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Time-Dependent Hartree-Fock Calculations for Multi-nucleon Transfer and Quasi-Fission Processes

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Time-dependent Hartree-Fock (TDHF) theory

describes Nuclear Dynamics without empirical parameters
other than Energy Functional that describes nuclear ground state.

TDHF equation

$$i\hbar \frac{\partial \phi_i(\boldsymbol{r}, \sigma, q, t)}{\partial t} = \hat{h}_{\text{Skyrme}}\left[\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu}\right] \phi_i(\boldsymbol{r}, \sigma, q, t)$$

$$\Phi(x_1, \cdots, x_N, t) = \frac{1}{\sqrt{N!}} \det\left\{\phi_i(x_j, t)\right\}$$

Applications for two distinct phenomena

- Nuclear Giant Resonance (linear response theory, RPA)
- Nucleus-nucleus collision at low energy (nonlinear dynamics, initial-value problem)

Realistic and systematic calculations become feasible thanks to developments of (super)computers,

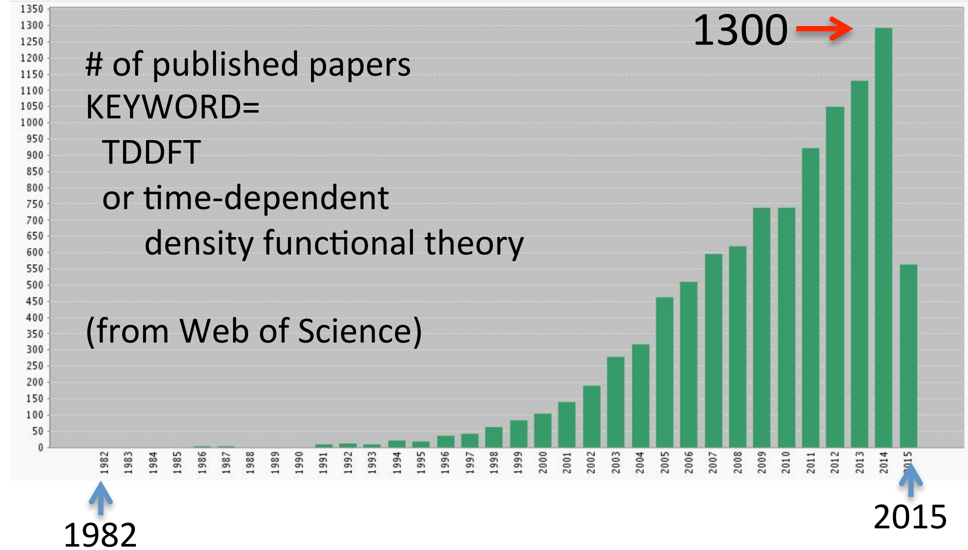
- use of complex and accurate Energy Functionals
- fully 3D calculations
- systematic calculations for various phenomena, fusion, transfer, quasi-fission, fission …

Common Theory in Other Fields

TDHF (Time-dependent Hartree-Fock)

TDDFT (Time-dependent Density Functional Theory)

developing as a universal theory for nonrelativisitc quantum dynamics of many-fermion systems



Long history in nuclear physics

One of the oldest simulation, $^{16}O - {}^{16}O$ fusion reaction:

H. Flocard, S.E. Koonin, M.S. Weiss, Phys. Rev.17(1978)1682.

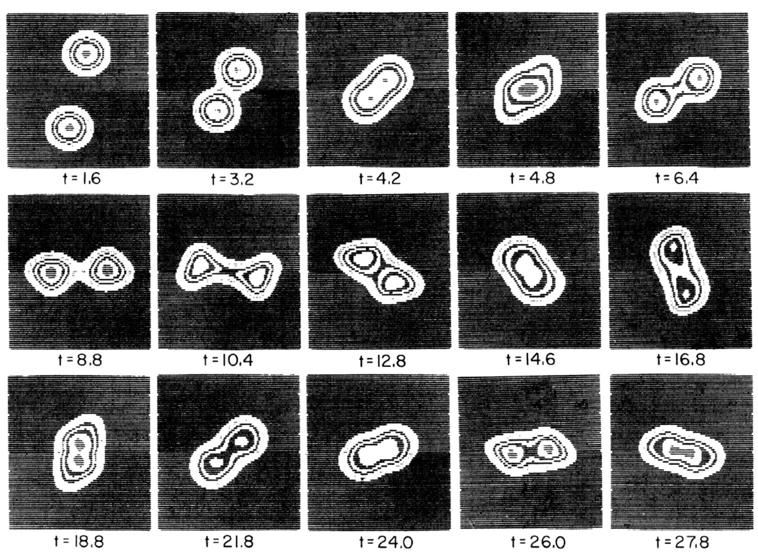
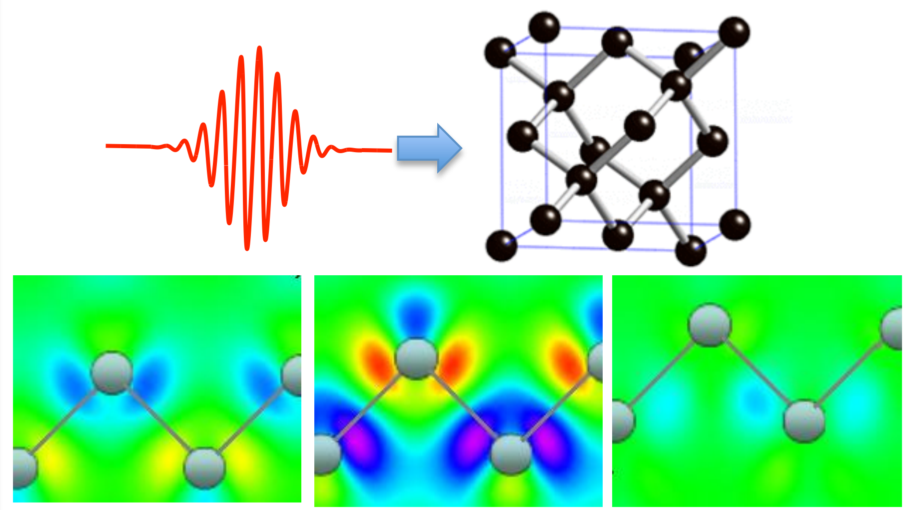


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + {}^{16}O$ collision at $E_{lab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

Applications in condensed matter physics, chemistry, and optical sciences (1990 -)



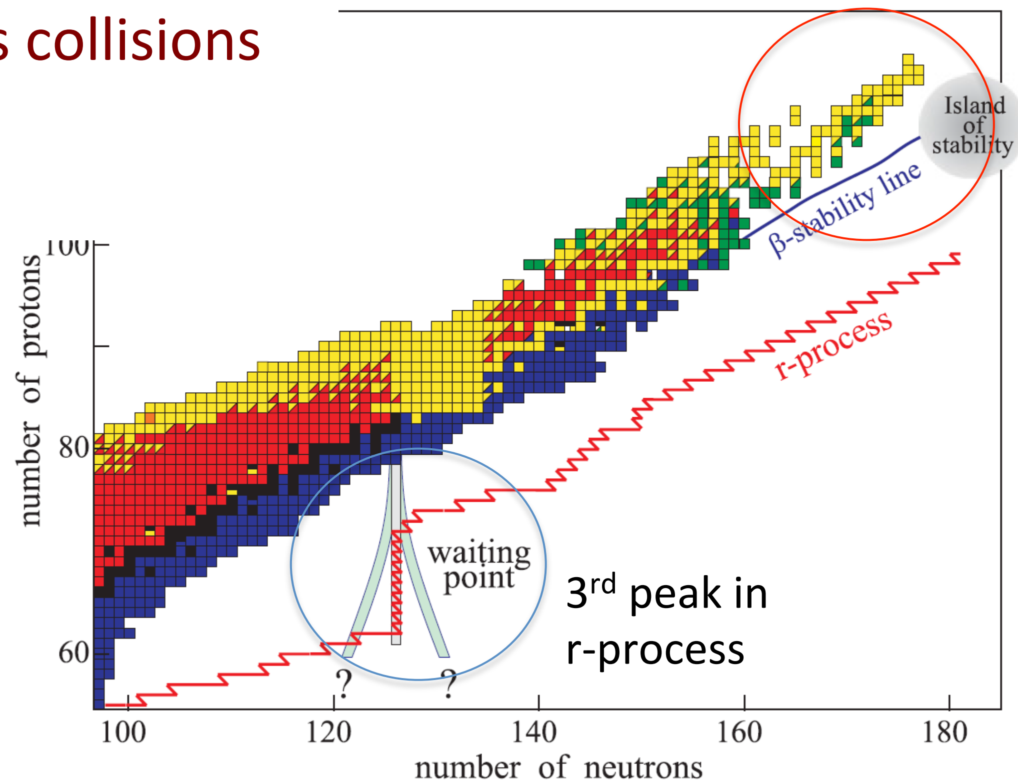
Electron dynamics in crystalline Silicon induced by laser pulse

I would like to talk on TDHF calculations for

Low-energy nucleus-nucleus collisions producing binary fragments

- (Multi-nucleon) transfer
- Quasi - fission

SHE production



Peripheral ⟷ Central

direct reaction, successive exchanges of nucleons

Neck formation and breaking

Fusion and quasi-fission for heavy nuclei

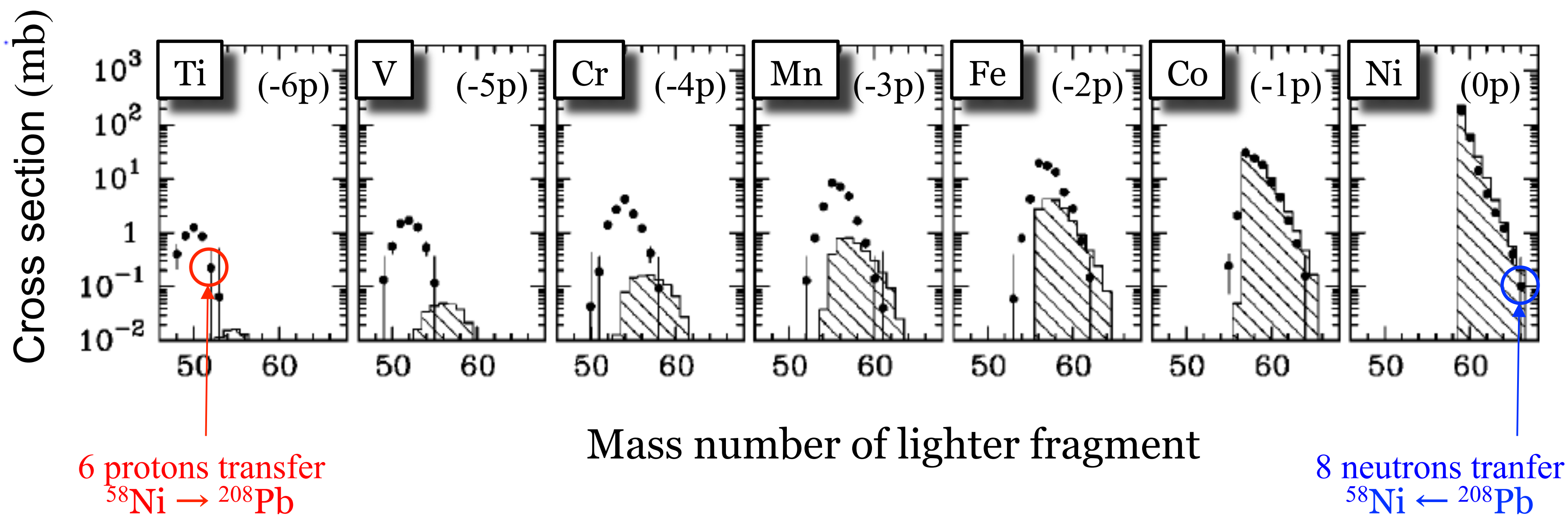
Multi-nucleon Transfer Reactions by TDHF

Consider the reaction,

$$^{58}_{28}\mathrm{Ni}_{30} + ^{208}_{82}\mathrm{Pb}_{126} \quad \text{at } E_{lab}=328.4 \text{ MeV}$$

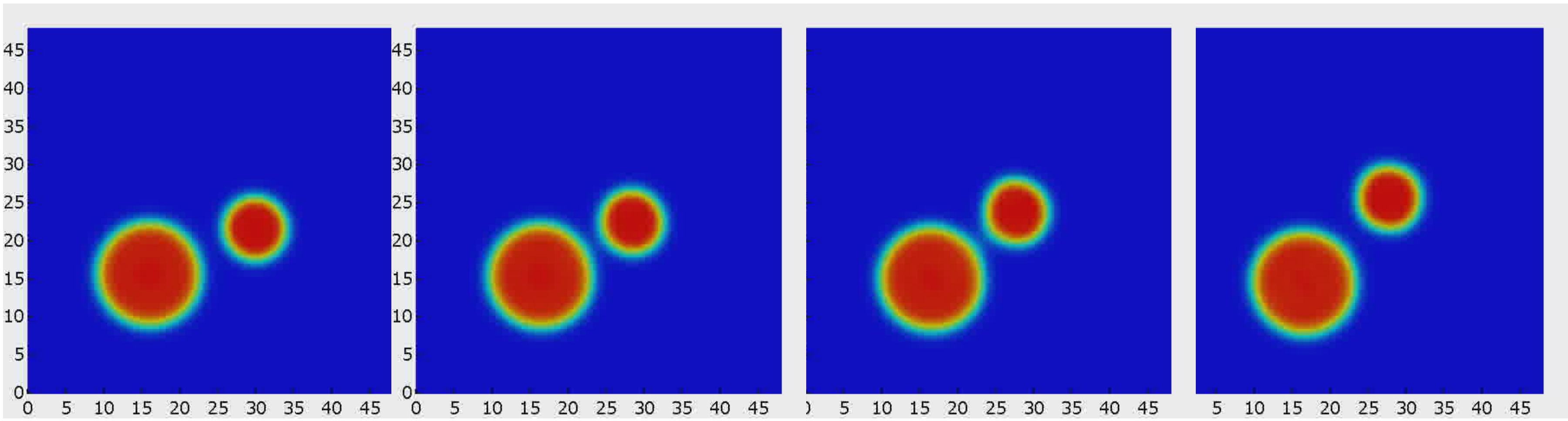
L. Corradi et al., Phys. Rev. C **66**, 024606 (2002)

Measurements vs Theory (Complex WKB model, single−nucleon transfer)

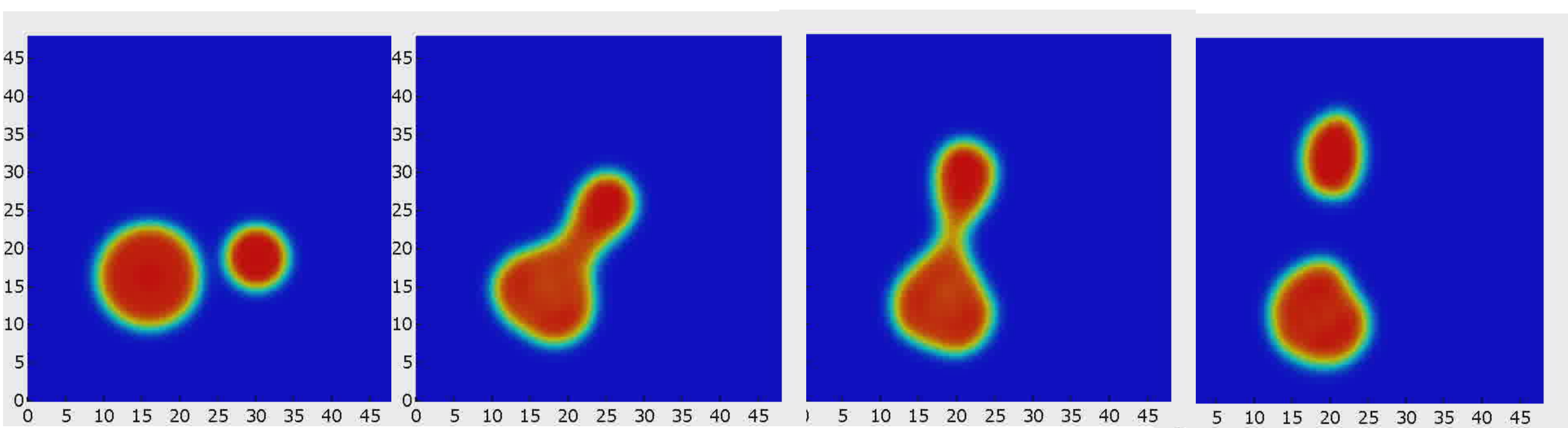


TDHF calculations for $^{58}Ni + ^{208}Pb$ at E_{lab}=328.4 MeV

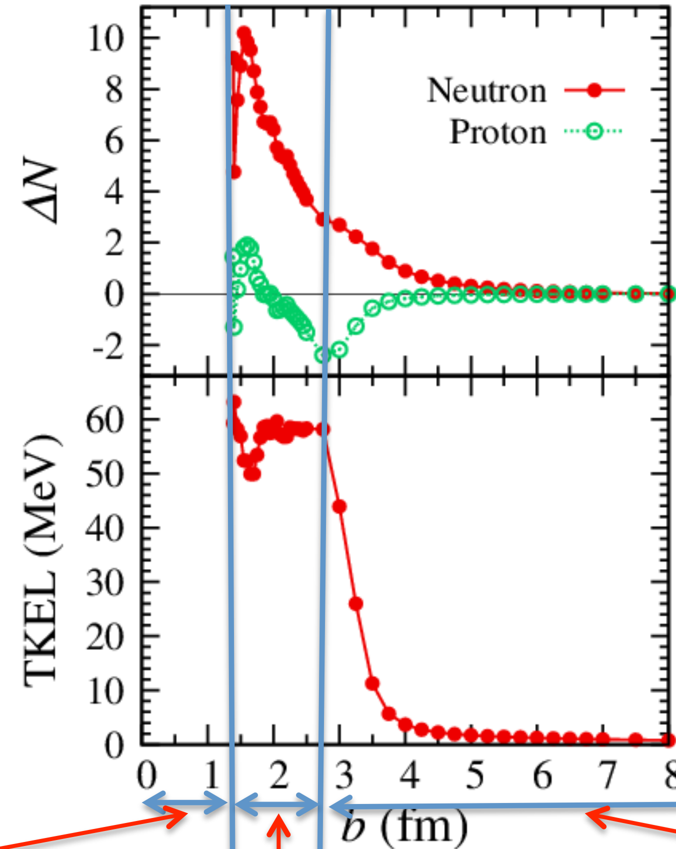
Large impact parameter (b=4.0 fm)
Transfer by (successive) single-nucleon exchanges



Small impact parameter (b=1.6fm)
Transfer by neck formation and breaking



^{58}Ni + ^{208}Pb
at E_{lab}=328.4 MeV



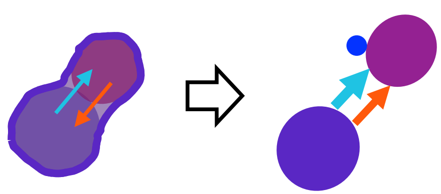
Average number of transferred nucleons (from Pb to Ni)

Total kinetic energy loss

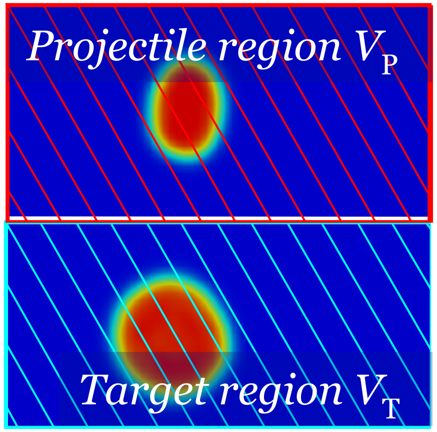
Fusion

Neck formation and breaking
Mass equilibrium
protons: Pb → Ni
neutrons: Pb → Ni

Successive nucleon exchange
Charge equilibrium
protons: Ni → Pb
neutrons: Pb → Ni



Calculate cross section from TDHF calculation, We need to know transfer probabilities, $P_n(b)$



Wave function in projectile (target) region is not an eigenstate of particle number

$$\left(\hat{N}_P + \hat{N}_T\right)\Phi(t) = \left(A_P + A_T\right)\Phi(t)$$

$$\hat{N}_P\Phi(t) \neq n\Phi(t)$$

Efficient projection method to calculate probabilities

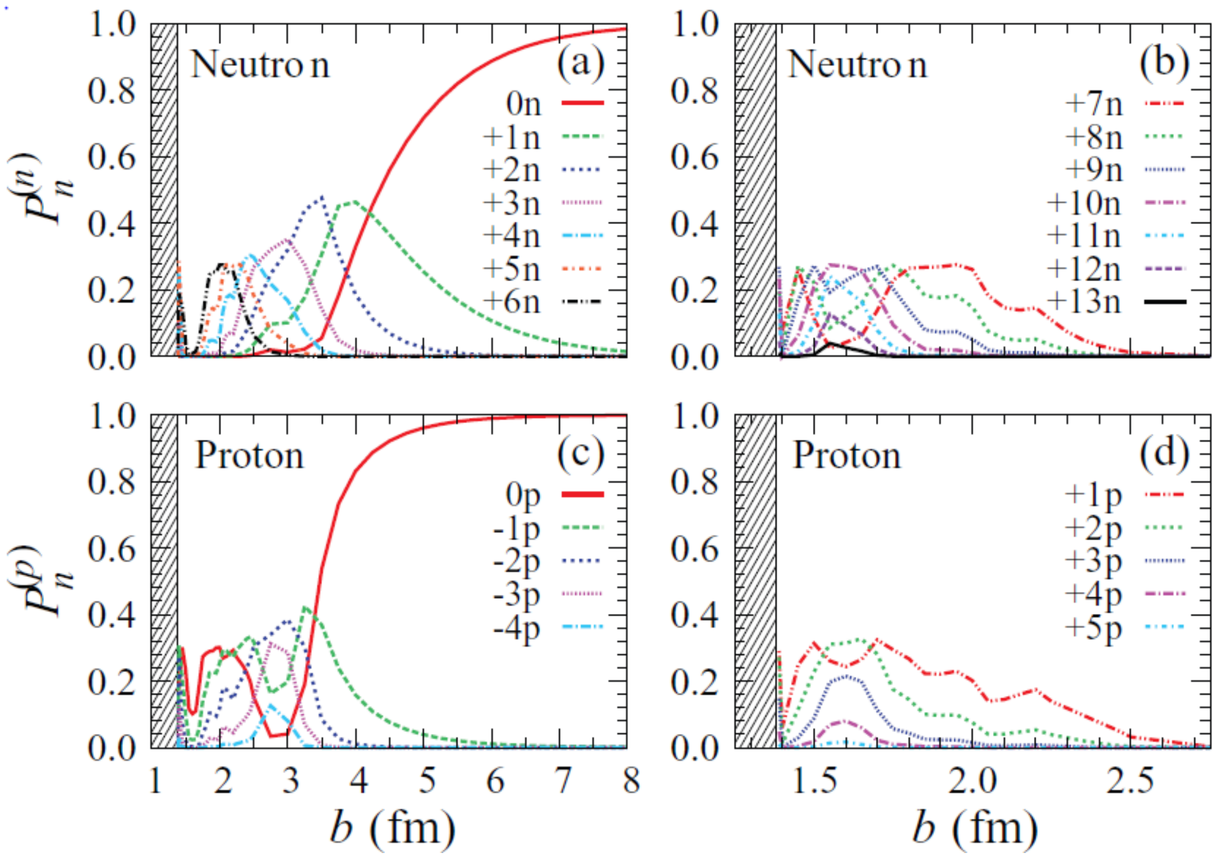
C. Simenel, Phys. Rev. Lett. **105**, 192701 (2010)

$$P_n(b) = \left\langle \Phi(t) \middle| \delta\left(\hat{N}_P - n\right) \middle| \Phi(t) \right\rangle$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{in\theta} \det\left\{ \left\langle \phi_i(t) \middle| \phi_j(t) \right\rangle_{V_T} + e^{-i\theta} \left\langle \phi_i(t) \middle| \phi_j(t) \right\rangle_{V_P} \right\}$$

^{58}Ni + ^{208}Pb at E_{lab}=328.4 MeV

Transfer probabilities $P_n(b)$
from TDHF wave function after collision



Neutron transfer always
Towards Pb → Ni

Proton transfer
In both directions

+ sign for Pb → Ni

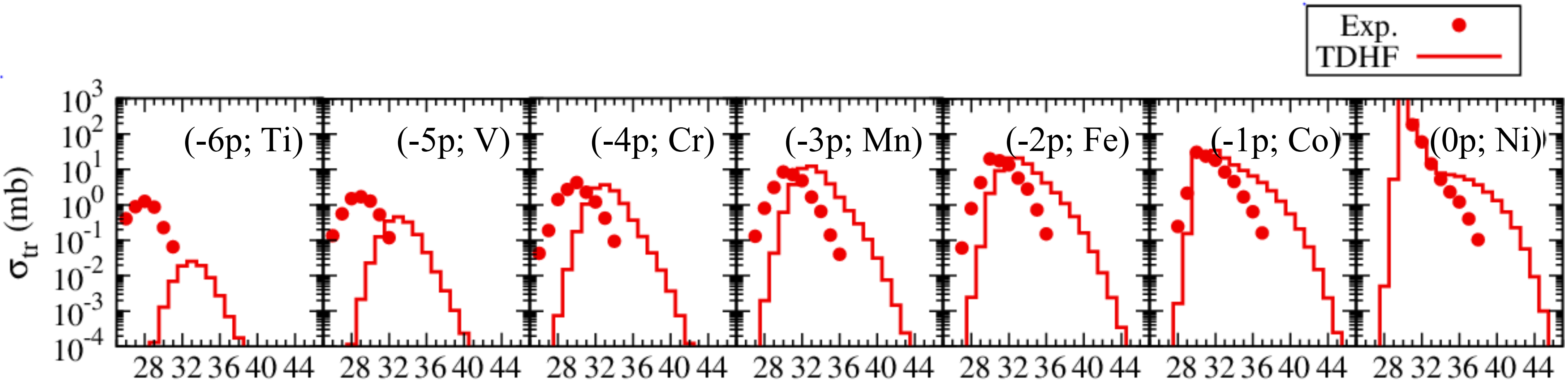
^{58}Ni + ^{208}Pb at E_{lab}=328.4 MeV

Cross section by TDHF

$$\sigma_{\rm tr}(Z,N) = 2\pi \int_{b_{\rm min}}^{\infty} b\, P_Z^{(p)}(b) P_N^{(n)}(b)\, db$$

$$P_Z^{(\rm p)} = \left\langle \Phi(t) \middle| \delta\left(\hat{N}_P - Z\right) \middle| \Phi(t) \right\rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{iZ\theta} \det\left\{ \left\langle \phi_i(t) \middle| \phi_j(t) \right\rangle_{V_T} + e^{-i\theta} \left\langle \phi_i(t) \middle| \phi_j(t) \right\rangle_{V_P} \right\}$$



Mass number of lighter fragment

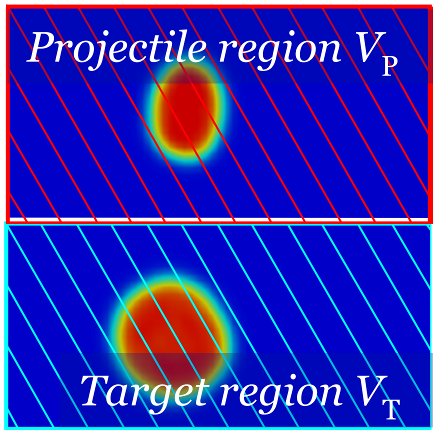
TDHF: K. Sekizawa and K. Yabana, Phys. Rev. C **88**, 014614 (2013)

Experiment: L. Corradi et al., Phys. Rev. C **66**, 024606 (2002)

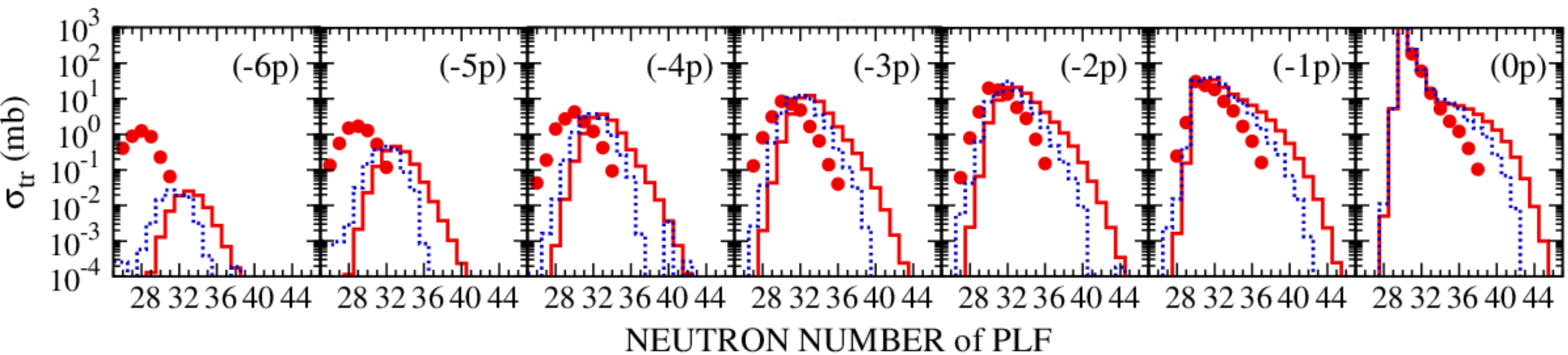
Estimation of slow neutron evaporation by statistical model

Calculate internal excitation energy of fragment
(Energy expectation value for number projected wave function)

K. Sekizawa, K. Yabana, Phys. Rev. C90, 064614 (2014)



$$E_n \equiv \frac{\langle \Phi | \hat{H}\, \hat{P}_n | \Phi \rangle}{\langle \Phi | \hat{P}_n | \Phi \rangle}$$
$$= \frac{1}{2\pi P_n} \int_0^{2\pi} d\theta\, e^{in\theta} \det B(\theta) \int_{V_P} d^3r\, \tilde{\mathcal{H}}(\boldsymbol{r}, \theta) + \frac{1}{2\pi P_n} \int_0^{2\pi} d\theta\, e^{in\theta} \det B(\theta) \int_{V_T} d^3r\, \tilde{\mathcal{H}}(\boldsymbol{r}, \theta)$$



After (blue) and before (red) evaporation effect

Summary of TDHF calculation for multi-nucleon transfer reaction

- Using projection operator method, we calculate and compare cross sections.

- TDHF reasonably describes transfer cross section for a few nucleon transfer but underestimate cross sections of large transferred nucleons.

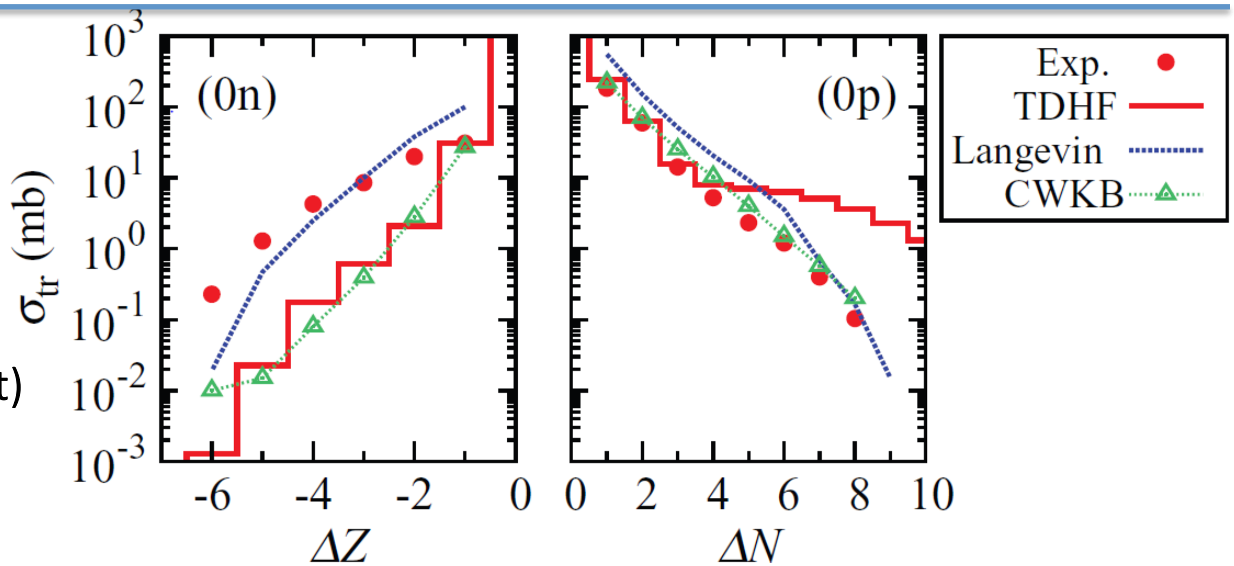
- Success and failure looks similar to other empirical calculations of GRAZING, CWKB.

- We should keep in mind that TDHF is known to underestimate variance (limitation for correlations).

$$\left\langle \hat{N} \right\rangle_{E,b} = \sum_n n P_n(b) \qquad \sigma^2_{E,b} = \left\langle \left(\hat{N} - \left\langle \hat{N} \right\rangle_{E,b} \right)^2 \right\rangle_{E,b} = \sum_n \left(n - \left\langle \hat{N} \right\rangle_{E,b} \right)^2 P_n(b)$$

$^{58}Ni + ^{208}Pb$
at E_{lab}=328.4 MeV

Comparisons among theories
(before evaporation treatment)



TDHF for quasi-fission processes

Fission before reaching equilibrium in collisions of heavy nuclei
where fusion hindrance is expected $Z_P Z_T > 1600$.

- Influence of shell effect (magic number)
- Sensitive to orientation of deformed nuclei
- Attracting interests to produce SHE and other unstable nuclei

Recently, successful descriptions by TDHF and collaborations with experiments have been reported,

A. Wakhle et.al, PRL113, 182502 (2014)
"Interplay between Quantum Shells and Orientation in Quasifission"

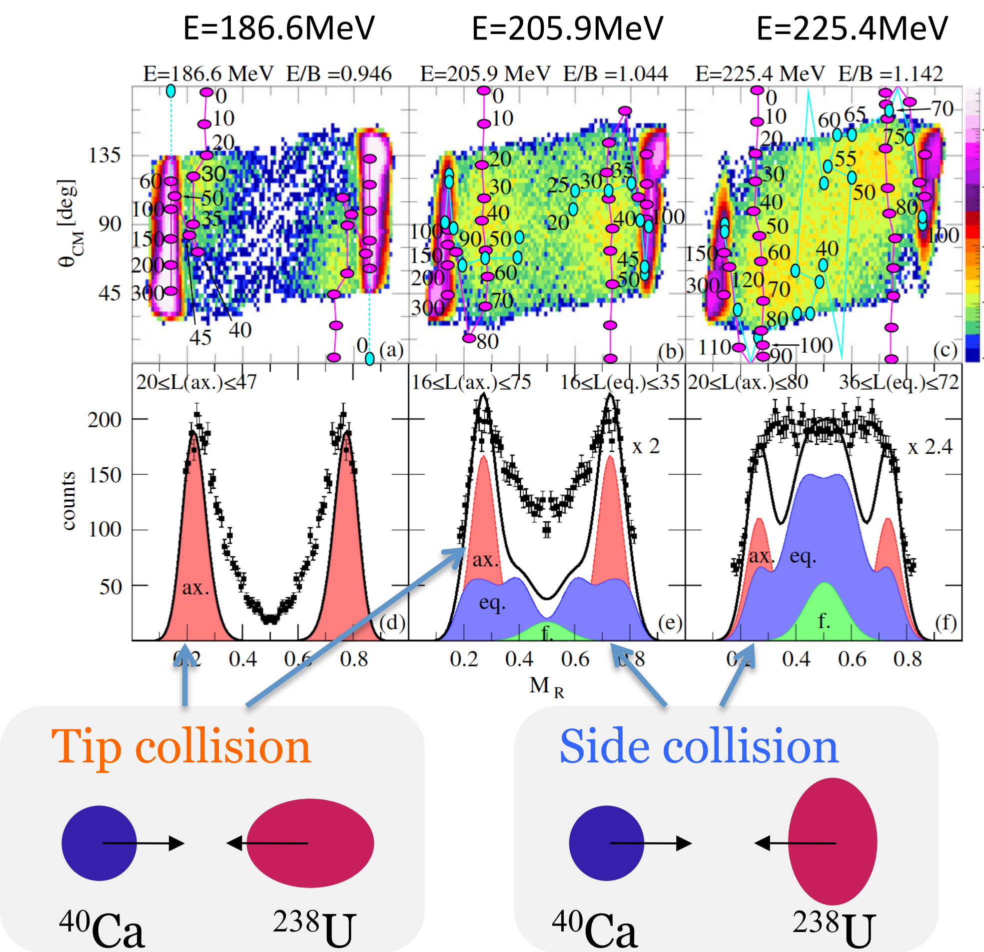
V.E. Oberacker et.al, PRC90, 054605(2014)
"Dissipative dynamics in quasifission"

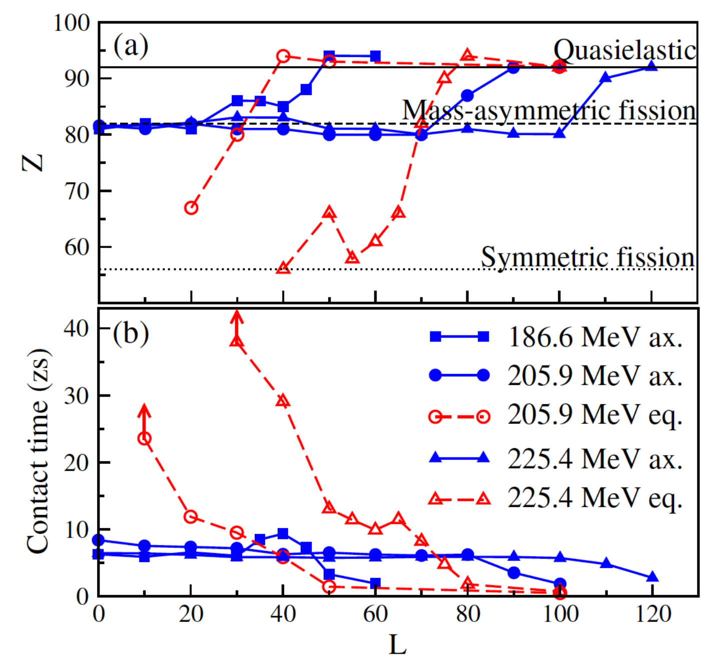
K. Hammerton et.al, PRC91, 041602 (2015)
"Reduced quasifission competition in fusion reactions forming neutron rich heavy elements"

PRL 113, 182502 (2014) PHYSICAL REVIEW LETTERS week ending 31 OCTOBER 2014

Interplay between Quantum Shells and Orientation in Quasifission

A. Wakhle, C. Simenel,* D. J. Hinde, M. Dasgupta, M. Evers, D. H. Luong, R. du Rietz, and E. Williams
Department of Nuclear Physics, Research School of Physics and Engineering, Australian National University, Canberra, Australian Capital Territory 2601, Australia



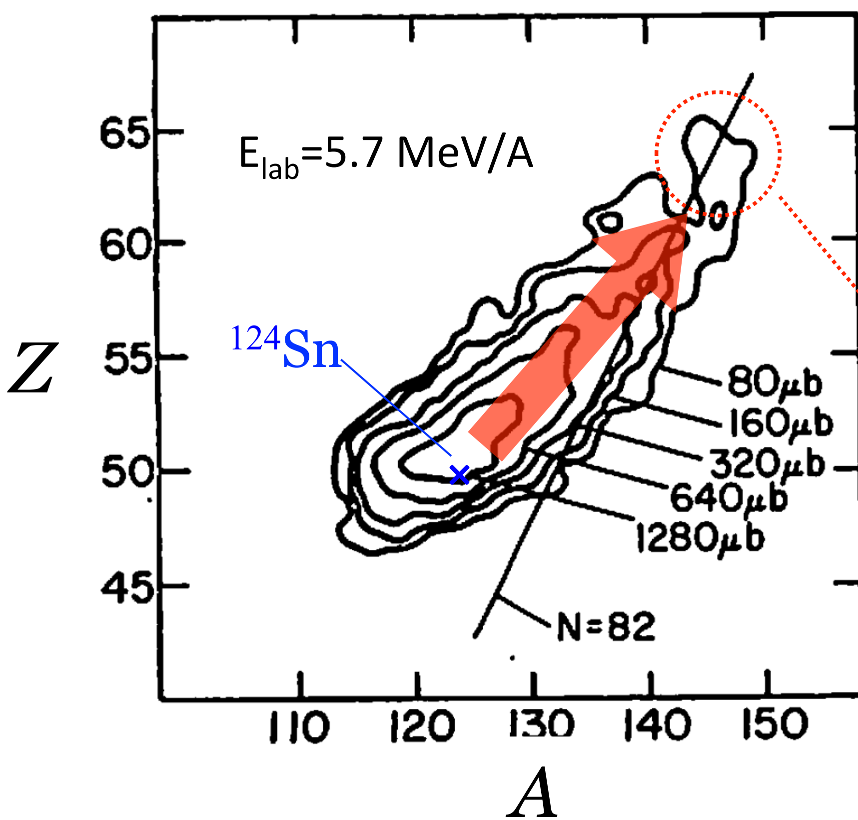


Fast fission in tip collision and producing Z=82 (magic) nuclei

We report our TDHF calculation for $^{238}U + ^{124}Sn$

- Effect of deformation and nuclear orientation on quasi-fission process
  Tip collision vs Side collision

- Energy dependence
  Inverse quasi-fission appears at higher incident energy



Early experiment reported

$^{238}U \rightarrow ^{124}Sn$

Neutron ~ 10 transferred

Proton ~ 15 transferred

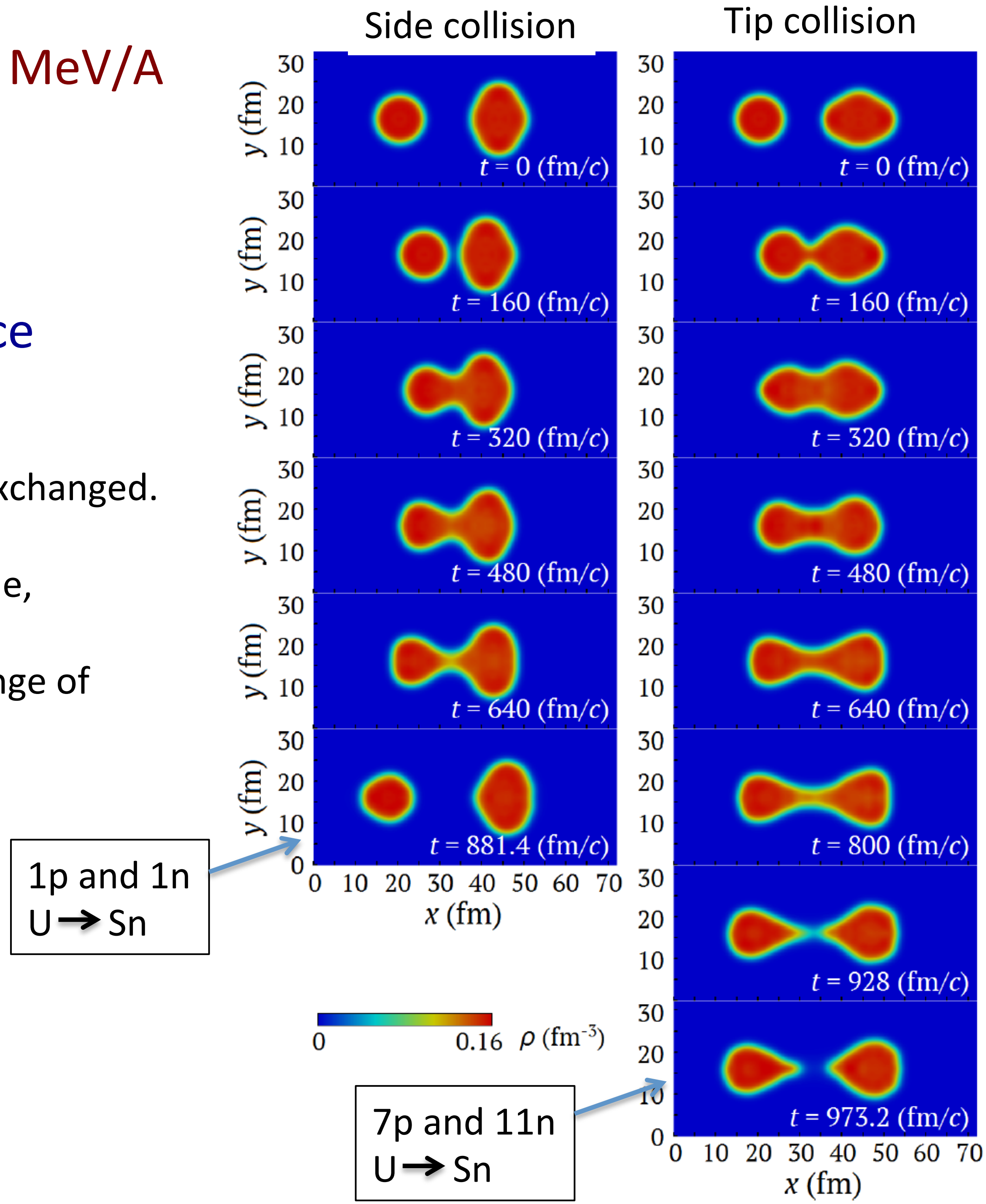
W. Mayer et al.,
Phys. Lett. **152B**, 162 (1985)

$^{238}U + ^{124}Sn$ at E_{lab}=5.7 MeV/A

Orientation dependence

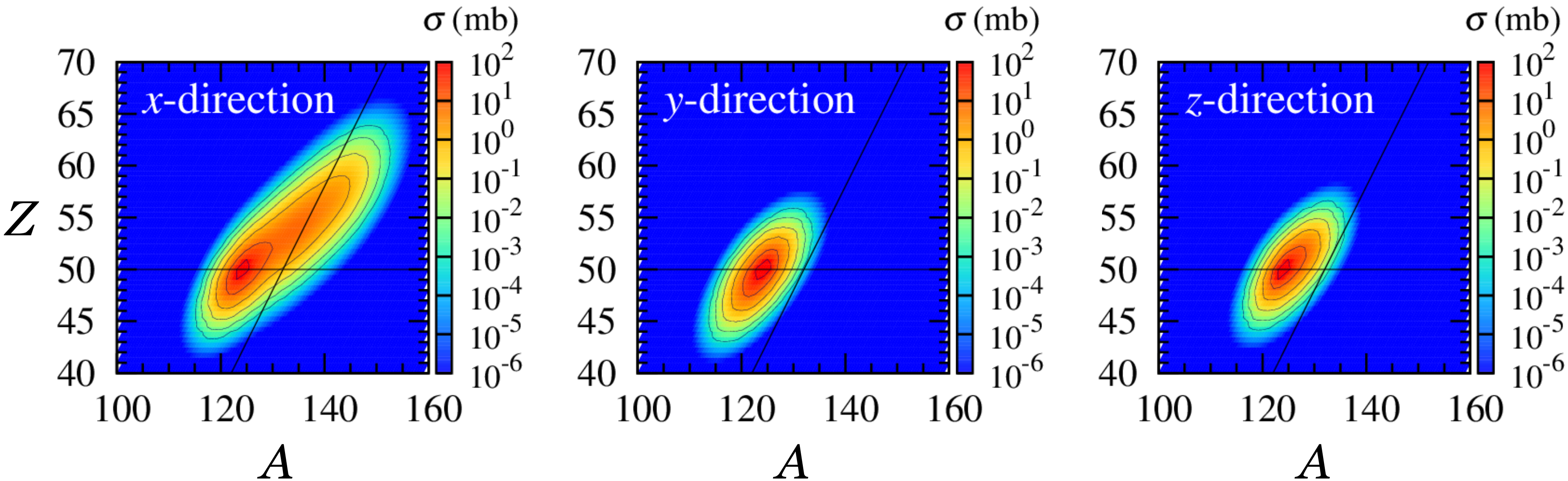
Side collision proceeds fast,
small number of nucleons exchanged.

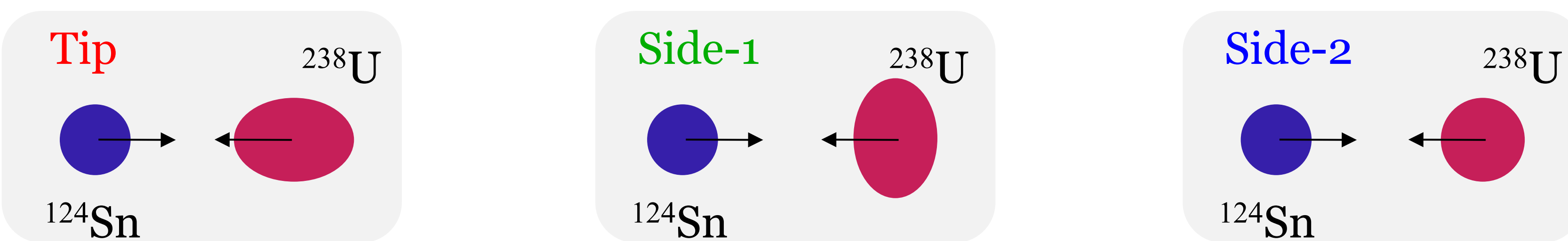
Tip collision takes longer time,
long neck is developed and
neck breaking causes exchange of
many nucleons.



Cross section by TDHF: ^{238}U + ^{124}Sn at E_{lab}=5.7 MeV/A

Production cross sections for lighter (^{124}Sn-like) fragments before evaporation





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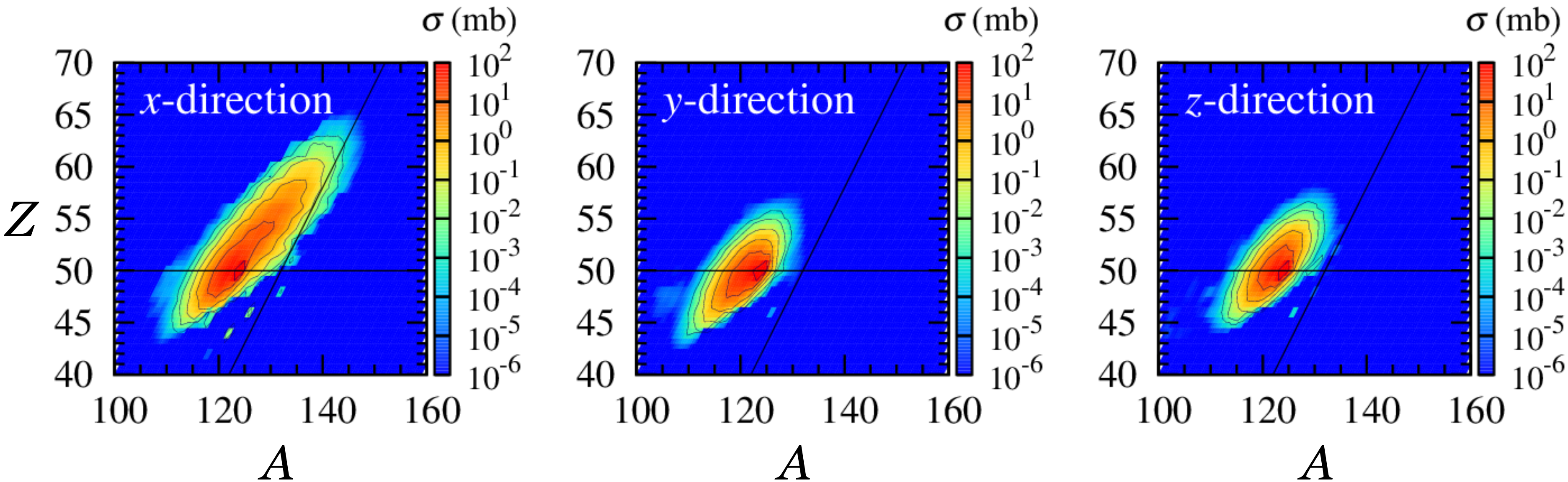

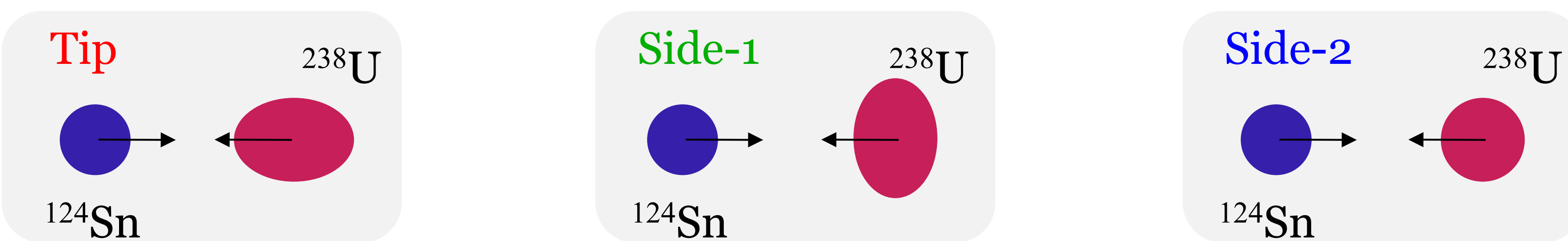

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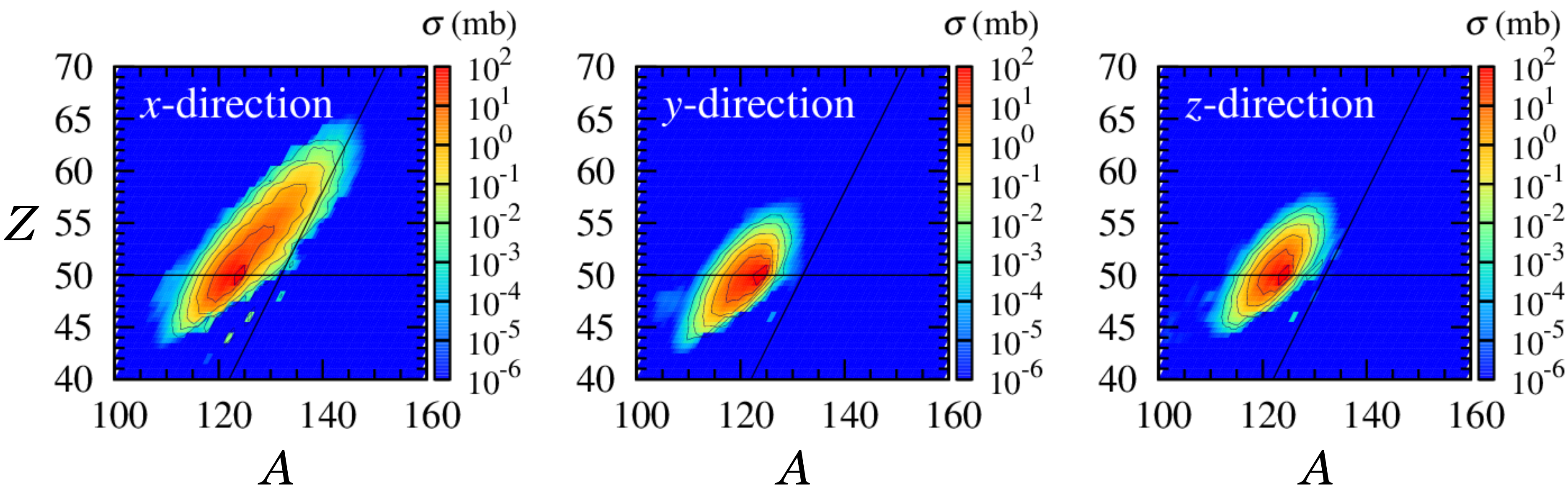
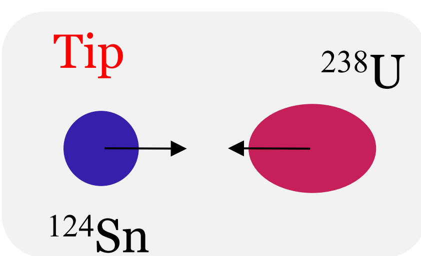
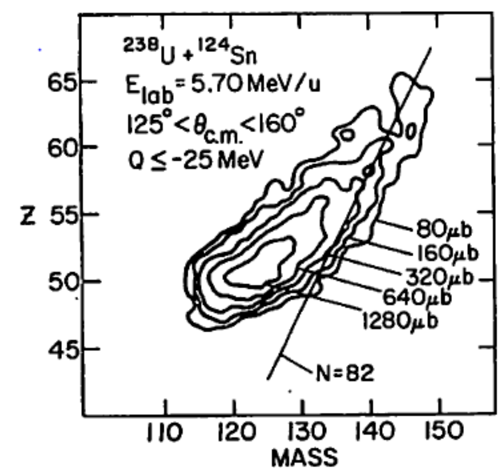




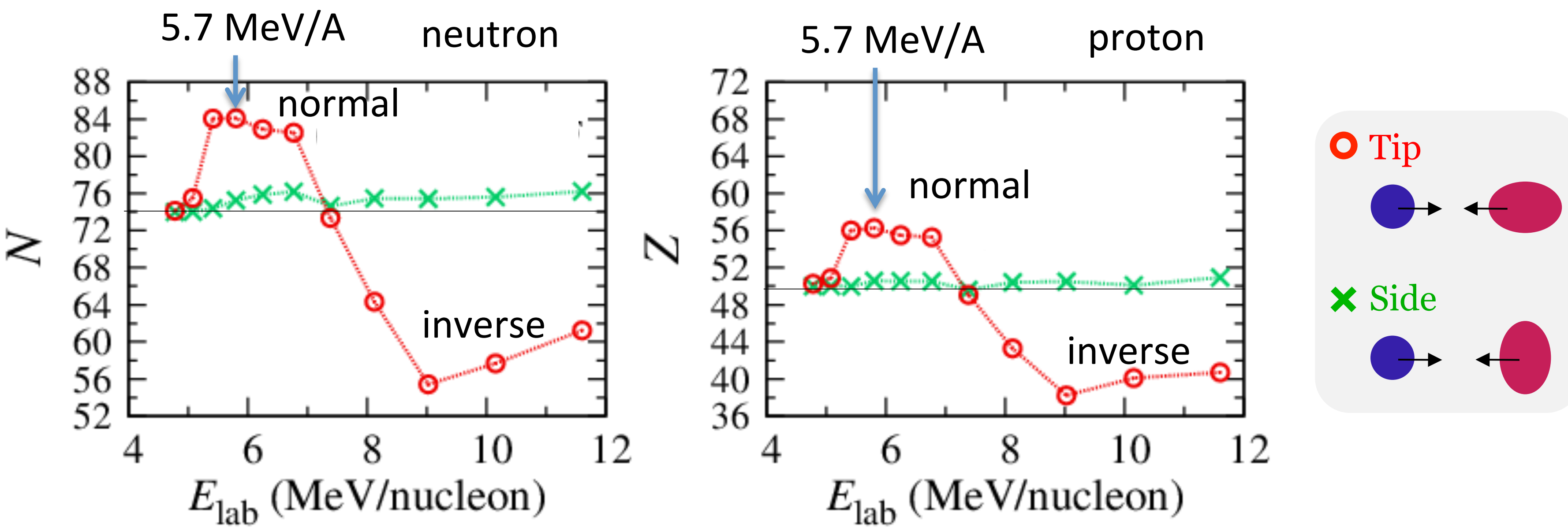
Measured flow of many protons can be explained by the neck formation and breaking in the tip collision.



Quasi-fission dynamics:

Systematic view changing energy and impact parameter

Average number of transferred nucleons, $^{238}U + ^{124}Sn$ (b=0)



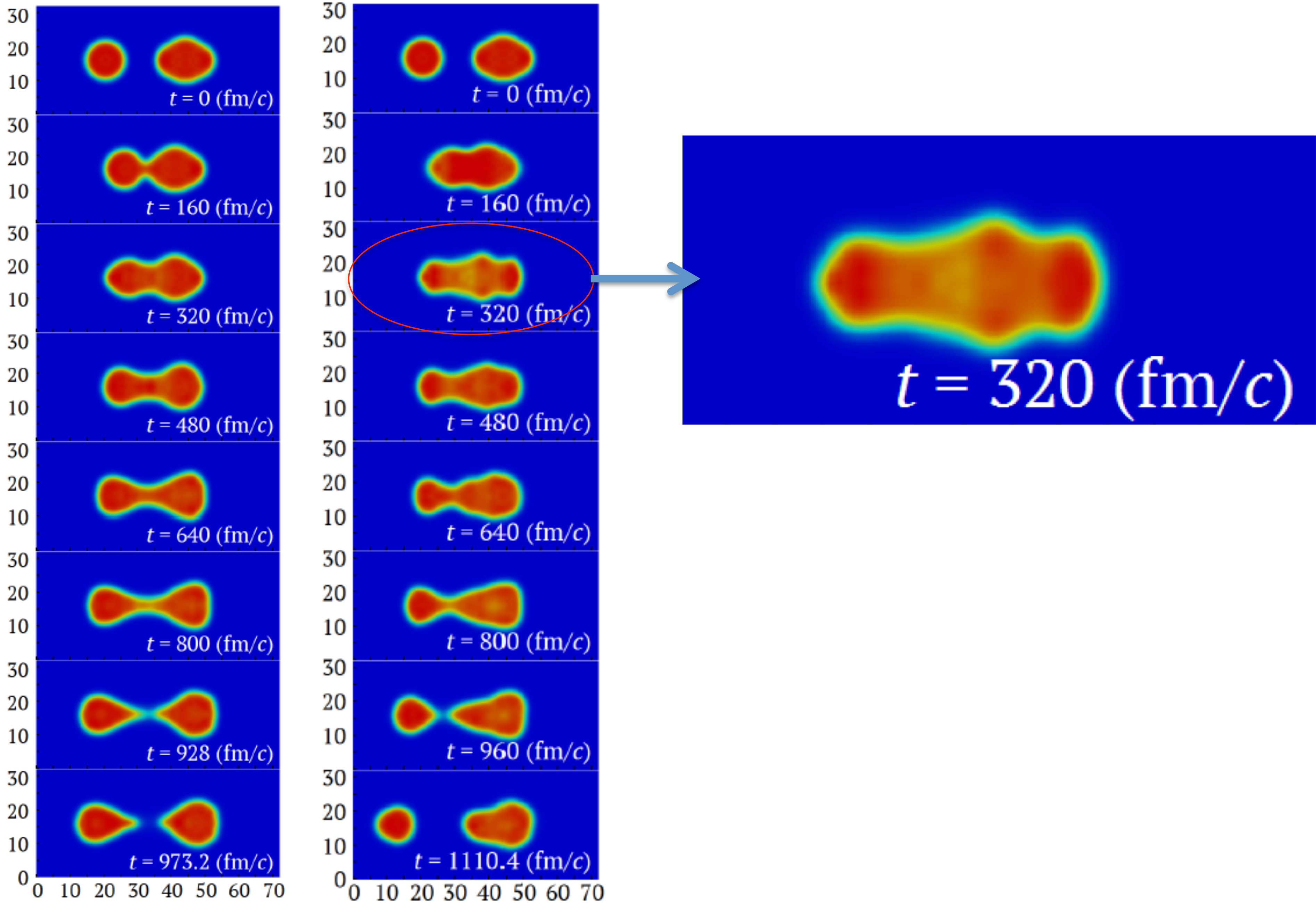
- In tip collisions above 7 MeV/A, both protons and neutrons transfer Sn → U (inverse quasi-fission)

- In side collisions, always small number of transferred nucleons

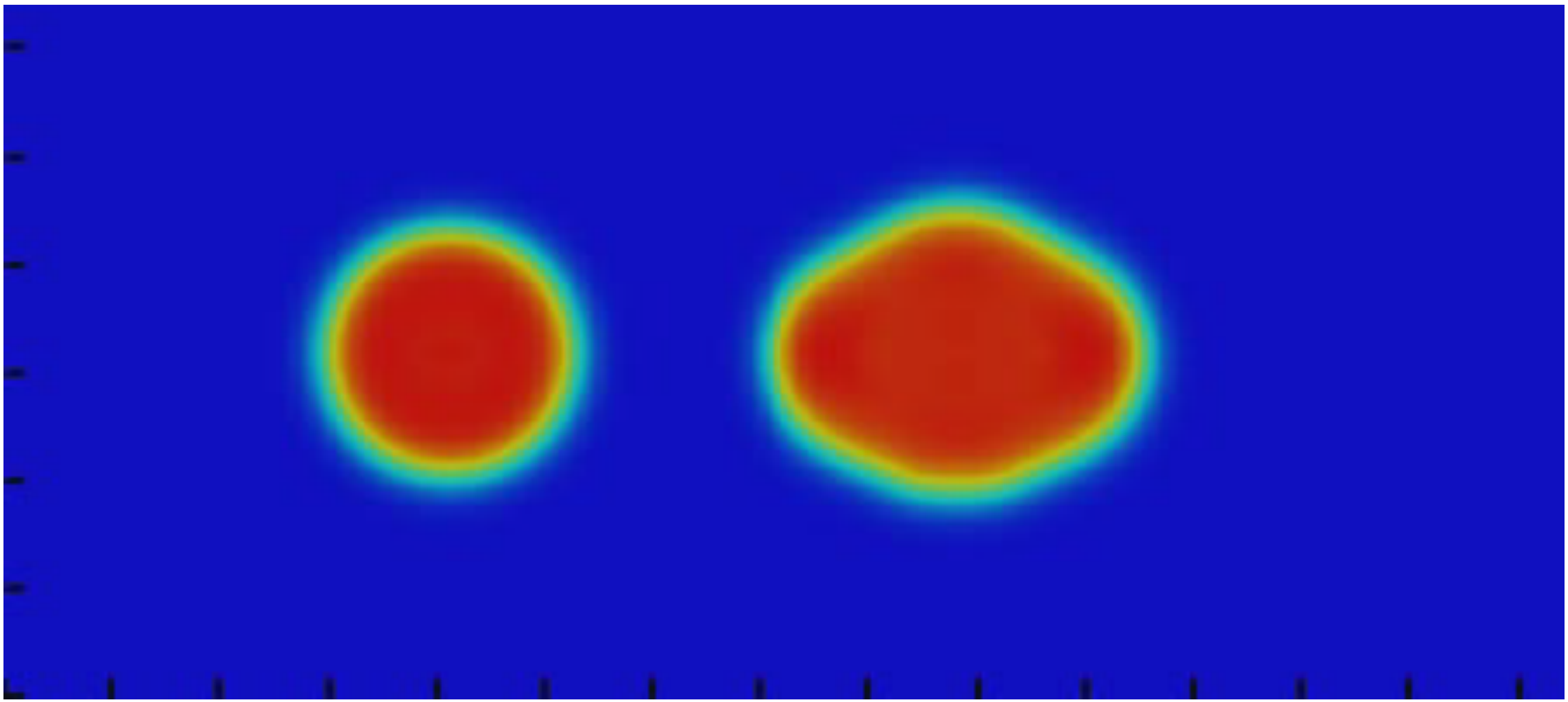
normal quasi-fission
E = 5.7 MeV/A

inverse quasi-fission
E = 9 MeV/A

$^{238}U + ^{124}Sn$ (b=0)



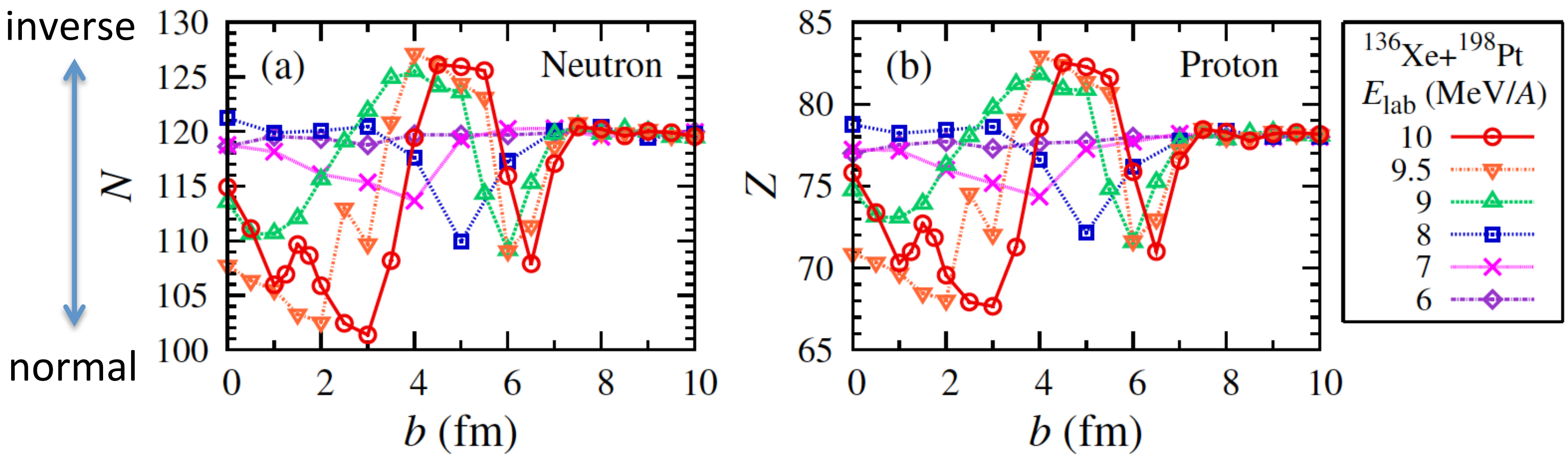
$^{238}U + ^{124}Sn$ E=9 MeV/A, b=0 fm



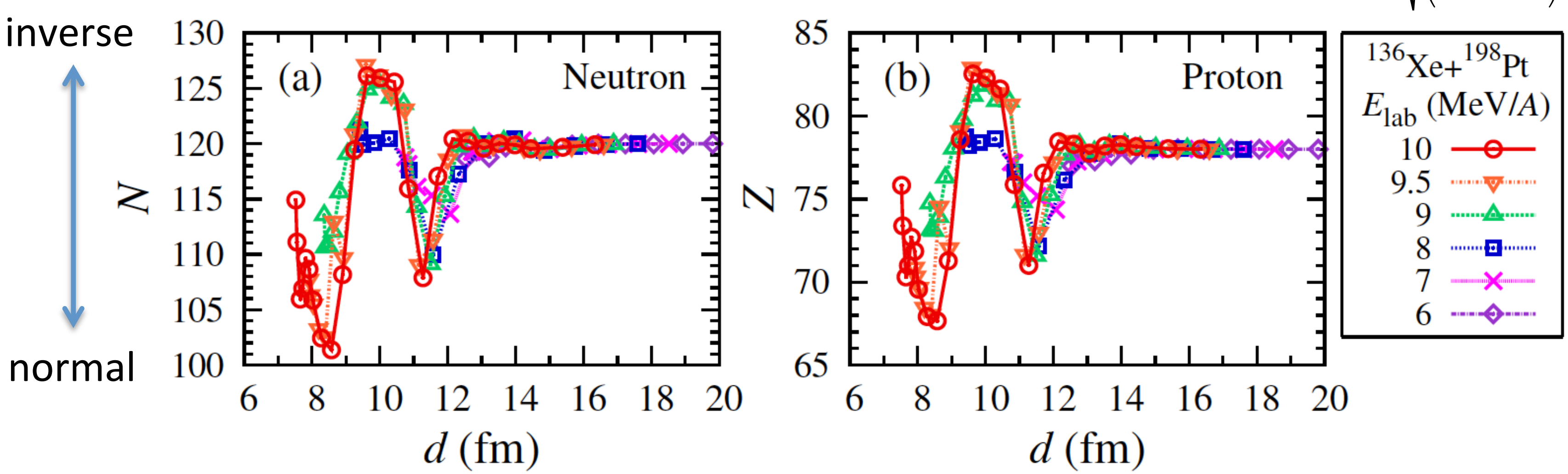
Origin of inverse quasi-fission: density wave initiates a development of a neck

Systematic calculations changing *E* and *b*: ^{136}Xe+^{198}Pt

Average N, Z of Pt-like fragment for various (E,b)



Same result plotted against d = distance of closest approach, $d = \frac{Z_P Z_T e^2}{2E} + \sqrt{\left(\frac{Z_P Z_T e^2}{2E}\right)^2 + b^2}$



Inverse quasi-fission is seen at a certain range of incident energy, radial dynamics is responsible.

Summary

TDHF calculation provide nuclear dynamics without empirical parameters specific to systems and dynamics.

TDHF for multi-nucleon transfer reactions

- describe cross sections reasonably for small number of transferred nucleons
  underestimate for channels involving large number of transferred nucleons
- Two dynamics competes:
  successive nucleon transfer at large impact parameter
  neck formation and breaking at small impact parameter

TDHF for quasi-fission

- describes subtle dynamics reflecting orientations of deformed nuclei, shell effect
- systematic calculation reveals appearance of inverse quasi-fission at higher energy

Future directions

- propose appropriate reactions producing SHE and r-process unstable nuclei.
- theories incorporating correlation beyond mean field are required.