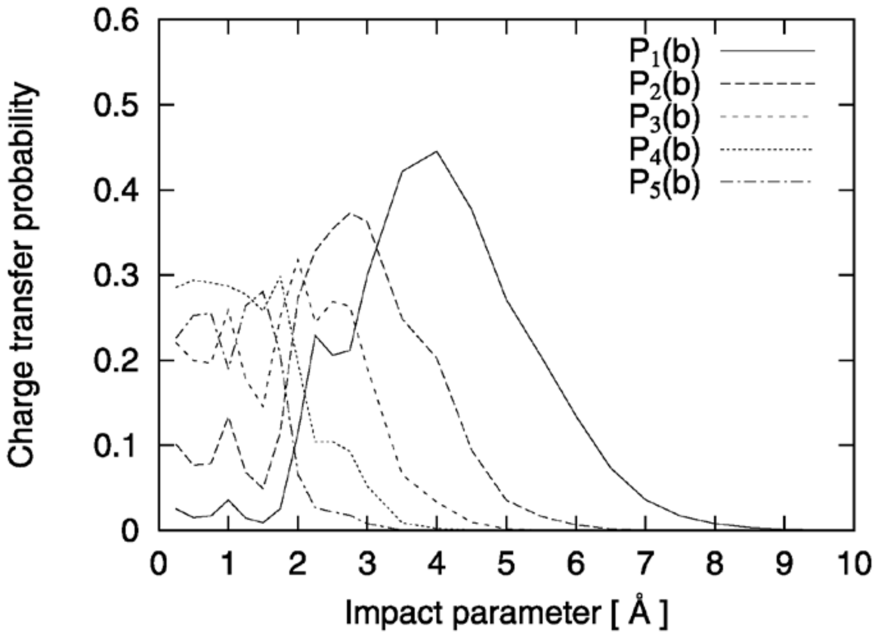
Charge transfer probability from final wave function

$P_n(b)$: n-electron removal probability from the target atom

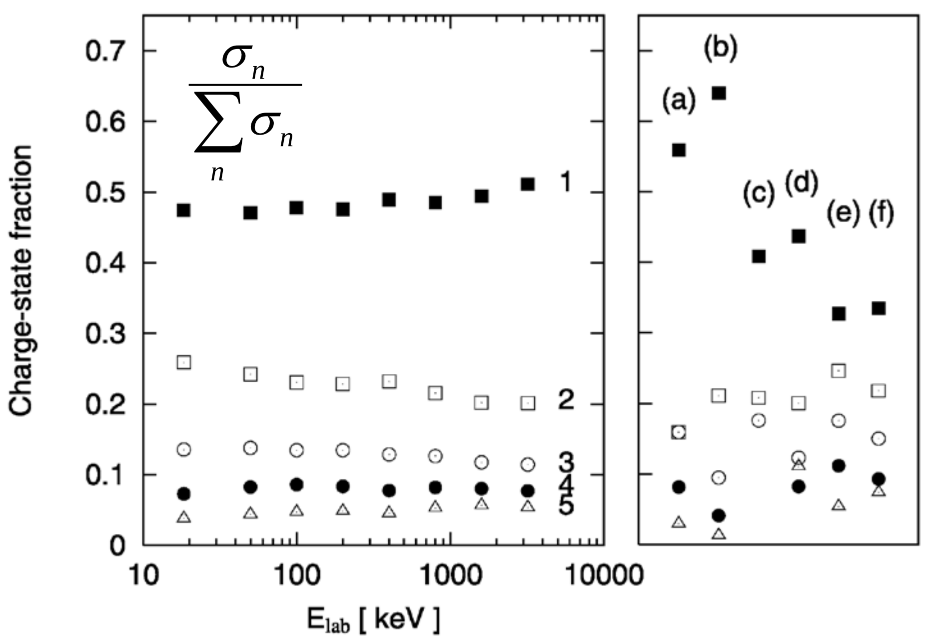
$$N_{av}(b) = \sum_{n=1}^{N} n P_n(b)$$ Average number

$$\sigma_n = \int db\, 2\pi b P_n(b)$$ Partial cross section

Ar-Ar^{8+} 18keV



Calculation Experiments



Time-dependent mean-field theory for ‘Transfer’ reaction

- Time-dependent mean-field theory for reactions

  Nucear reaction : fusion, deep inelastic collision

  Atomic collision : multi-electron transfer

- How to calculate transfer probability?

  Method developed in atomic collision

  Projection operator technique to define transfer probability

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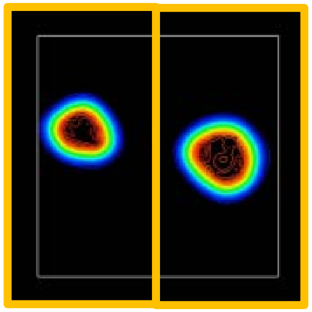
How to define probability distribution of nucleon number ?

A : Projectile region



B : Target region

Final wave function

$$\Psi_{\mathrm{final}}\left(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{A_P+A_T}\right)$$

Decompose wave function according to how many nucleons in spatial region A

$$\Psi_{\mathrm{final}} = \Psi_{n=0} + \Psi_{n=1} + \cdots + \Psi_{n=N_A-1} + \Psi_{n=N_A} + \Psi_{n=N_A+1} + \cdots + \Psi_{n=N_A+N_B}$$

Then one may define probability distribution of nucleon number by

$$P_n = \langle \Psi_n | \Psi_n \rangle$$

Decomposition looks like a projection procedure,

$$\Psi_n = \delta\left(n - \hat{N}_A\right)\Psi_{\mathrm{final}}$$

$$P_n = \left\langle \Psi_{\mathrm{final}} \left| \delta\left(n - \hat{N}_A\right) \right| \Psi_{\mathrm{final}} \right\rangle$$

$$\hat{N}_A = \int_A d\vec{r}\,\psi^+(\vec{r})\psi(\vec{r})$$

Alternative (equivalent) definition of probability distribution

One may start from a normalization relation,

$$1 = \int d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}\left(r_1, r_2, \cdots, r_{N_A+N_B}\right) \right|^2$$

Decomposing integral region into A and B,

$$1 = \left(\int_A d\vec{r}_1 + \int_B d\vec{r}_1 \right) \cdots \left(\int_A d\vec{r}_{N_A+N_B} + \int_B d\vec{r}_{N_A+N_B} \right) \left| \Psi_{\text{final}}\left(r_1, r_2, \cdots, r_{N_A+N_B}\right) \right|^2$$

$$= \sum_{\tau_i = A\,\text{or}\,B} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_{N_A+N_B}} d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}\left(r_1, r_2, \cdots, r_{N_A+N_B}\right) \right|^2$$

One may define probability distribution by,

$$P_n = \sum_{\tau_i = A\,\text{or}\,B,\, A\,\text{appers}\,n\,\text{times}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_{N_A+N_B}} d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}\left(r_1, r_2, \cdots, r_{N_A+N_B}\right) \right|^2$$

$$\sum_n P_n = 1$$

This is equivalent to the previous definition.

We have two equivalent expressions for nucleon number distributions.

$$P_n = \langle \Psi_{\text{final}} | \delta(n - \hat{N}_A) | \Psi_{\text{final}} \rangle$$
$$= \sum_{\tau_i = A \text{ or } B,\, A \text{ appears } n \text{ times}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_{N_A+N_B}} d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}(r_1, r_2, \cdots, r_{N_A+N_B}) \right|^2$$

How to calculate probability distribution for Slater determinant

$$\Psi_{\text{final}}(r_1, r_2, \cdots, r_{N_A+N_B}) = \frac{1}{\sqrt{(N_A + N_B)!}} \det\{\psi_i(\vec{r}_j, t)\}$$

the single-particle orbitals extends both spatial regions of A and B.

$$\psi_i(\vec{r}_j, t) = \psi_i^A(\vec{r}_j, t) + \psi_i^B(\vec{r}_j, t)$$

$$\langle \psi_i | \psi_j \rangle = \underbrace{\int_A d\vec{r}\, \psi_i^*(\vec{r}, t) \psi_j(\vec{r}, t) + \int_B d\vec{r}\, \psi_i^*(\vec{r}, t) \psi_j(\vec{r}, t)}_{\langle \psi_i | \psi_j \rangle_A \;+\; \langle \psi_i | \psi_j \rangle_B} = \delta_{ij}$$

Nucleon number distribution for a Slater determinant

$$P_n = \sum_{\tau_i = A \text{ or } B,\, A \text{ appears } n \text{ times}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_{N_A+N_B}} d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}(r_1, r_2, \cdots, r_{N_A+N_B}) \right|^2$$
$$= \sum_{\tau_i = A \text{ or } B,\, A \text{ appears } n \text{ times}} \det\left\{ \langle \psi_i | \psi_j \rangle_{\tau_i} \right\}$$

Need to calculate $2^{N_A+N_B}$ determinants

H.J. Ludde, R.M. Dreizler, J. Phys. B16, 3973 (1983)

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$$P_n = \sum_{\tau_i = A \text{ or } B,\ A \text{ appers } n \text{ times}} \int_{\tau_1} d\vec{r}_1 \cdots \int_{\tau_{N_A+N_B}} d\vec{r}_{N_A+N_B} \left| \Psi_{\text{final}}\left(r_1, r_2, \cdots, r_{N_A+N_B}\right) \right|^2$$

$$= \sum_{\tau_i = A \text{ or } B,\ A \text{ appers } n \text{ times}} \det\left\{ \left\langle \psi_i \middle| \psi_j \right\rangle_{\tau_i} \right\}$$

Need to calculate $2^{N_A+N_B}$ determinants

Computationally too demanding for N>20

C. Simenel, Phys. Rev. Lett 105, 192701 (2010)

$$P_n = \left\langle \Psi_{\text{final}} \middle| \delta\left(n - \hat{N}_A\right) \middle| \Psi_{\text{final}} \right\rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta \, e^{in\theta} \det\left\{ \left\langle \psi_i \middle| \psi_j \right\rangle_B + e^{-i\theta} \left\langle \psi_i \middle| \psi_j \right\rangle_A \right\}$$

discretization of 100 is sufficient

➡ Need to calculate only 100 determinants!

Feasible for any number of nucleons

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TDHF calculation for ^{40}Ca + ^{124}Sn (E_{lab}=170 MeV)

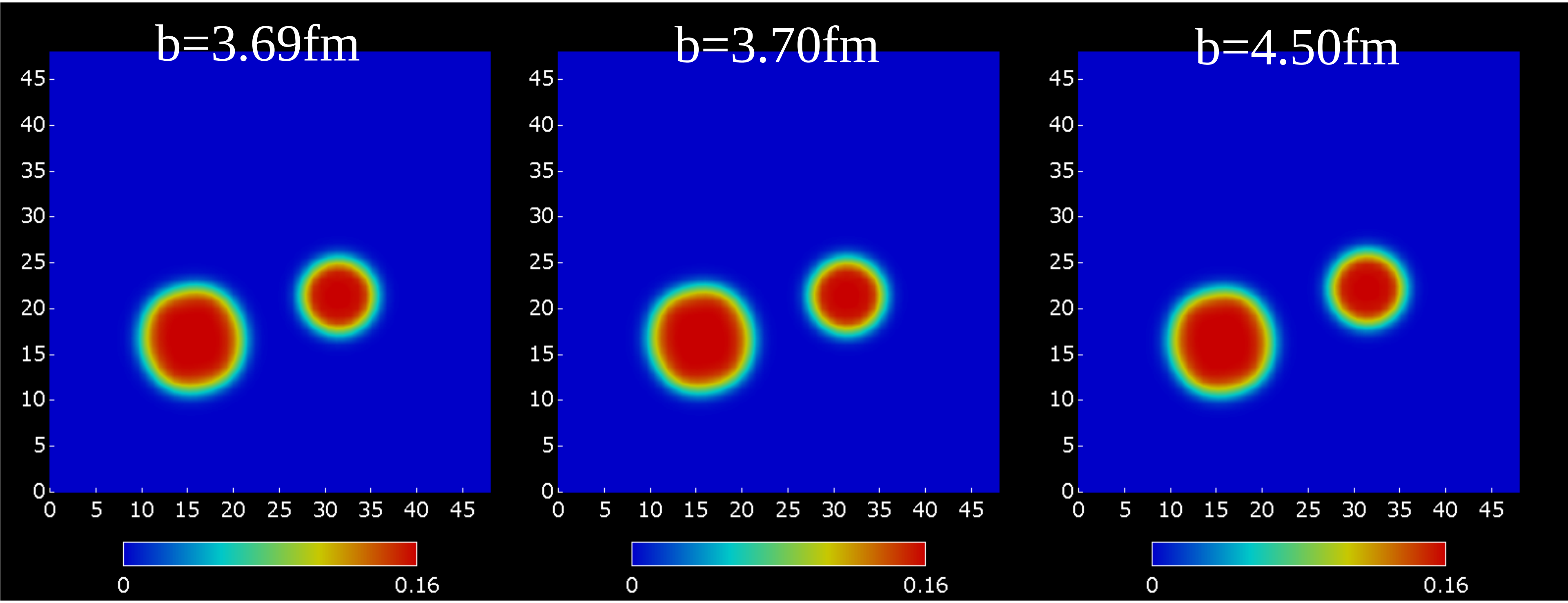
CM energy slightly higher than Coulomb barrier

3D grid, $60 \times 60 \times 26$ grid points ($48 \times 48 \times 20.8$ fm, $\Delta x = 0.8$ fm)

Skyrme SLy5 force

Calculations achieved $0 < b < 10$ fm

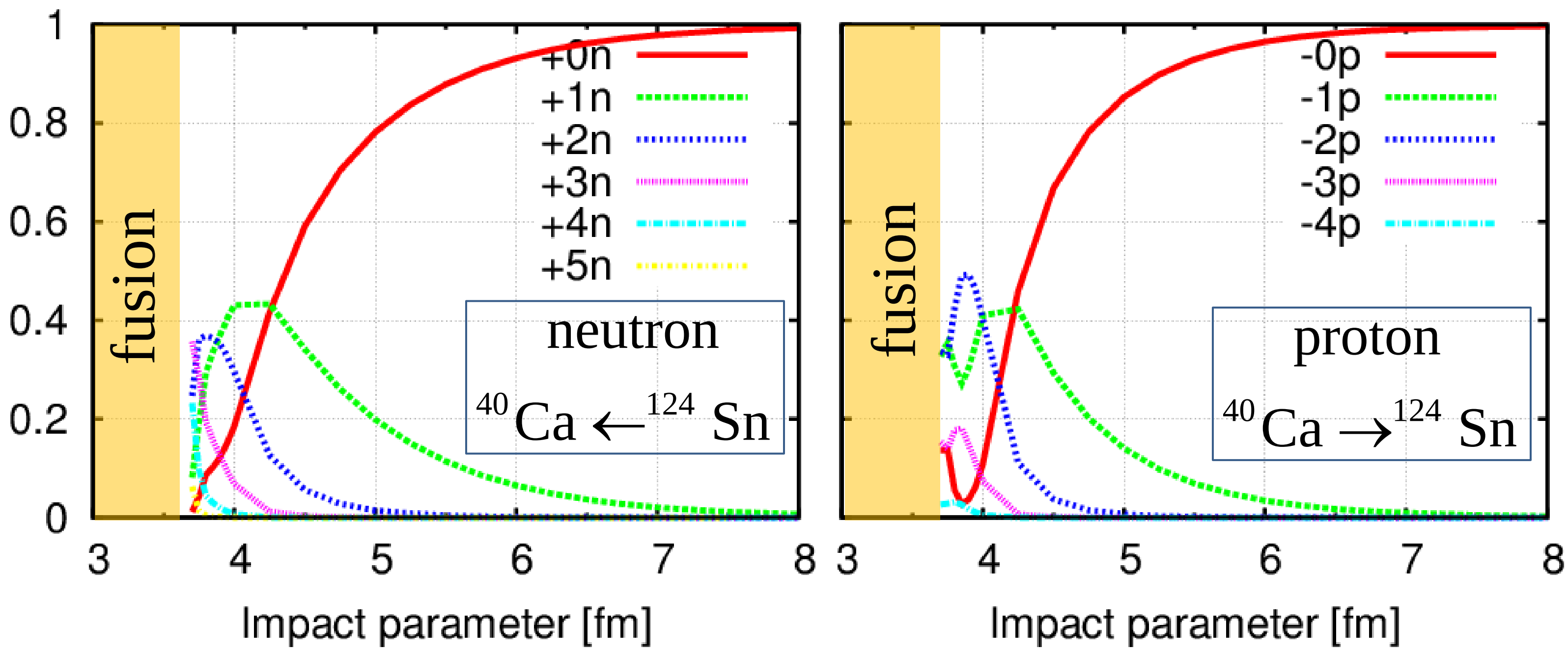
Fusion ($b \leq 3.69$ fm), Binary final state ($b \geq 3.70$fm)



$\langle \Delta N \rangle = 2.93, \langle \Delta Z \rangle = -1.55$ $\langle \Delta N \rangle = 0.45, \langle \Delta Z \rangle = -0.37$

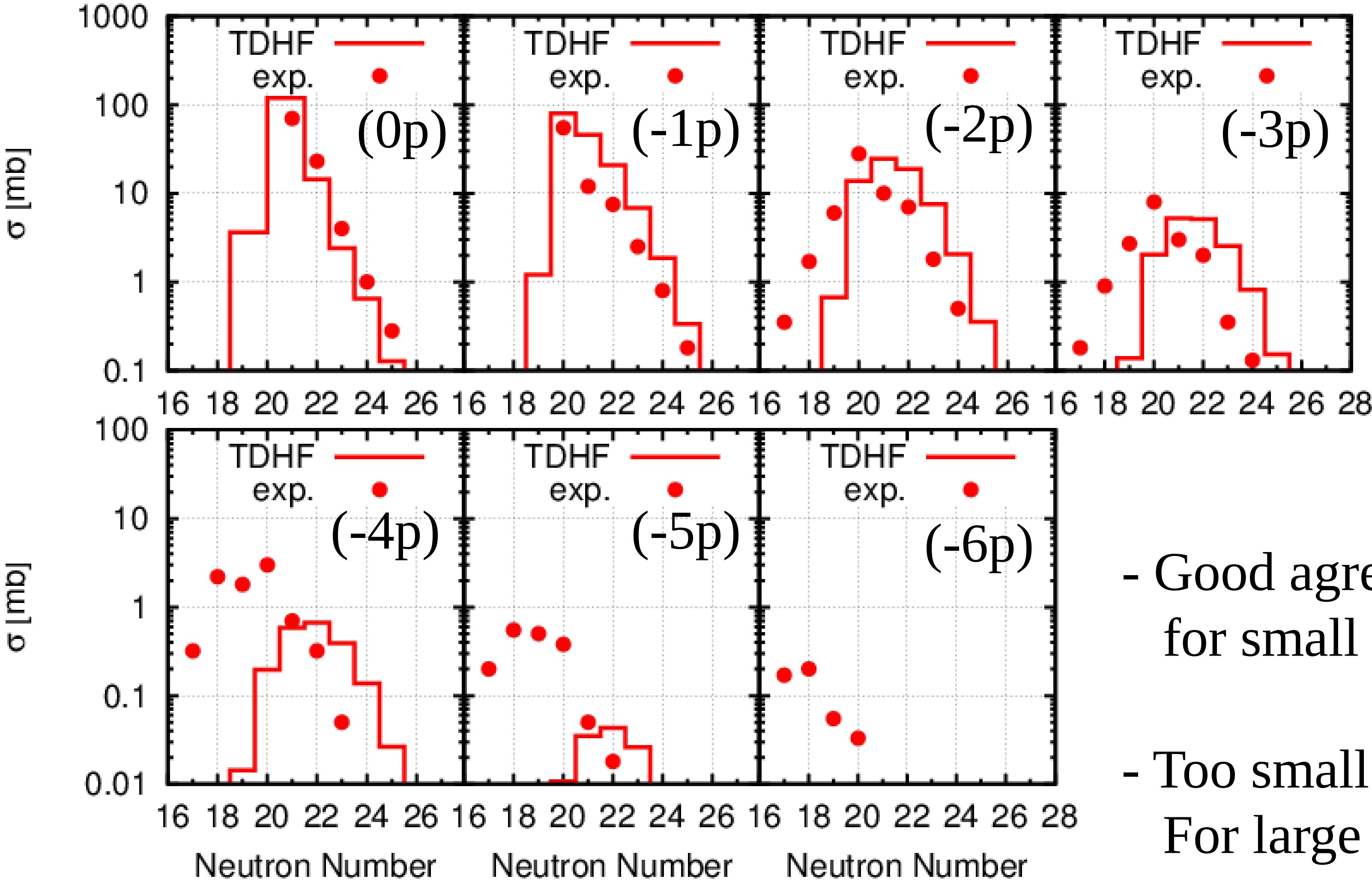
Multi-nucleon transfer probability : $^{40}Ca + ^{124}Sn$ (E_{lab}=170 MeV)

$$P_n = \left\langle \Psi_{\text{final}} \middle| \delta\left(n - \hat{N}_A\right) \middle| \Psi_{\text{final}} \right\rangle$$
$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{in\theta} \det\left\{ \left\langle \psi_i \middle| \psi_j \right\rangle_B + e^{-i\theta} \left\langle \psi_i \middle| \psi_j \right\rangle_A \right\}$$



Cross section, comparison with measurement: ^{40}Ca + ^{124}Sn (E_{lab}=170 MeV)

Experiment. L. Corradi et.al, Phys. Rev. C54, 201 (1996)



- Good agreement for small N_p

- Too small σ For large N_p

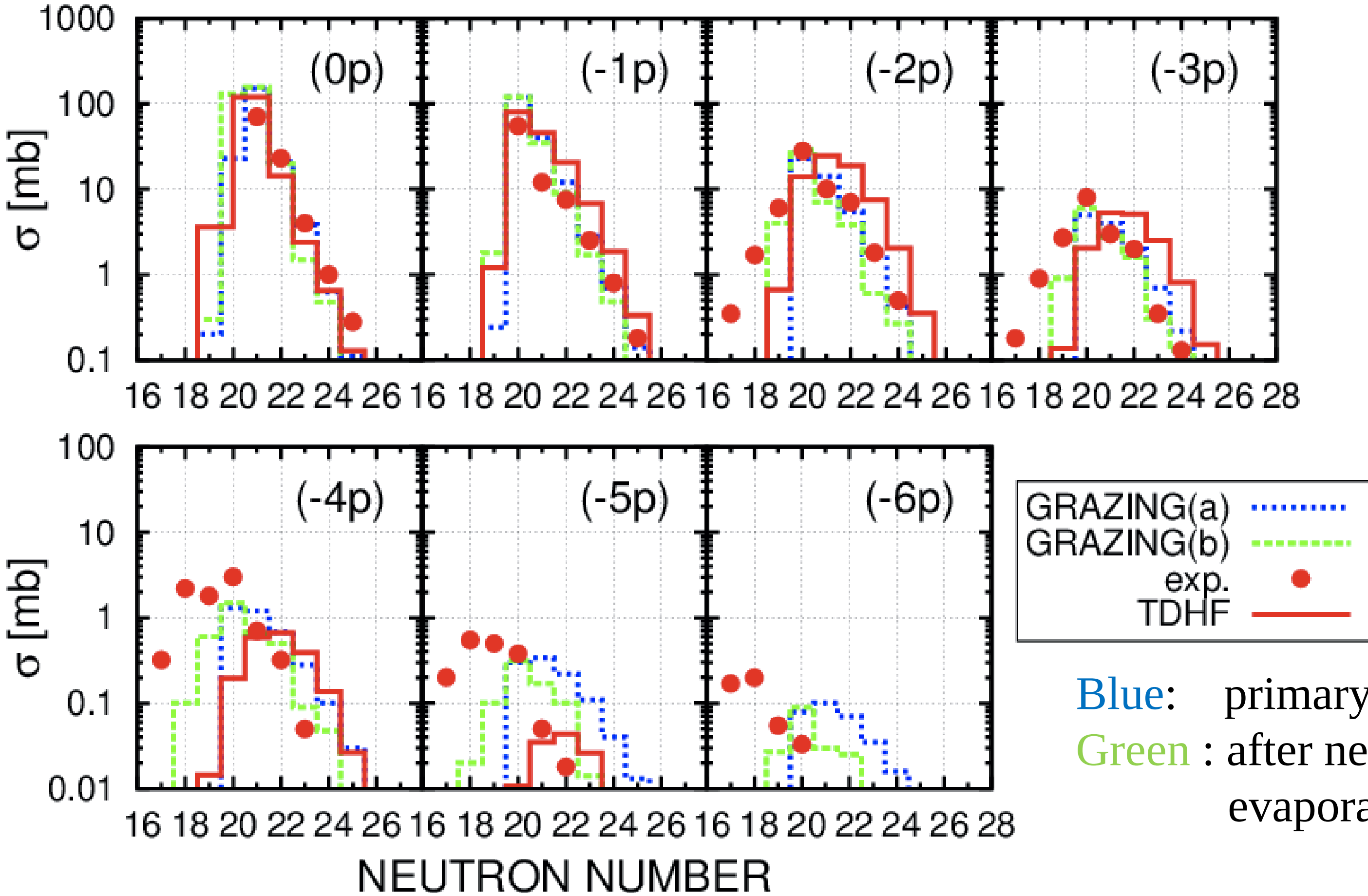
Comparison with other theory : GRAZING

$^{40}Ca + ^{124}Sn$ (E_{lab}=170 MeV)

A. Winther, Nucl. Phys. A572, 191 (1994)

Based on the framework of direct reaction theory
Nucleon transfer is treated, to some extent, statistically
(average transfer probability times density of states)

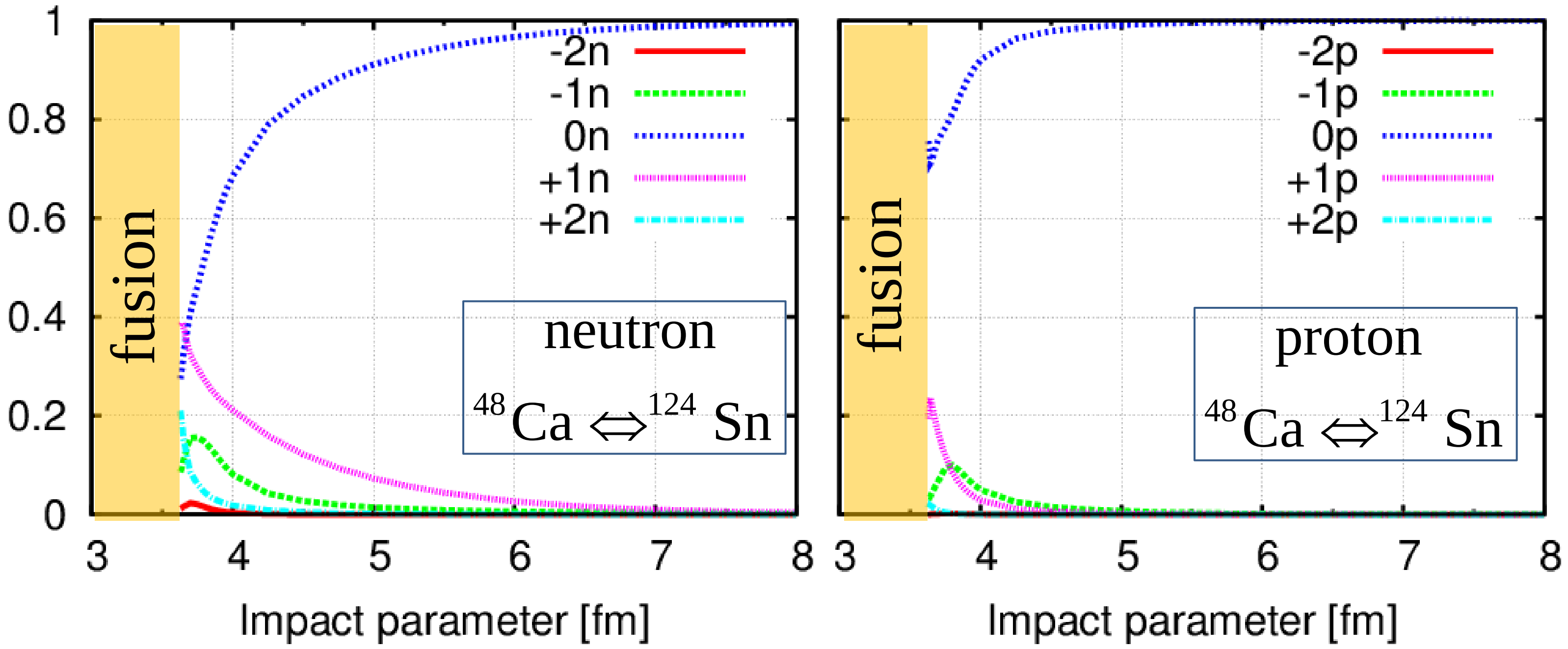
Experiment. L. Corradi et.al, Phys. Rev. C54, 201 (1996)



Blue: primary
Green : after neutron evaporation

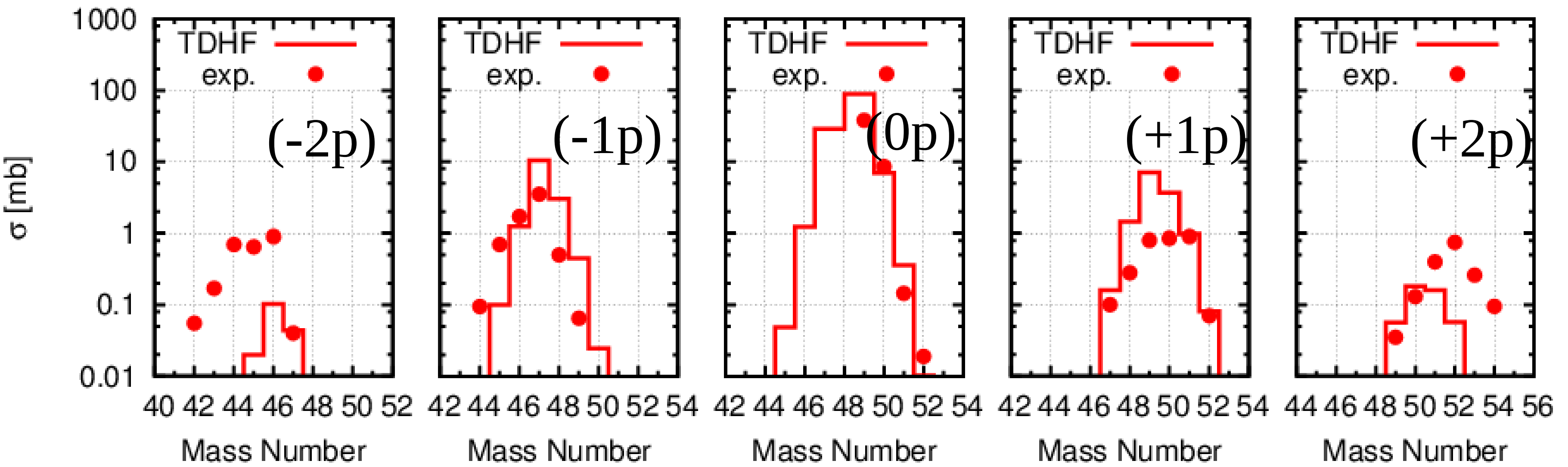
Another example: $^{48}Ca + ^{124}Sn$ (E_{lab}=174 MeV)

Almost the same N/Z ratio



Cross section, comparison with measurement: $^{48}Ca + ^{124}Sn$ (E_{lab}=174 MeV)

Experiment. L. Corradi et.al, Phys. Rev. C56, 938 (1997)



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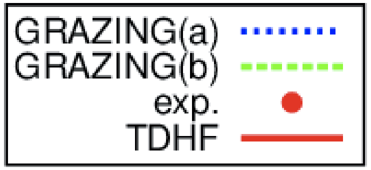

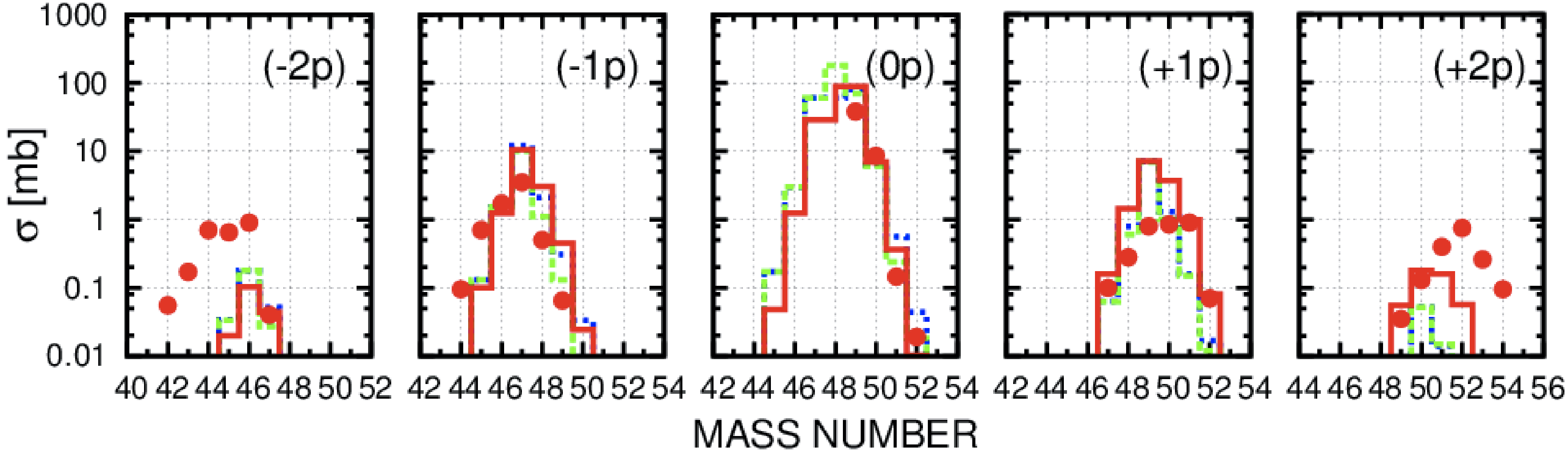

Experimentally, α-transfer ($\Delta N=\Delta Z=2$) dominates for +-2p channel.

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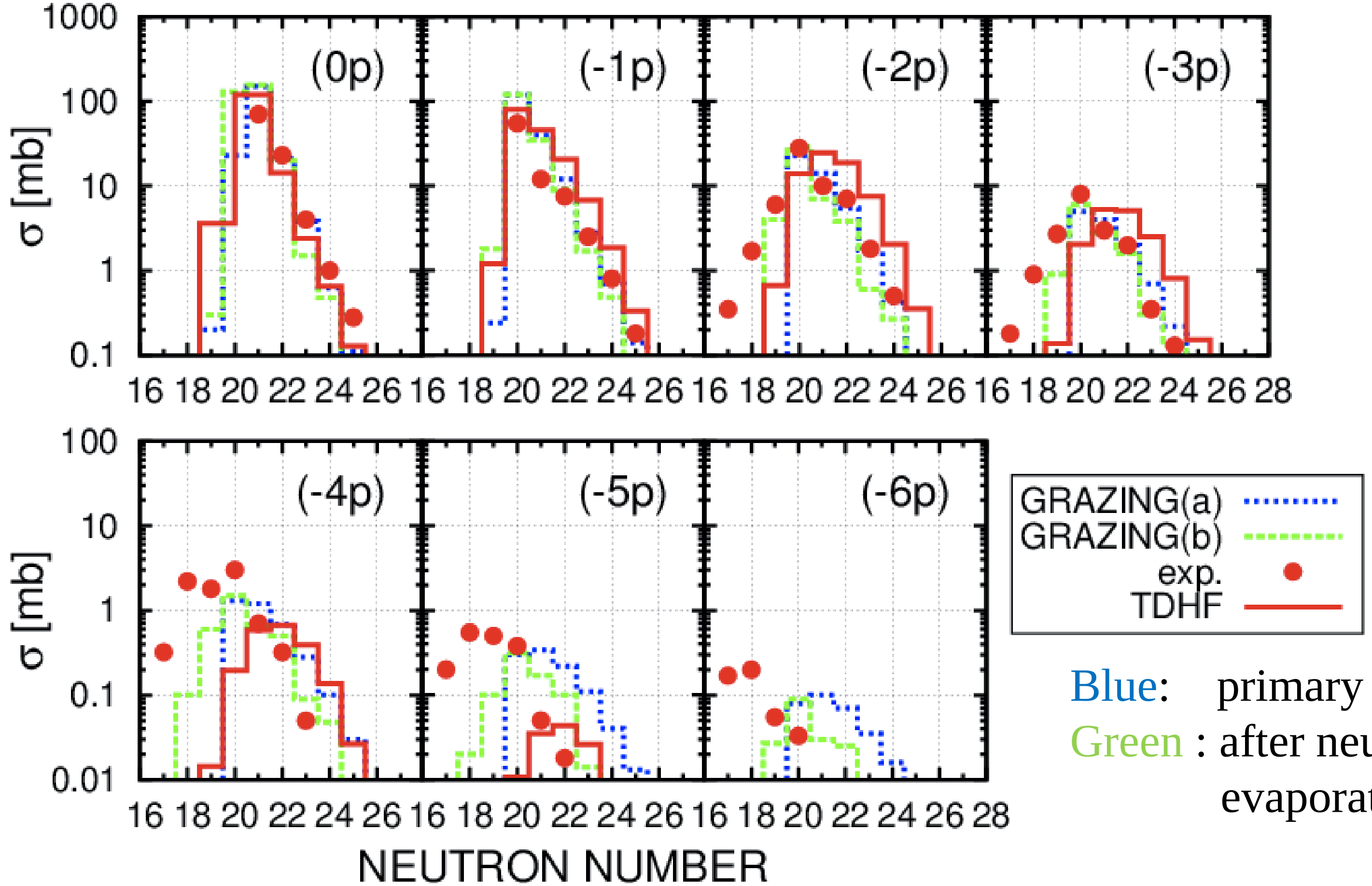

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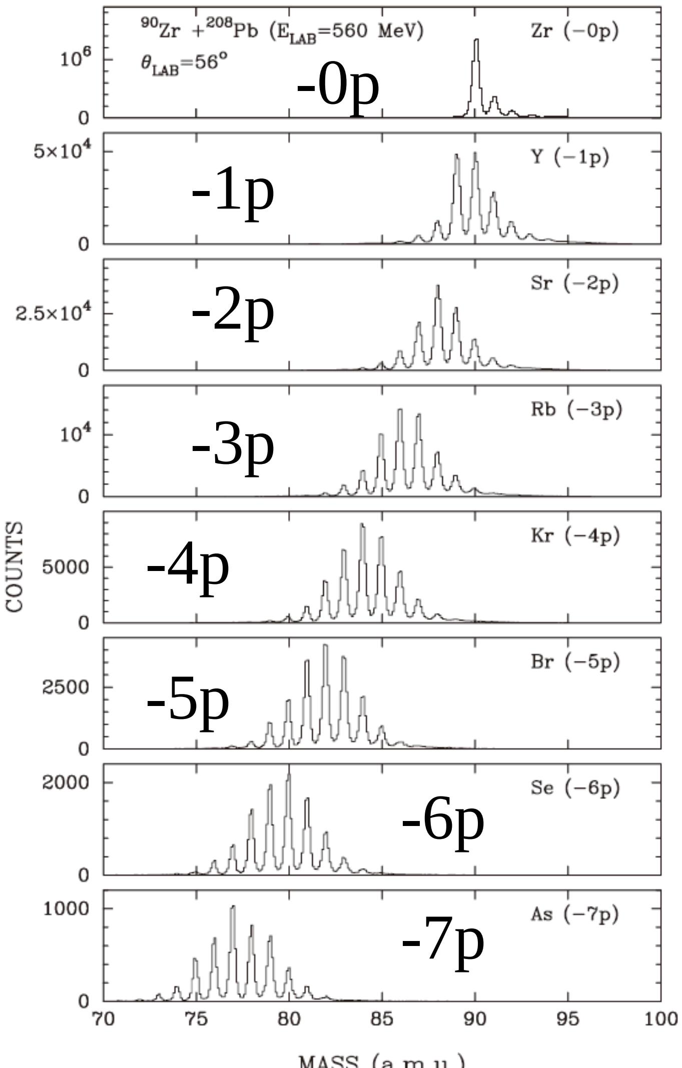
Absence of p-n correlation in TDHF calculation

$$\Psi\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A_P+A_T}\right)=\Psi^{proton}\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_Z\right)\Psi^{neutron}\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N\right)$$

$$P\left(N_n,N_p\right)=P_n(N_n)P_p(N_p)$$



$^{90}Zr + ^{208}Pb$

(E_{lab}=560MeV, θ_{lab}=56°)

S. Szilner et.al, Phys. Rev. C76, 024604 (2007)

- Experimentally, single collision (measurement with fixed scattering angle) shows correlation between removed proton and neutron numbers.

Is it possible to incorporate p-n correlation in one-body TDHF dynamics?

Summary

I discussed how to define and calculate transfer probability from TDHF calculation.

The framework by C. Simenel works well for heavy ion collision.

Application to ^{40,48}Ca + ^{124}Sn collision around Coulomb barrier

- Reasonable reproduction of cross section except for many-nucleon transfer cases
- Absense of p-n correlation behavior in the TDHF (and GRAZING)
  - neutron evaporation ?
  - genuine many-body correlation during dynamics?

Next and future:

- To clarify what determines transferred nucleon number from TDHF dynamics
- Investigate final nuclear states in more detail (excitation energy, angular momentum,…)
- Which reaction will be useful to produce neutron-rich nuclei?