Microscopic Heavy-Ion Potentials Based on TDHF

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Many-Body Fusion and Fission

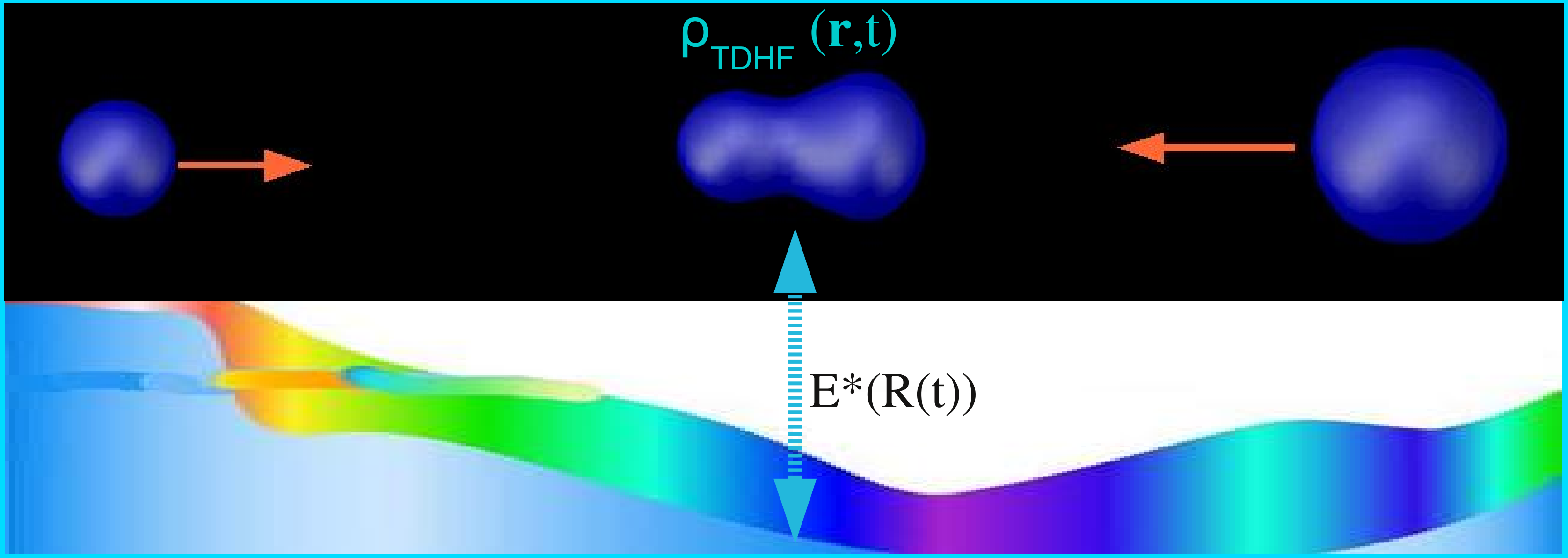
- No practical ab-initio many-body theory for fusion exists

- All approaches involve two prongs
  a) Calculate an ion-ion barrier (usually one-dimensional)
    - Phenomenological (Wood-Saxon, Proximity, Folding, Bass, etc.)
    - macroscopic-microscopic methods using collective variables
  b) Employ quantum mechanical tunneling methods for the reduced one-body problem (WKB, IWBC)

- Incorporate quantum mechanical processes by hand
  a) Neutron transfer
  b) Few excitations of the entrance channel nuclei (CC)

Microscopic Collective Dynamics Based on TDHF

- ➔ Obtain collective dynamics (density evolution) from TDHF
  - system selects its evolutionary path via time-dependent action
- ➔ Find lowest energy of the system compatible with TDHF density
- ➔ Need a method to extract internal excitation energy while holding the instantaneous densities and currents constrained



Quasi-Static Energy Surface

Density-Constraint

Lowest energy collective state corresponding to TDHF state |Φ(t)>:

Solution of Hartree-Fock equations

$$< \Phi_{\rho,\mathbf{j}} | a_h^\dagger a_p \hat{H} | \Phi_{\rho,\mathbf{j}} >= 0$$

Subject to constraints

$$< \Phi_{\rho,\mathbf{j}} | \hat{\rho}(\mathbf{r}) | \Phi_{\rho,\mathbf{j}} >= \rho(\mathbf{r},t)$$

$$< \Phi_{\rho,\mathbf{j}} | \hat{\jmath}(\mathbf{r}) | \Phi_{\rho,\mathbf{j}} >= \mathbf{j}(\mathbf{r},t)$$

TDHF

$$E_{coll}(\rho(\mathbf{r},t),\mathbf{j}(\mathbf{r},t)) =< \Phi_{\rho,\mathbf{j}} | \hat{H} | \Phi_{\rho,\mathbf{j}} >$$

$$E^* = E_{TDHF} - E_{coll}$$

Total conserved TDHF energy

Static collective state corresponding to TDHF state |Φ(t)>:

Solution of Hartree-Fock equations

$$< \Phi_{\rho} | a_h^\dagger a_p \hat{H} | \Phi_{\rho} >= 0$$

Subject to constraints

$$< \Phi_{\rho} | \hat{\rho}(\mathbf{r}) | \Phi_{\rho} >= \rho(\mathbf{r},t)$$

$$< \Phi_{\rho} | \hat{\jmath}(\mathbf{r}) | \Phi_{\rho} >= 0$$

$$E_{DC}(\rho(\mathbf{r},t)) =< \Phi_{\rho} | \hat{H} | \Phi_{\rho} >$$

$$E_{coll} = E_{kin}(\rho(t),\mathbf{j}(t)) + E_{DC}(\rho(\mathbf{r},t))$$

Ion-Ion Potential and Excitation Energy

Collective Potential

Collective energy has kinetic and static part

$$E_{coll} = E_{kin}(\rho(t), \mathbf{j}(t)) + E_{DC}(\rho(\mathbf{r}, t)) \longrightarrow V_{coll} \propto E_{DC}$$

Contains binding energies

$$V(R(t)) = E_{DC}(\rho(r,t)) - E_{A_1} - E_{A_2} \longrightarrow \text{Subtract binding energies}$$

Label it with ion-ion separation at time t

Correct asymptotic behavior – no normalization or scaling

$$E_{DC}(R_{max}) = E_{A_1} + E_{A_2} + V_{Coulomb}(R_{max}) \longrightarrow V(R_{max}) = V_{Coulomb}(R_{max})$$

Excitation Energy

$$E^*(R(t)) = E_{TDHF} - E_{coll} = E_{TDHF} - E_{kin}(\rho(t), \mathbf{j}(t)) - E_{DC}(\rho(t))$$

Approximate expression for collective kinetic energy

$$E_{kin}(\rho(t), \mathbf{j}(t)) \approx \frac{\hbar^2}{2m} \int d^3r\, \mathbf{j}(t)^2 / \rho(t)$$

Implementation

Generalize the ordinary method of constraints

- for a single constraint → $\hat{H} \to \hat{H} + \lambda \hat{Q}$

- for a set of constraints → $\hat{H} \to \hat{H} + \sum_i \lambda_i \hat{Q}_i$

- for density constraint → $\hat{H} \to \hat{H} + \int d^3r\, \lambda_q(r)\, \hat{\rho}_q(r)$

Works as efficiently as a single constraint

- numerical method for steering the solution to TDHF density is in:

1. Cusson, Reinhard, Maruhn, Strayer, Greiner, *Z. Phys. A* **320**, 475 (1985)
2. Umar, Strayer, Cusson, Reinhard, Bromley, *Phys. Rev. C* **32**, 172 (1985)

DC-TDHF Method for Ion-Ion Potentials

➔ Completely microscopic description of ion-ion potential barriers

➔ Includes all dynamical entrance channel effect through density

➔ Incorporates energy dependence of barriers

➔ Successful in obtaining realistic fusion barriers whenever the participating nuclei are well described by Skyrme-HF

➔ Obtain fusion cross-sections via IWBC

➔ Average over all orientations for deformed nuclei

(e.g. if one of the nuclei is axially symmetric)

$$\sigma_f(E_{c.m.}) = \int_0^1 d\cos(\beta)\, P(\beta)\, \sigma(E_{c.m.},\beta)$$

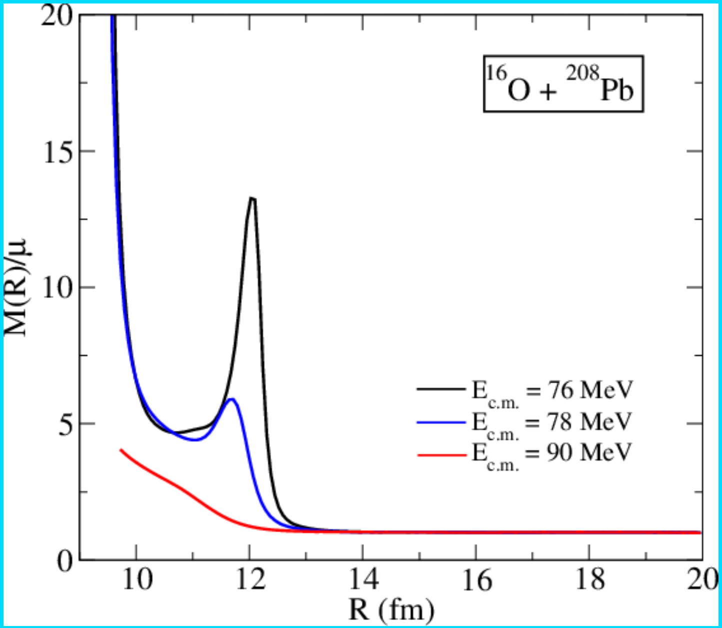
DC-TDHF + IWBC

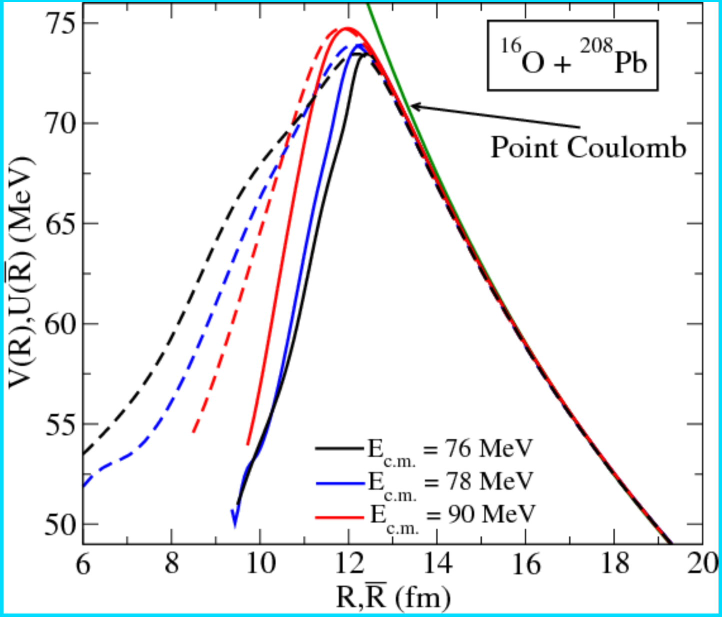
From Coulomb excitation

Umar & Oberacker,
PRC 73, 054607 (2006)
PRC 74, 024606 (2006)
PRC 74, 021601(R) (2006)
PRC 74, 06160 (R) (2006)
PRC 76, 014614 (2007)
PRC 77, 064605 (2008)
EPJA 39, 243 (2009)
JPG 36, 025101 (2009)

Umar, Oberacker, Maruhn, Reinhard, ...
EPJA 37, 245 (2008); PRC 82. 034603 (2010); PRC 81, 064607 (2010);
PRC 80, 041601(R) (2009); PRL 104, 212503 (2010)

Dynamical Effective Mass





$$E_{c.m.} = \frac{1}{2} M(R)\,\dot{R}^2 + V(R)$$

TDHF DC-TDHF

$$M(R) = \frac{2\left(E_{c.m.} - V(R)\right)}{\dot{R}^2}$$

- Transform effect to potential

$$d\bar{R} = \left(\frac{M(R)}{\mu}\right)^{\frac{1}{2}} dR$$

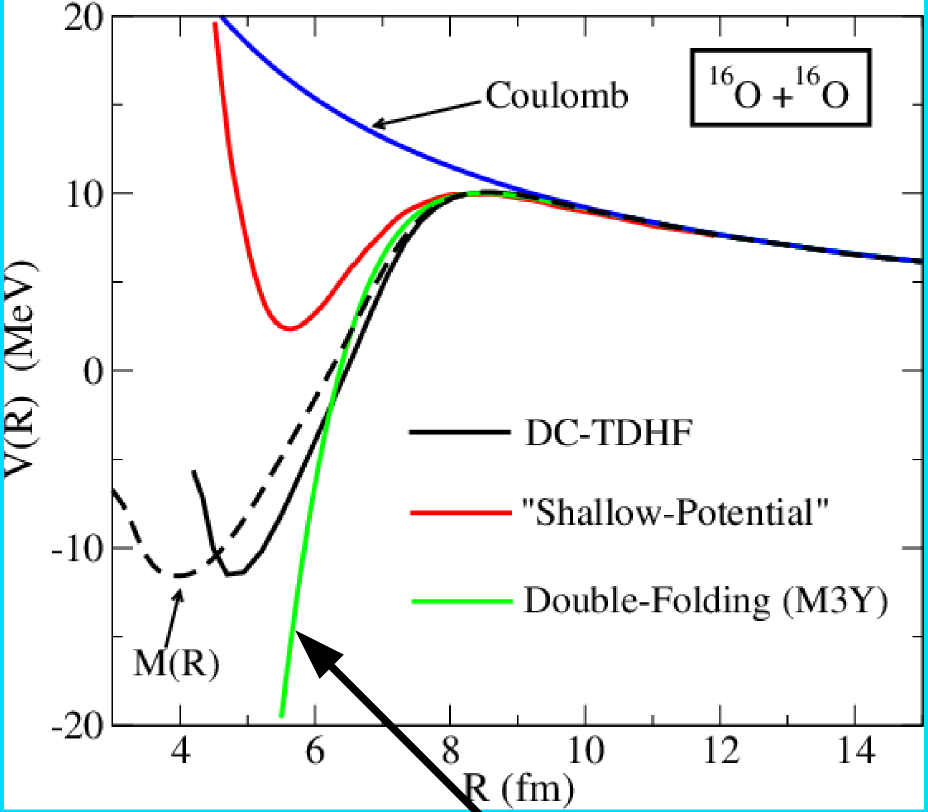
$$V(r) \rightarrow U(\bar{R}) \qquad M(\bar{R}) = \mu$$

New Generation TDHF Code

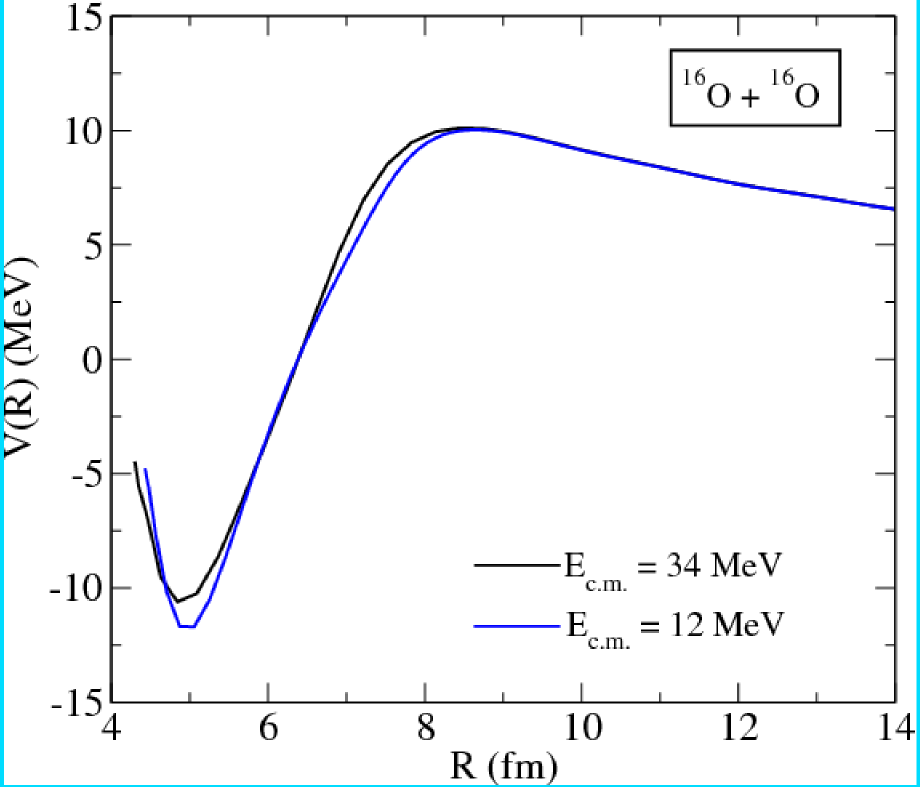
- Unrestricted **3-D Cartesian** geometry
  - No fixed reaction plane
  - No reflection symmetry (+z/-z)
- **Basis-Spline** discretization for high accuracy
- Programmed in **Fortran 95** and **OMP**
- Use of modern **Skyrme** forces with **all** the terms (time even/odd)
- **No time-reversal** symmetry assumed
- It is possible to calculate cross sections for deformed nuclei

Comparison to Other Fusion Potentials

- DC-TDHF potential contains no parameters and normalization (SLy4)



Frozen density

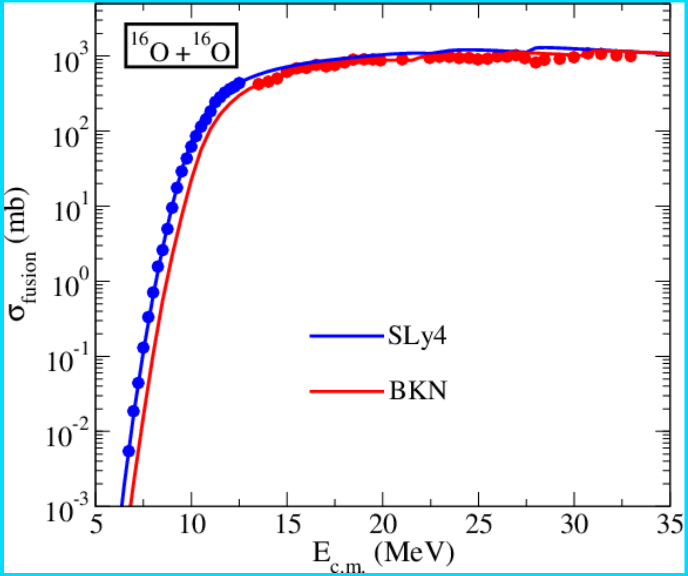


Energy dependence:
For light systems energy dependence is small

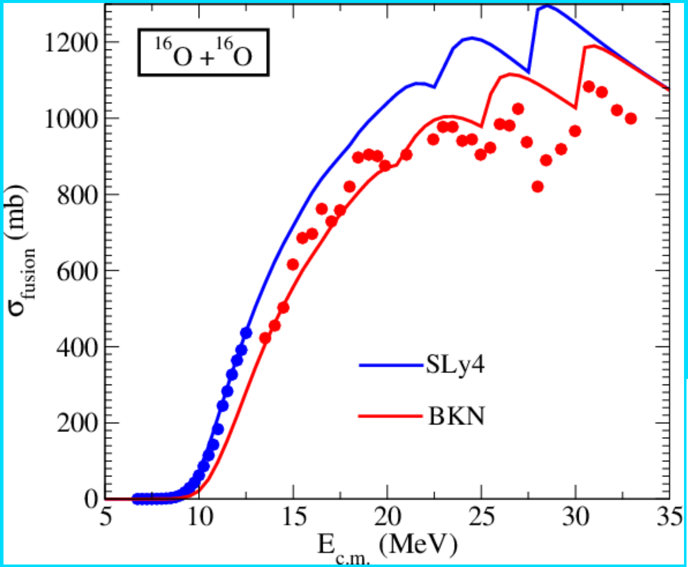
Double folding: M3Y effective NN interaction, exp densities
Shallow-Potential: H. Esbensen, PRC 77, 054608 (2008)

- Coulomb tails always accurate to 50-150 keV

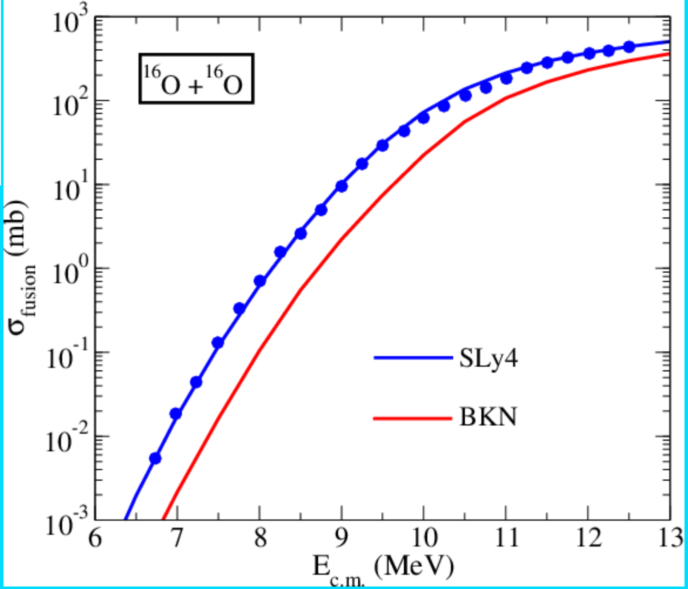
Fusion Cross-Sections



- Energies multiple times the barrier height (10 Mev)
- Do better around barrier top and below

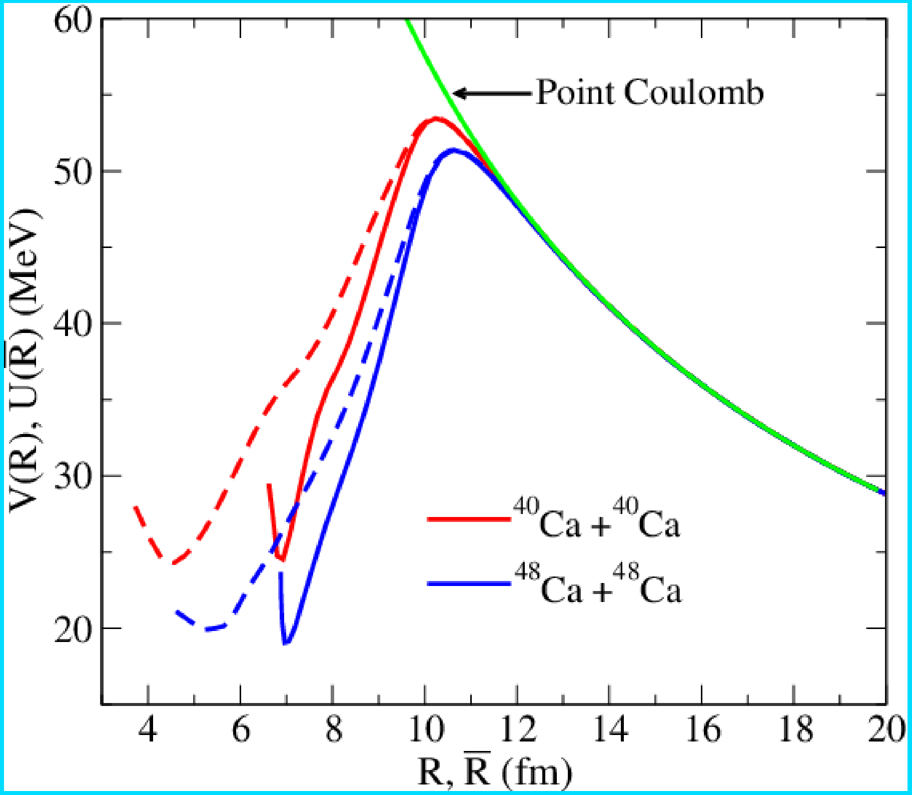


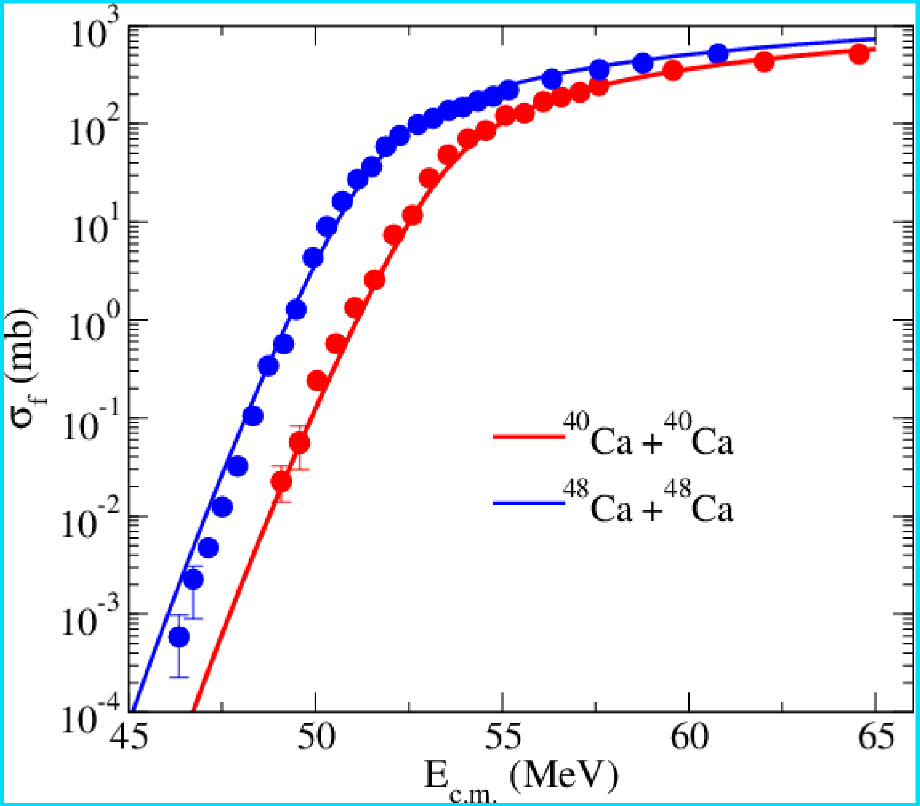
Subbarrier



- Calculate x-section using IWBC method
- Gross-structure due to changing L_{max} as E_{cm} increases

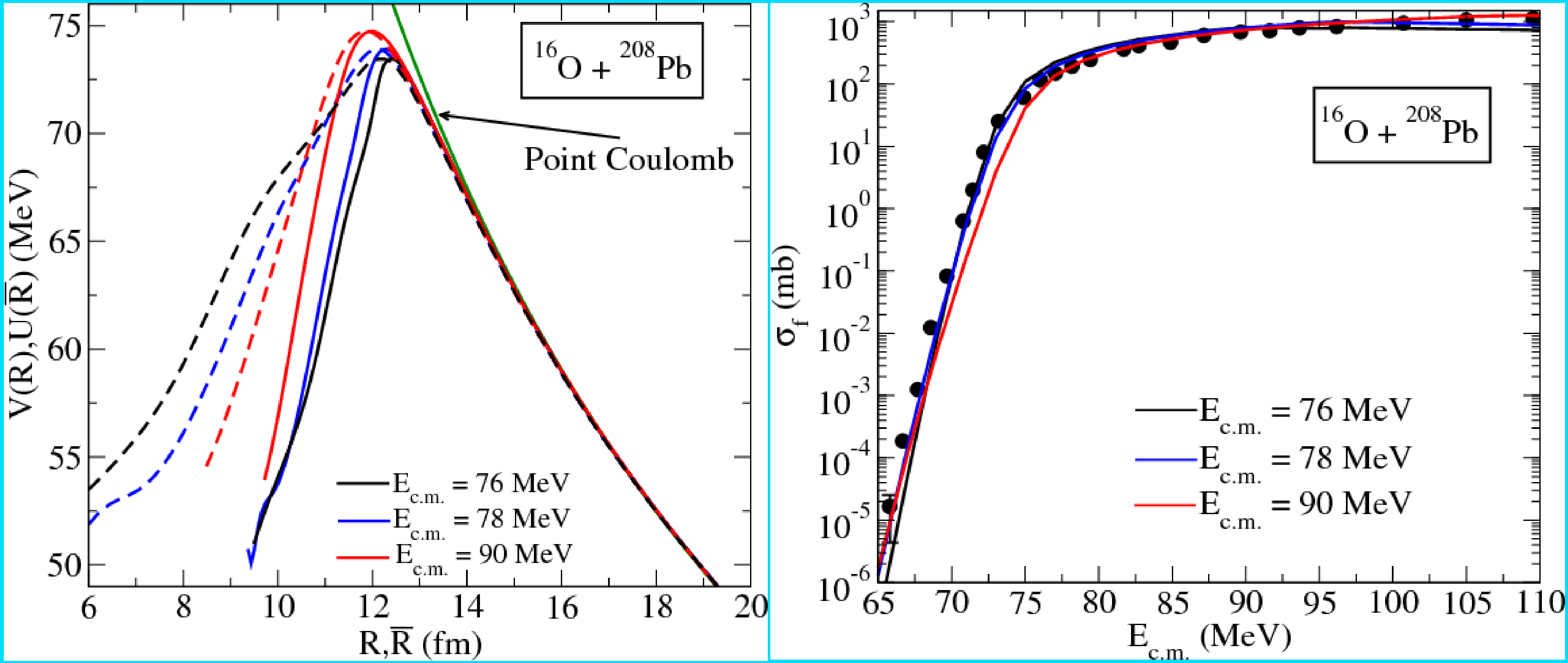
Ca + Ca Fusion





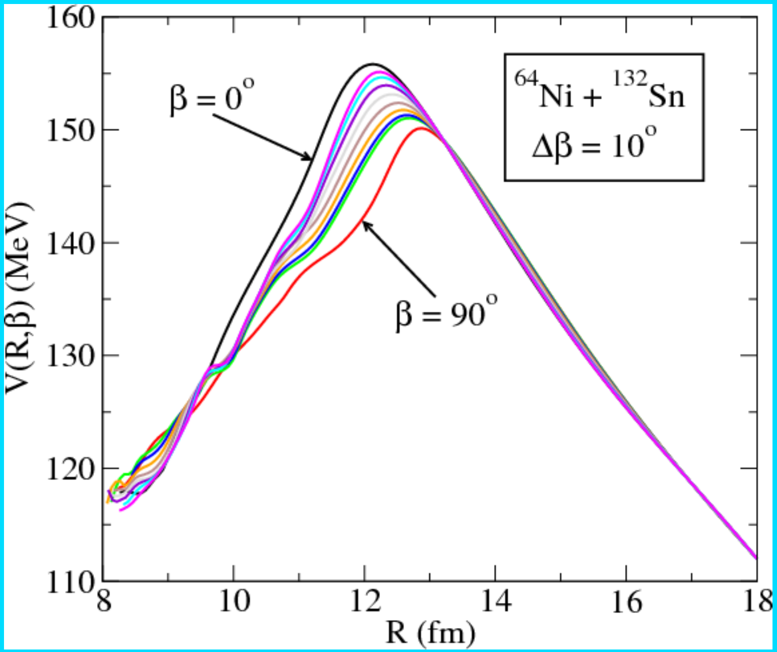
- 40Ca and 48Ca usually in Skyrme fits (here SLy4)
- 40Ca+40Ca result slightly better than 48Ca+48Ca

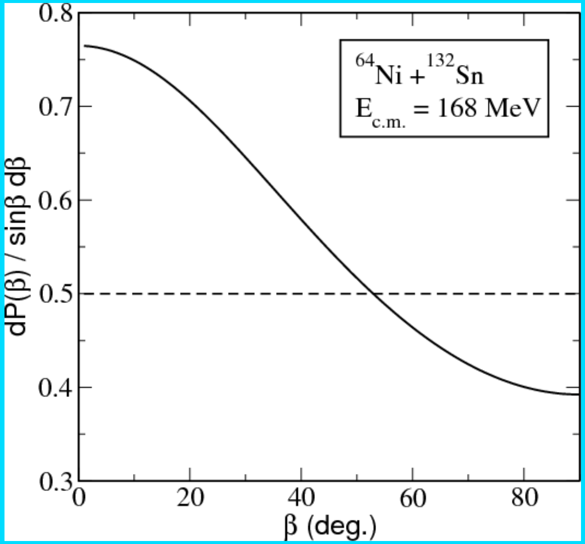
$^{16}O + ^{208}Pb$ Fusion Cross-Section

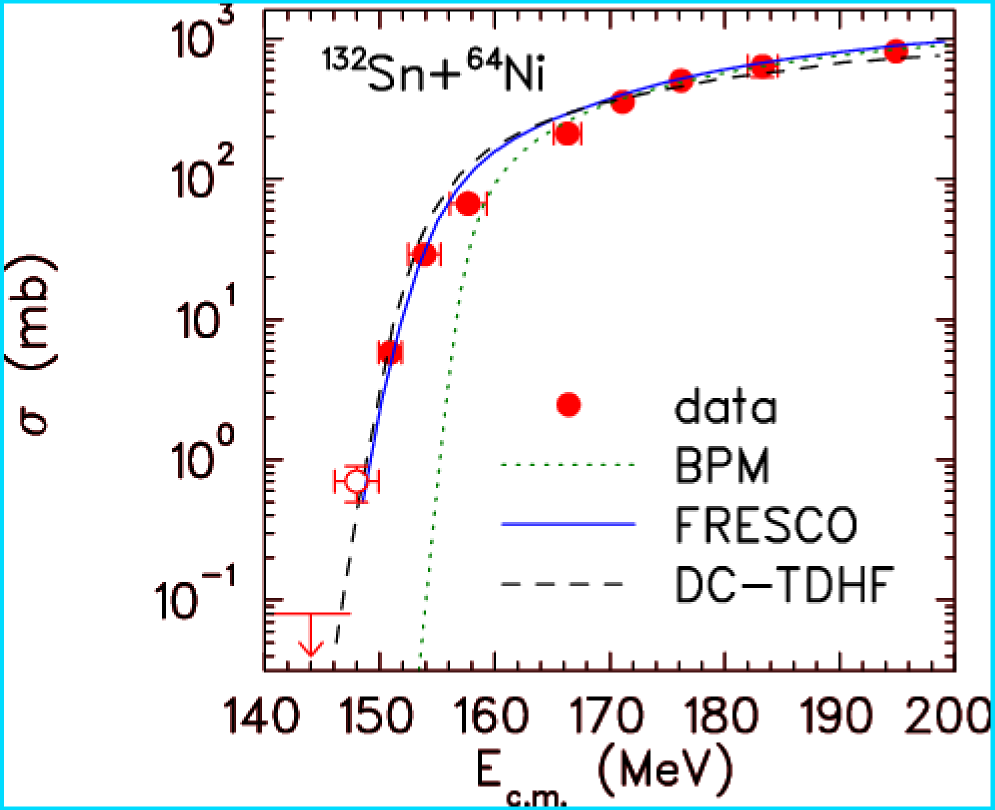


Umar, Oberacker, *EPJA* **39**, 243 (2009)

^{64}Ni + ^{132}Sn Complete Set of Barriers







- Use IWBC
- Average over orientations

$$\sigma_f(E_{c.m.}) = \int_0^1 d\cos(\beta) P(\beta) \sigma(E_{c.m.}, \beta)$$

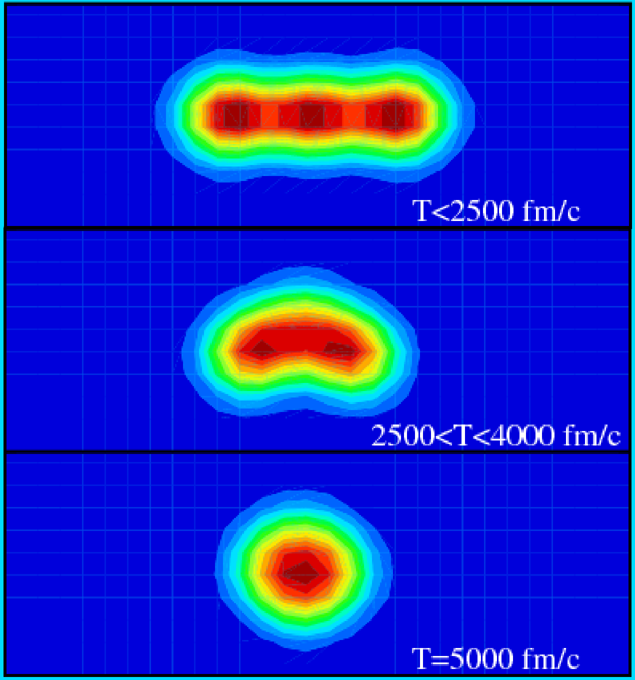
Exp.: J.F. Liang *et al.*, PRL 91, 152701 (2003); PRC 75, 054607 (2007)

Umar and Oberacker, *Phys. Rev. C* **76**, 014614 (2007)

Formation of ^{12}C In the Universe (also ^{16}O)

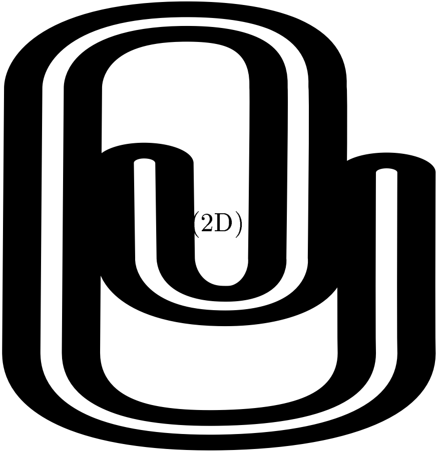
- ^{8}Be has 10^{-16}s lifetime and not found in nature
- In stars due to ^{4}He abundance small amount of ^{8}Be always present
- ^{4}He+^{8}Be combine to form resonant state of ^{12}C
- Excited state decays to ground state via an intermediate state
- Use TDHF to study the dynamics of this collision

See Movies

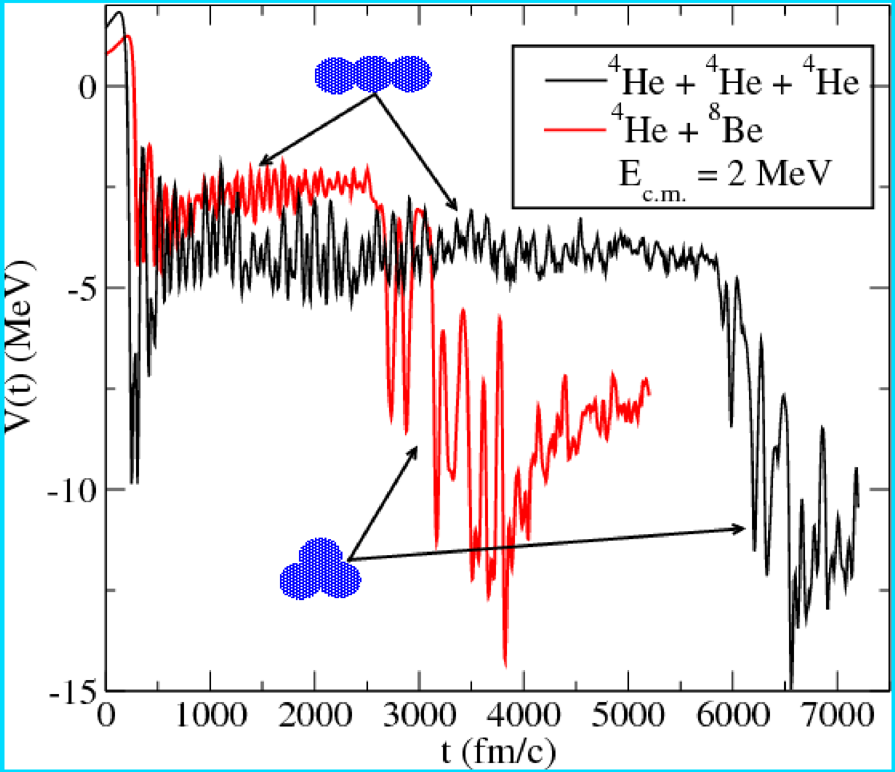


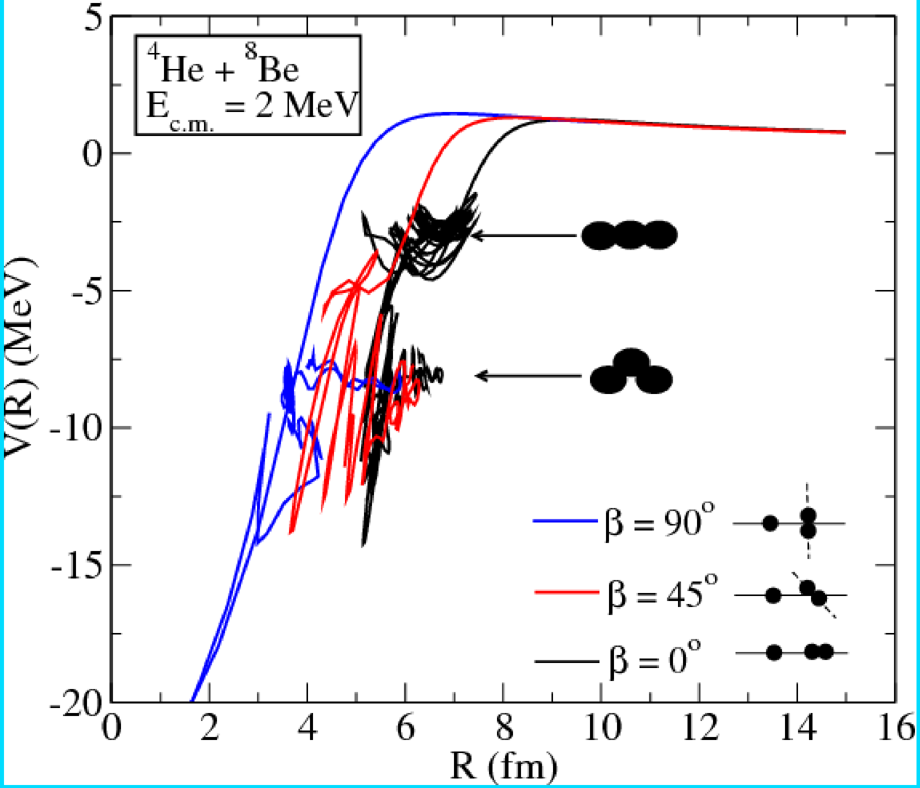
Umar, Maruhn, Itagaki, Oberacker
Phys. Rev. Lett. **104**, 212503 (2010)

$\alpha -^8 Be$ $E_{cm} = 2\ MeV$

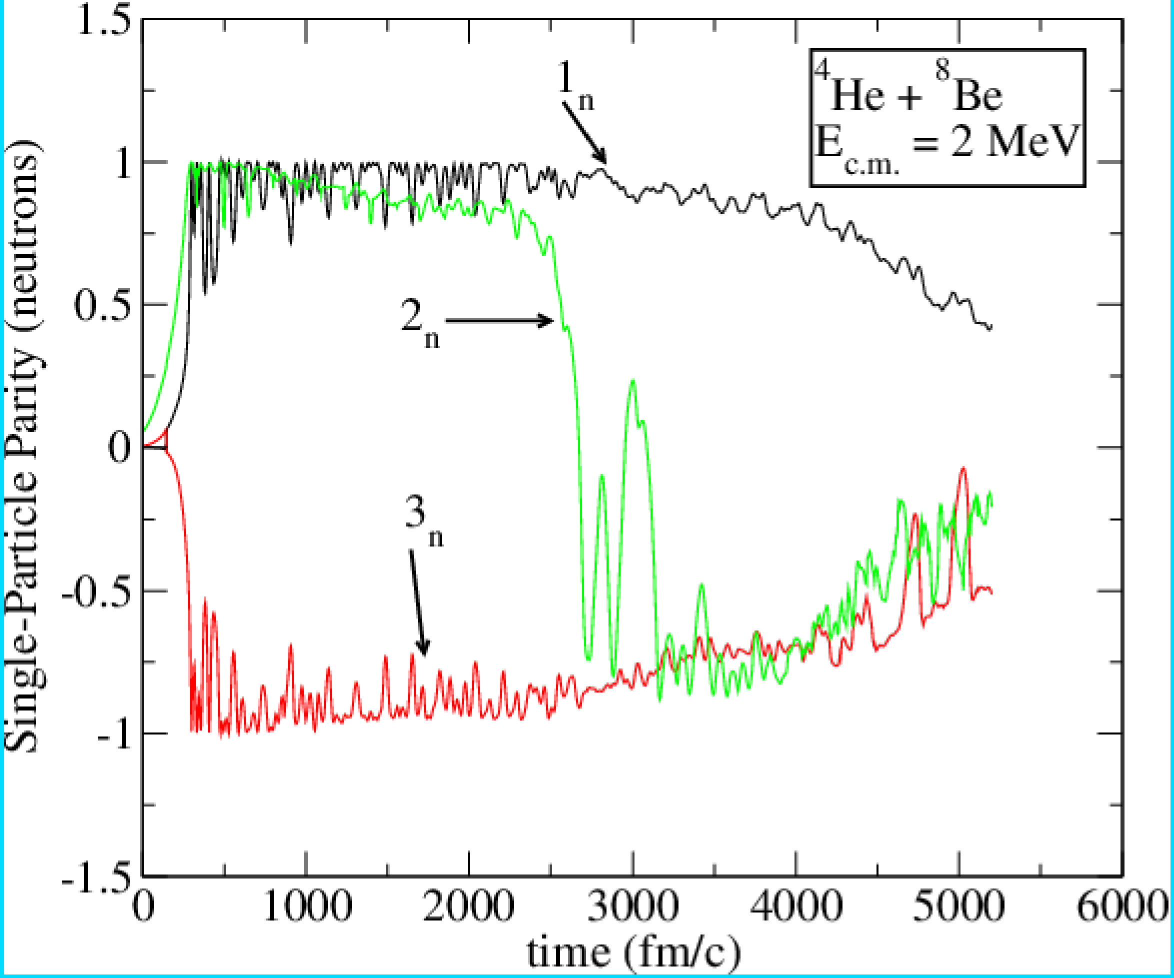


Dynamics of Transition

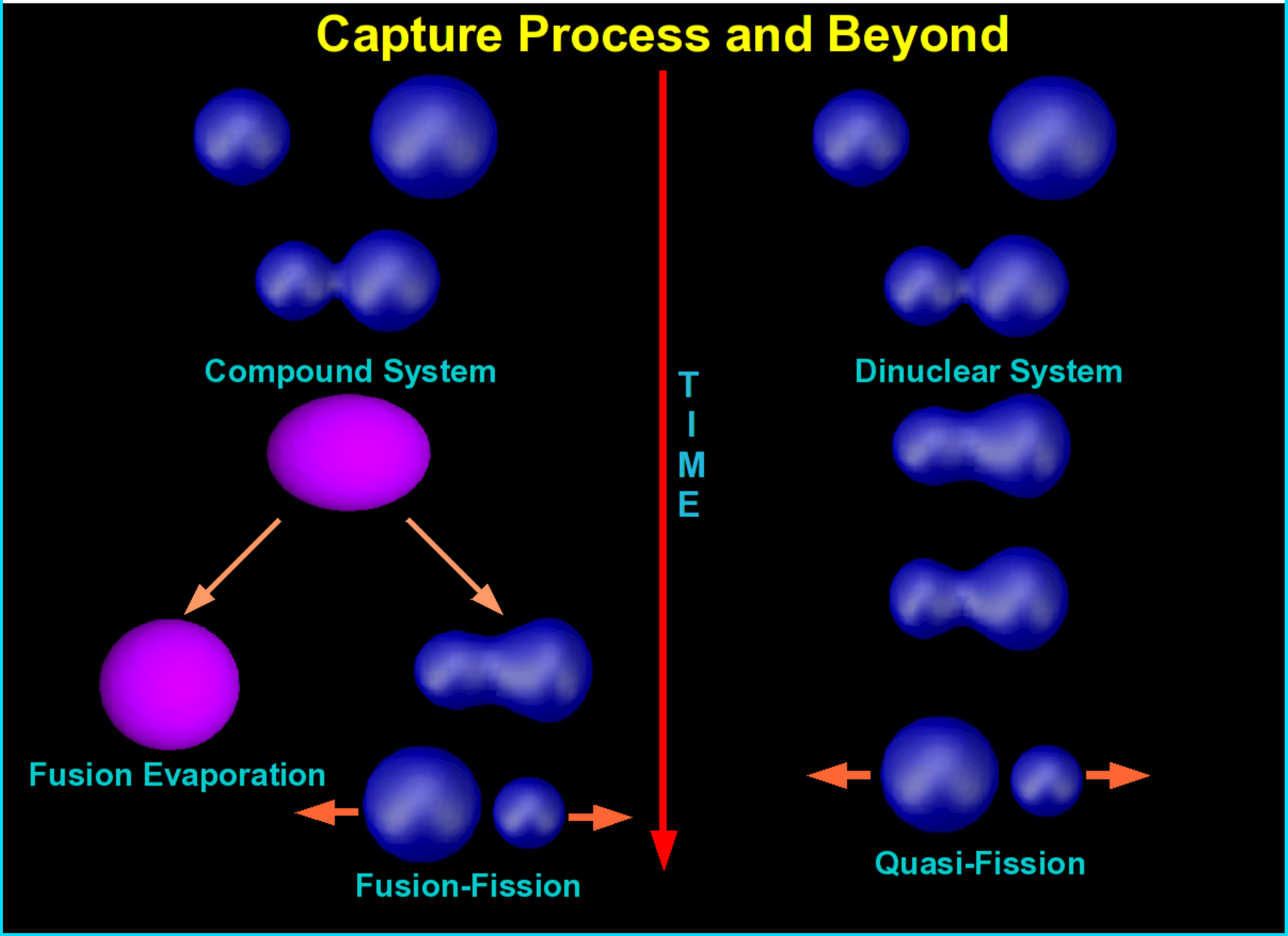




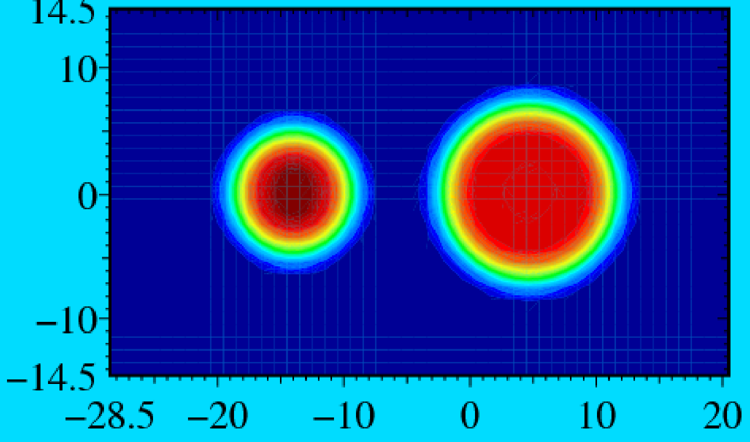
Parity Evolution



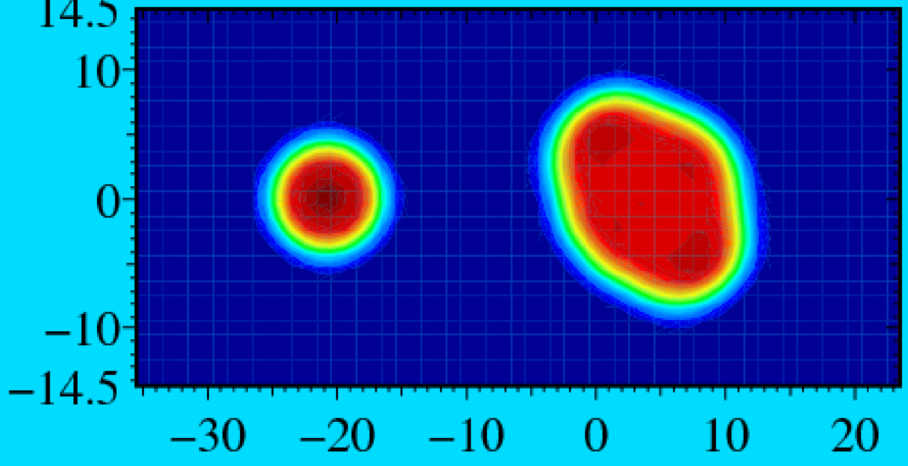
Dynamics of Heavy Systems



Cold and Hot Fusion of Heavy Systems



^{70}Zn+^{208}Pb



^{48}Ca+^{238}U (β=45°)

Heavy nuclei exhibit a very different behavior in forming a composite system

Light-Medium Mass Systems

$$\sigma_{capture} \approx \sigma_{ER} \approx \sigma_{fusion}$$

- Fission and quasi-fission negligible
- Simple V(R) for composite system

Heavy Systems

$$\sigma_{capture} = \sigma_{QF} + \sigma_{FF} + \sigma_{ER}$$

- Quasi-fission dominant
- Di-nuclear composites common
- A multi-stage V(R)
- QF may masquerade as DI

Excitation Energy

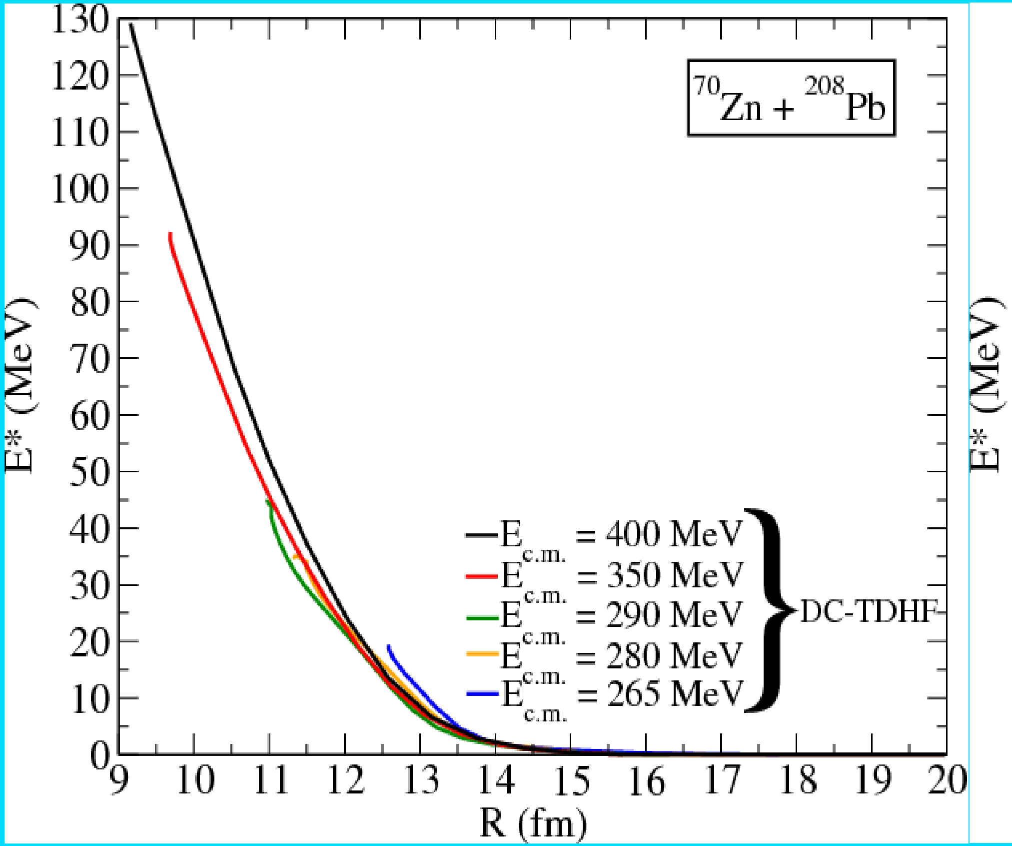
- ➔ Excitation energy is an important indicator of reaction dynamics
- ➔ Superheavy formations are very sensitive to excitation energy
- ➔ Indicator of temperature for compound configurations
- ➔ Traditional knowledge based on initial and final reaction products:

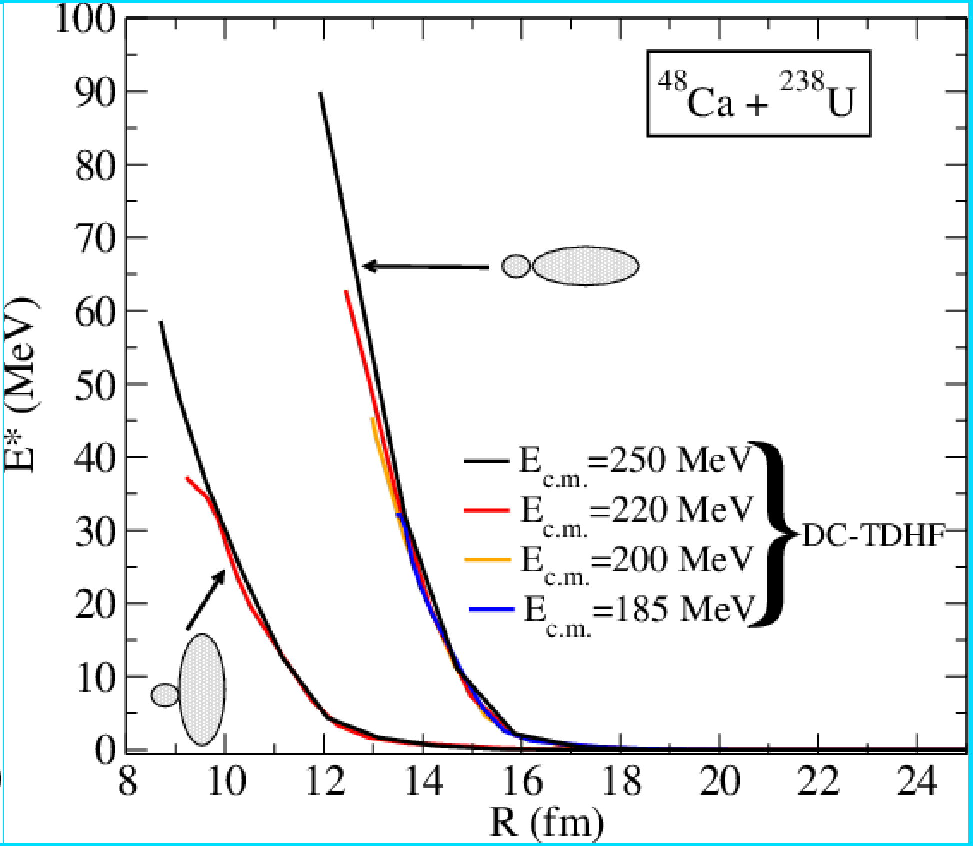
$$\boxed{E^{*} = E_{c.m.} + Q_{gg}}$$

- ➔ Time evolution of excitation energy could tell us about the survival of intermediate configurations
- ➔ Density constraint makes this calculation possible via TDHF

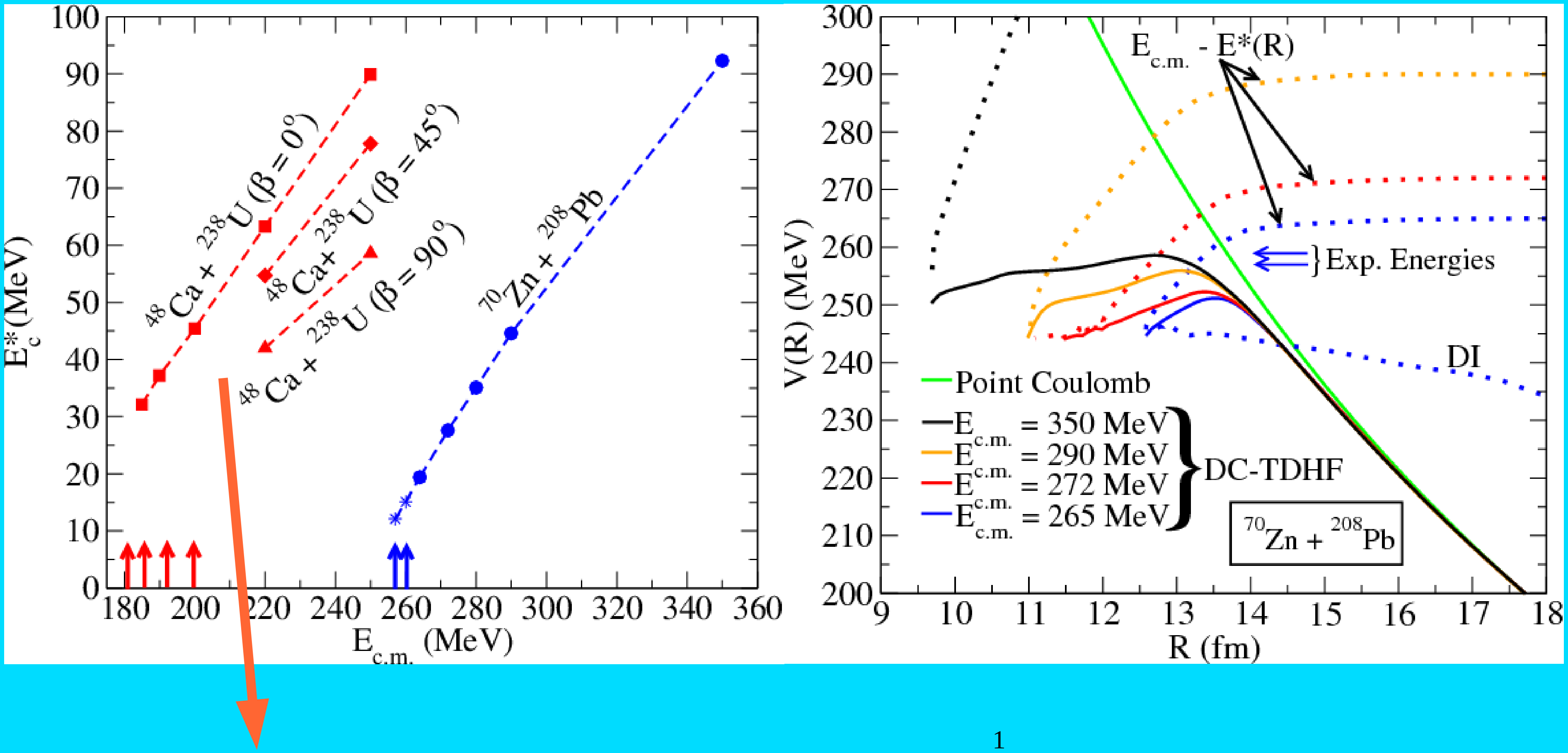
Excitation Energies at Capture Point

- ➔ Experimentally cited excitation energy $E^{*}_{\rm exp} = E_{c.m.} + Q_{\rm gg}$
- ➔ We calculate excitation energy as a function of R(t)



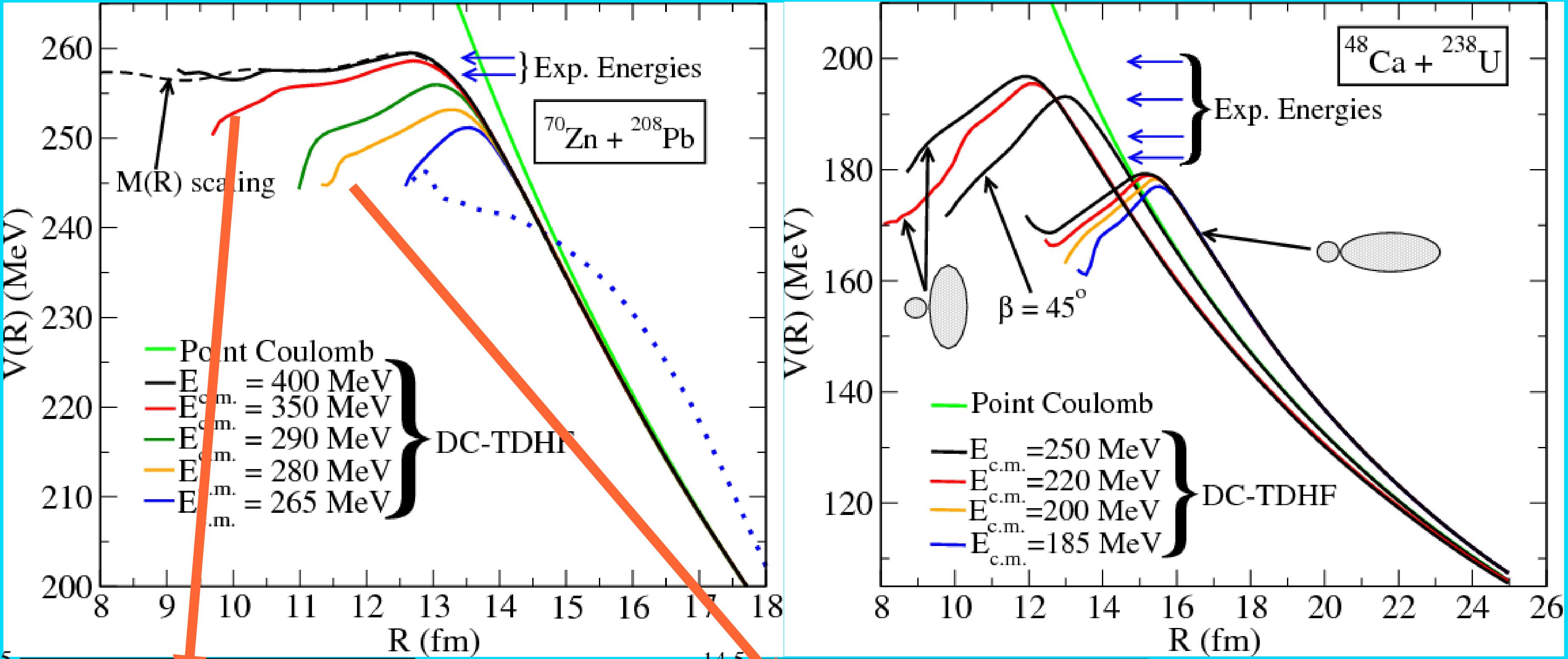


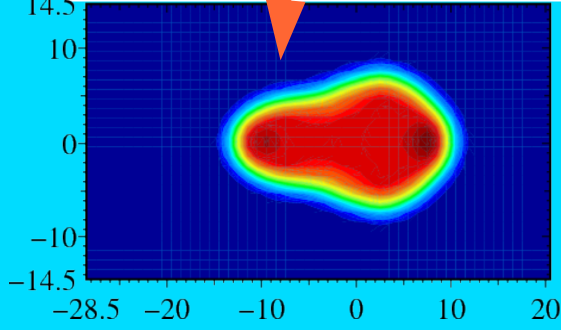
Excitation Energies



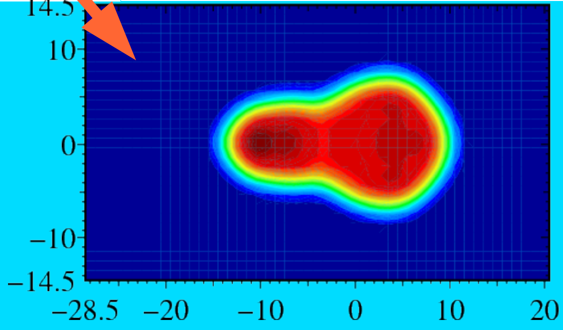
Should be alignment averaged: $E^*(E_{c.m.}) = \int_0^1 d\beta \sin(\beta) P(\beta) E^*(E_{c.m.},\beta)$

Potentials





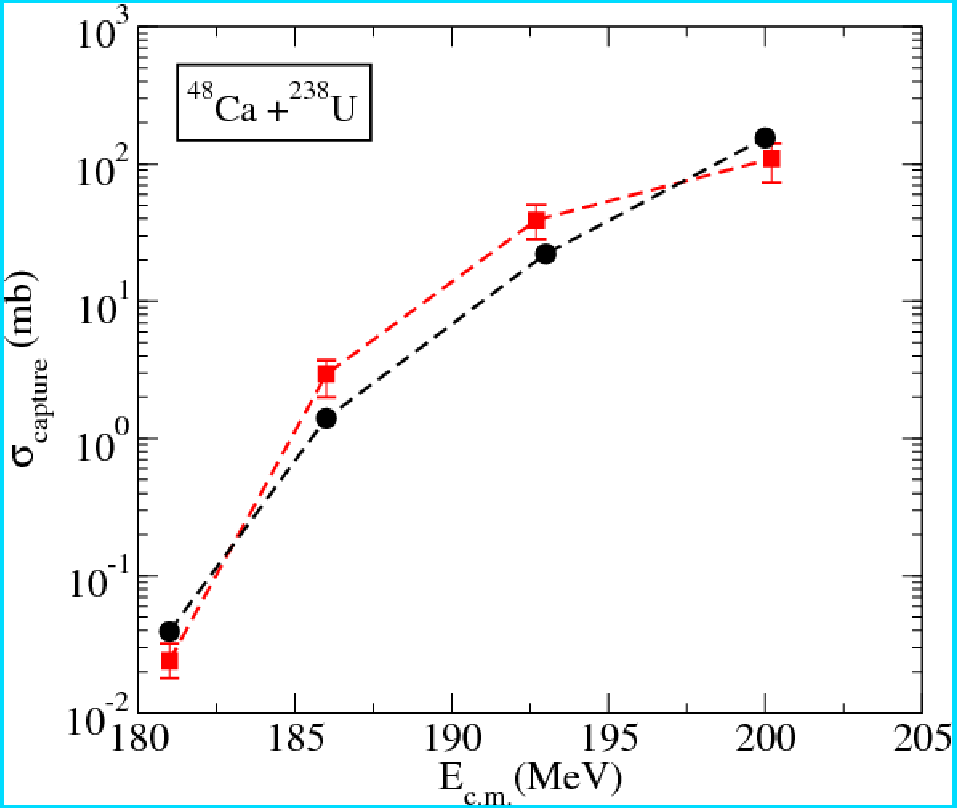
- Cores join
- Capture



- Cores remain distinct
- Nucleons exchanged
- b>0 deep-inelastic

Cross-Sections

Umar, Oberacker, Maruhn, Reinhard, PRC 81, 064607 (2010)



➔ **Angle average ^{238}U alignment:**
- significantly reduces x-section

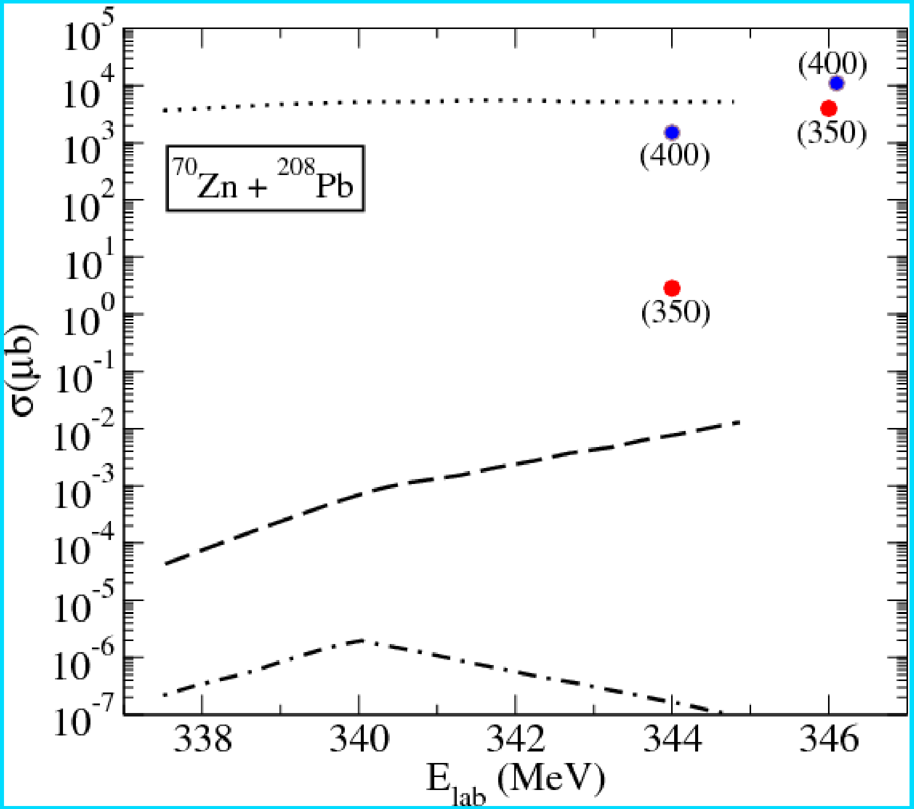
$$\sigma_f(E_{c.m.}) = \int_0^1 d\beta \sin(\beta) P(\beta) \sigma(E_{c.m.}, \beta)$$

- x-section falls rapidly for $\beta > 10^\circ$
- sin(β) multiply small angles
- P(β) is in the range 0.4-0.6

Experimental data (private communication):
1. Yu. Ts. Oganessian, *Phys. Rev. C* **70**, 064609 (2004)
2. Yuri Oganessian, *J. Phys. G: Nucl. Part. Phys.* **34**, R165 (2007)

Cross-Sections

Umar, Oberacker, Maruhn, Reinhard, PRC 81, 064607 (2010)



➔ Could not find data for capture x-section

➔ Calculated capture x-section (reproducing one σ_{ER} x-section value.)

G. Giardina, S. Hofmann, A.I. Muminov, and A.K. Nasirov, *Eur. Phys. J. A* **8**, 205 (2000)

Experiments:

1. S. Hofmann et al., *Rev. Mod. Phys.*, **72**, 733 (2000)
2. S. Hofmann et al., *Eur. Phys. J. A* **14**, 147 (2002)

Neutron Transfer in TDHF

- Recent studies show that TDHF description of HI collisions is most accurate for the entrance channel dynamics:

  Umar, Oberacker, *J. Phys. G* **36**, 025101 (2009)
  Guo, Maruhn, Reinhard, Hashimoto, *Phys. Rev. C* **77**, 041301 (2008)

- Recent DD-TDHF studies show good agreement with friction models

  Kouhei Washiyama, Denis Lacroix, and Sakir Ayik, *Phys. Rev. C* **79**, 024609 (2009)

- One of the processes that influence fusion is neutron transfer

- Investigate neutron transfer in TDHF (semi-classical) and compare with QM model calculations:

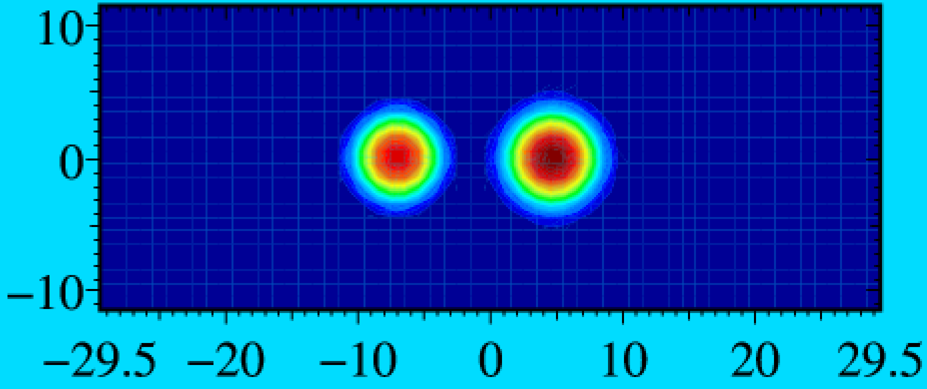
  V. I. Zagrebaev, V. V. Samarin, and W. Greiner, *Phys. Rev. C* **75**, 035809 (2007)

Umar, Oberacker, Maruhn, *Eur. Phys. J. A* **37**, 245 (2008)

Two Neutron-Rich Systems Above/Below the Barrier

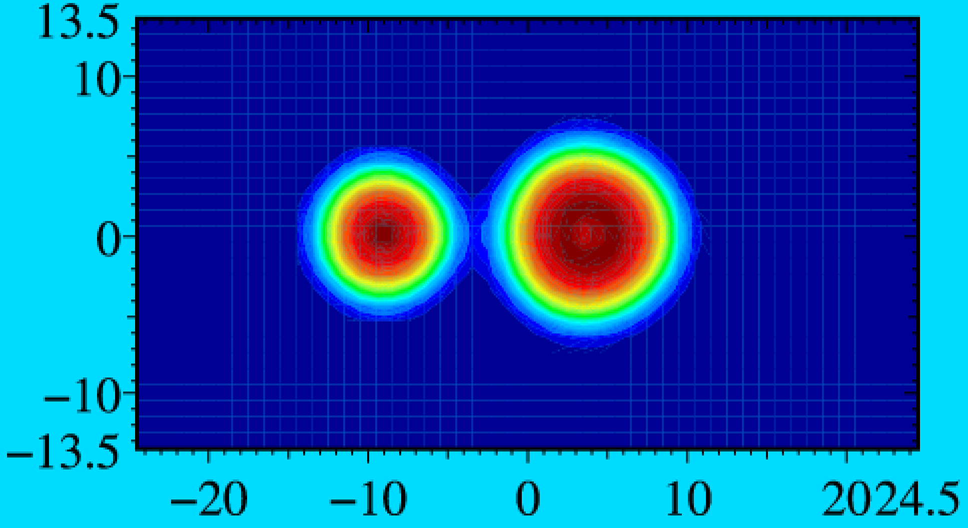
- ^{16}O+^{24}O at E_{cm}= 8 MeV (below effective barrier)

Closest approach →

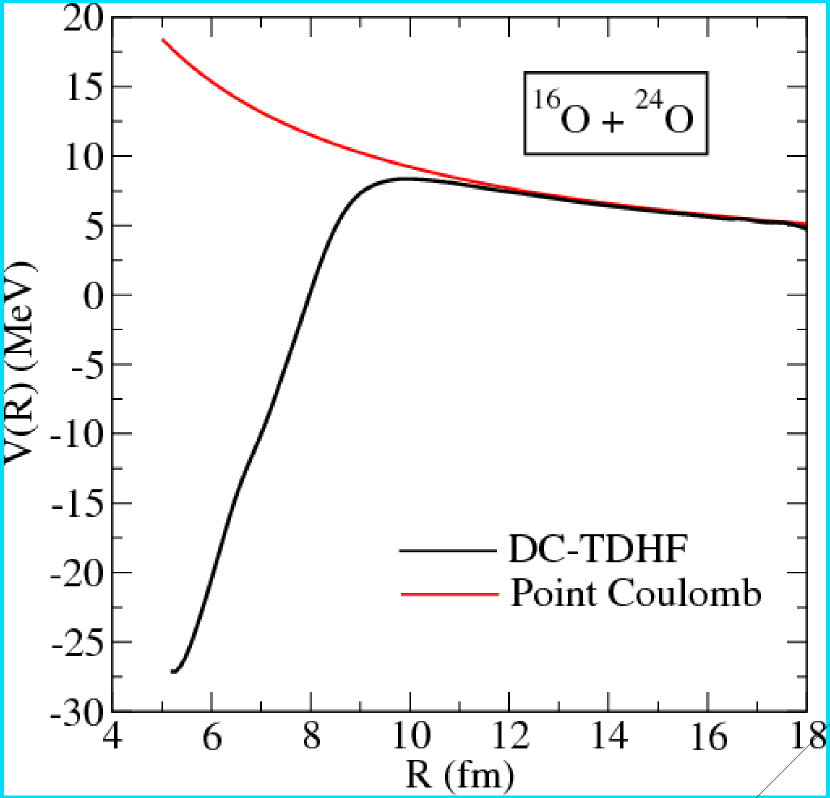


- ^{40}Ca+^{96}Zr at E_{cm}= 91 MeV (below effective barrier)

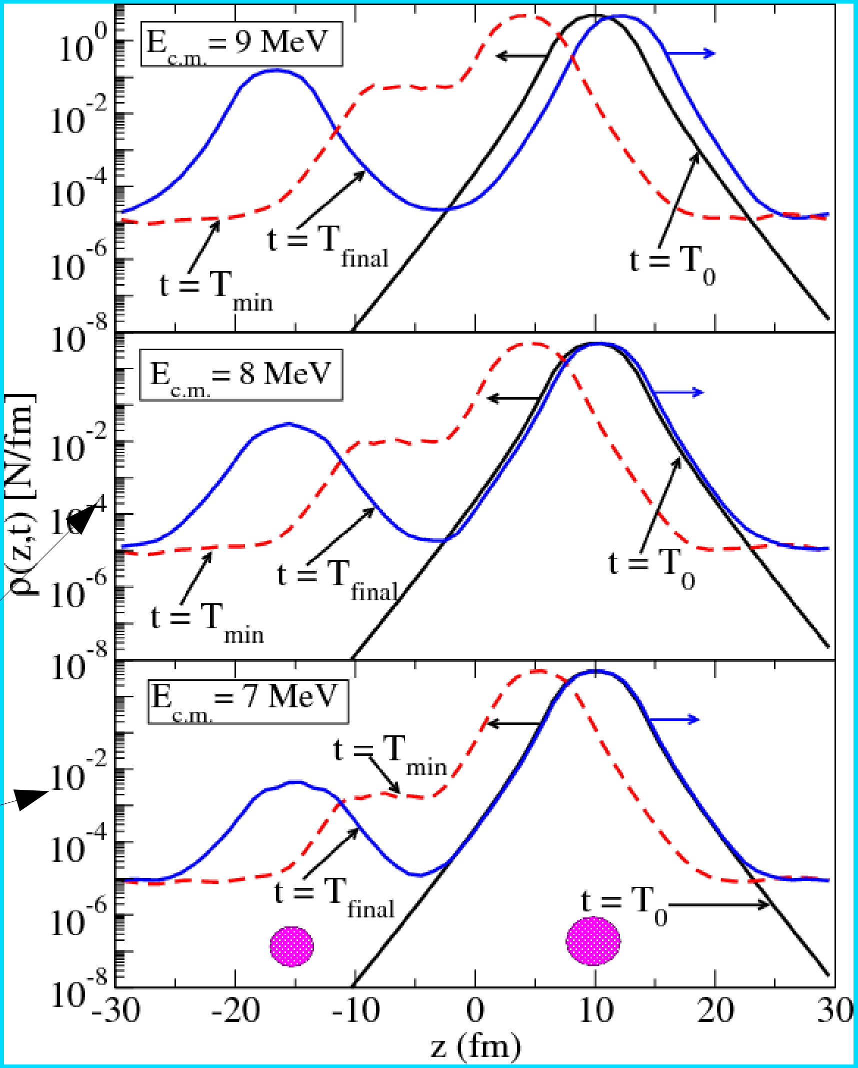
Closest approach →



Analyze Transfer at Single-Particle Level



^{24}O

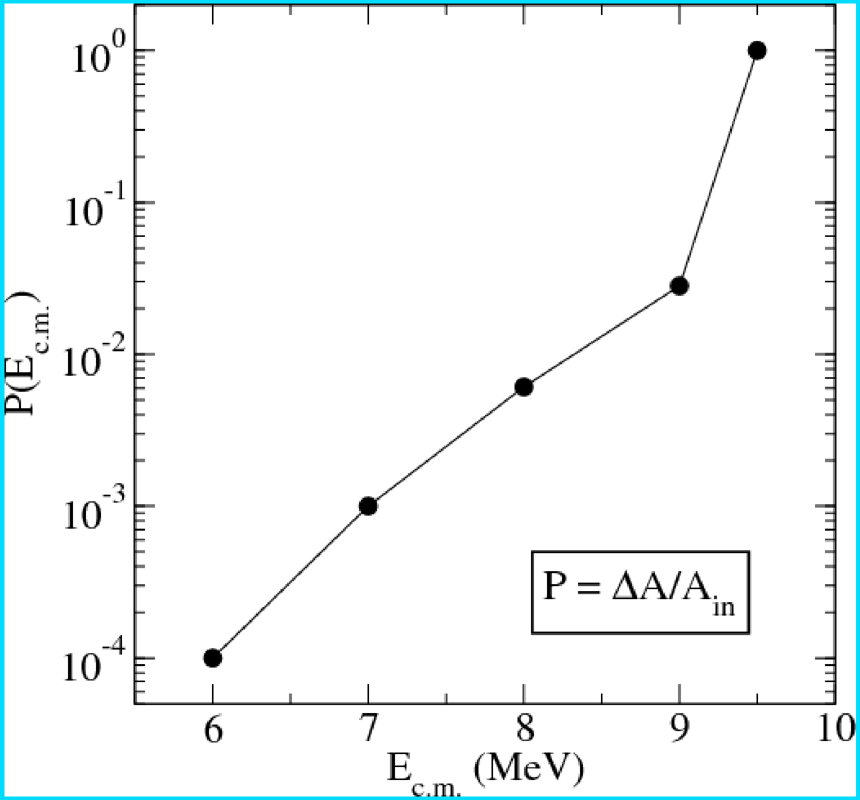


$$\rho(z,t)=\int dx \int dy\, \rho(x,y,z,t)$$

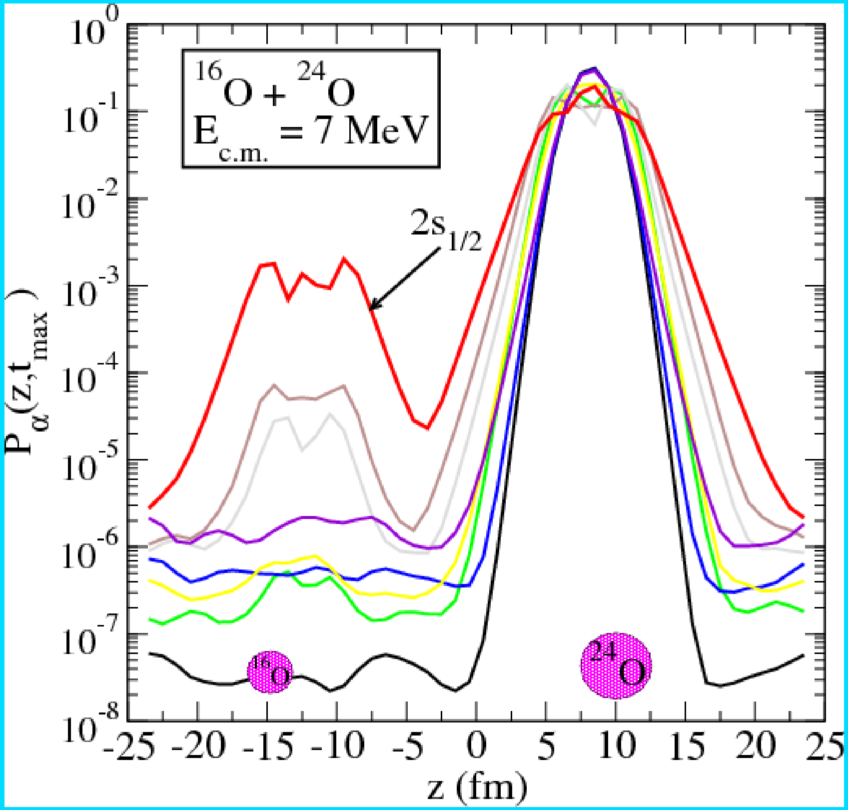
Below the barrier!

- Long after recoil we have non-zero neutron probability left at ^{16}O

Transfer Probability Below the Effective Barrier

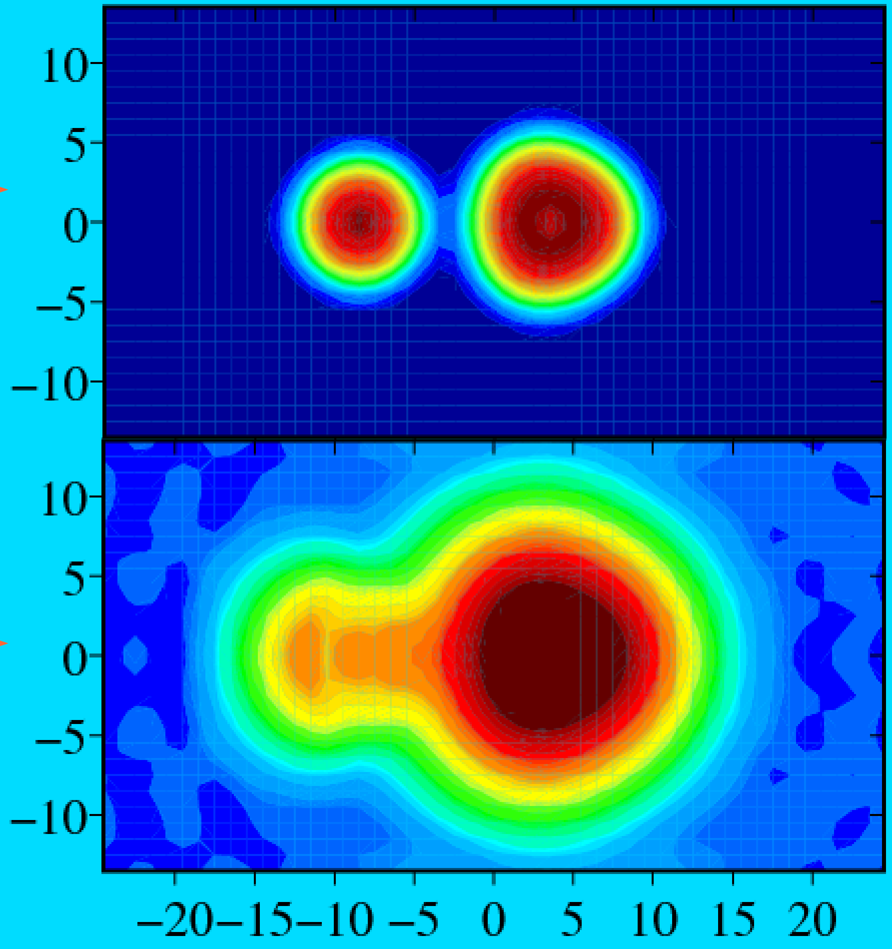


^{24}O



- In a many-body system different states will see different barriers TDHF can simulate some aspects of this physics

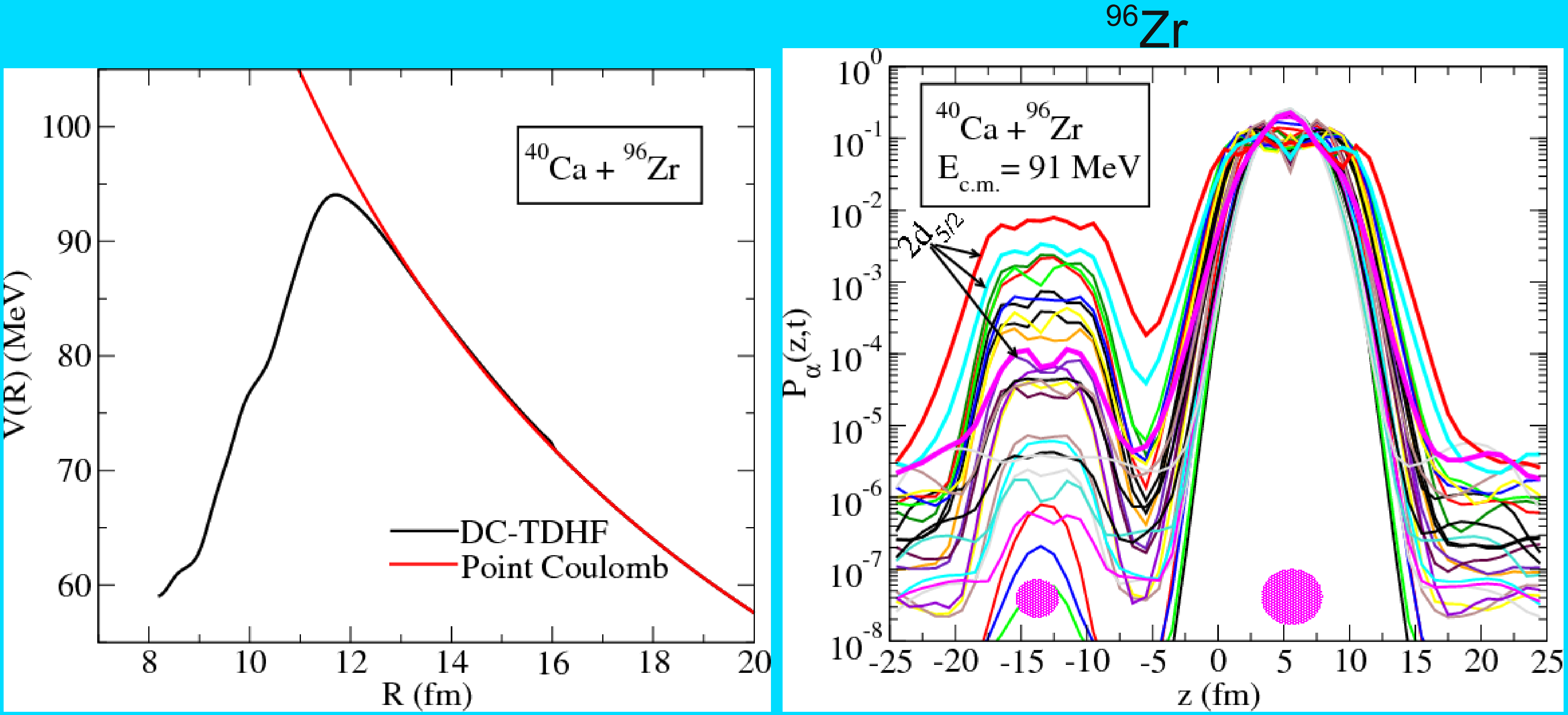
^{40}Ca+^{96}Zr System at E_{cm} = 91 MeV



Closest approach
(normal plot)

Closest approach
(log plot, only ^{96}Zr)

Transfer Probability Below the Effective Barrier



- Sub-states of $2d_{5/2}$ dominate the transfer
- Our results in agreement with quantum mechanical model:

  V. I. Zagrebaev, V. V. Samarin, and W. Greiner, *Phys. Rev. C* **75**, 035809 (2007)

Conclusions

- There is mounting evidence that TDHF dynamics give a good description of the early-stages of low-energy HI collisions
- We have developed powerful methods for extracting more information from the TDHF dynamical evolution (V(R), M(R), E*, etc.)
- Although heavy systems pose a greater challenge, such microscopic calculations may provide an insight into these collisions
- Effort needed to incorporate deformation and scattering information in to the Skyrme parametrization