Dynamics of Quasifission in TDHF Theory

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Collaborators:

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Erlangen:	P.-G. Reinhard		

Topics Covered:

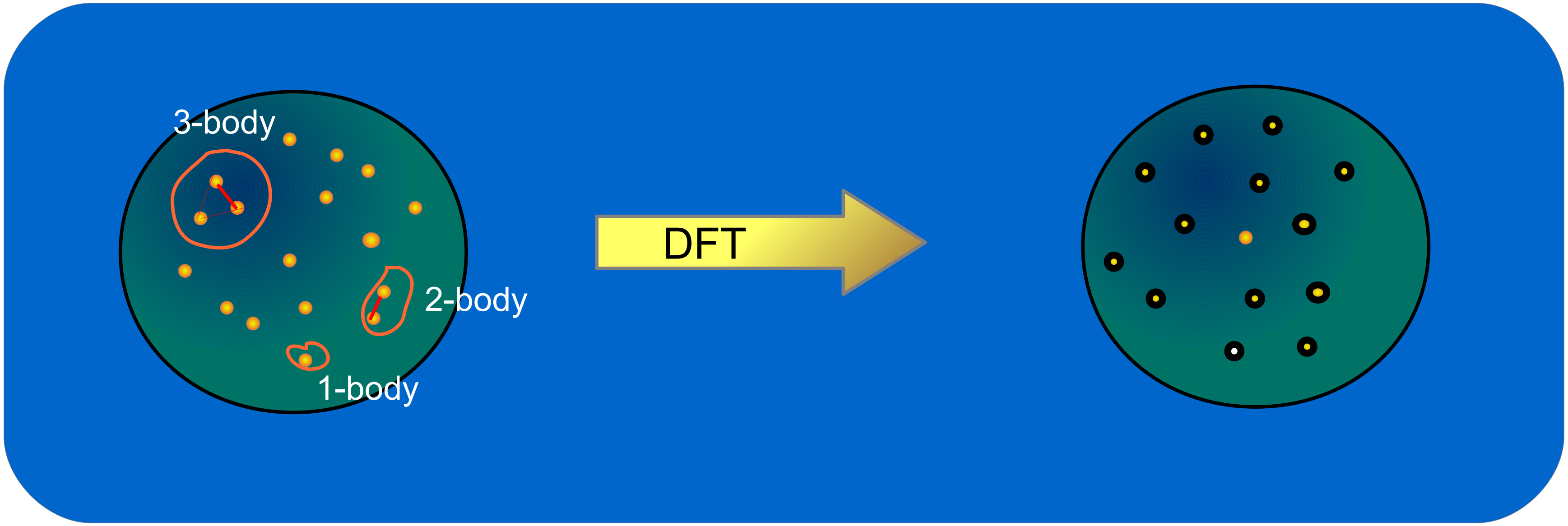
Time-dependent DFT theory (TDHF)
Capture (DC-TDHF)
Quasifission using TDHF

- $^{40,48}Ca + ^{238}U$
- $^{48}Ca + ^{249}Bk$ *(preliminary)*
- $^{50,54}Cr + ^{180,186}W$

Dynamical moment of inertia, E, T*
P_{CN} from TDHF
Dynamics of Fission (time permitting)

VANDERBILT UNIVERSITY Research supported by: U.S. Department of Energy, Division of Nuclear Physics

Nuclear Mean Field or Energy Density Functional (EDF)



ab-initio

$$\langle \Psi | H | \Psi \rangle = E$$

Mean-field - EDF

$$\Psi \rightarrow \Phi_{Slater}$$

$$H \rightarrow H_{eff}$$

$$E = \langle \Phi | H_{eff} | \Phi \rangle = \int d^3 r \ \{ H(\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu} \ ; \boldsymbol{r}) + H_{Coulomb}(\rho_p) \}$$

Single-(one-) particle density *etc.* in terms of s.p. states

$$\rho_q(\boldsymbol{r}) = \sum_{i=1}^{A} \sum_{\sigma} \varphi_i^*(\boldsymbol{r}, \sigma, q) \varphi_i(\boldsymbol{r}, \sigma, q)$$

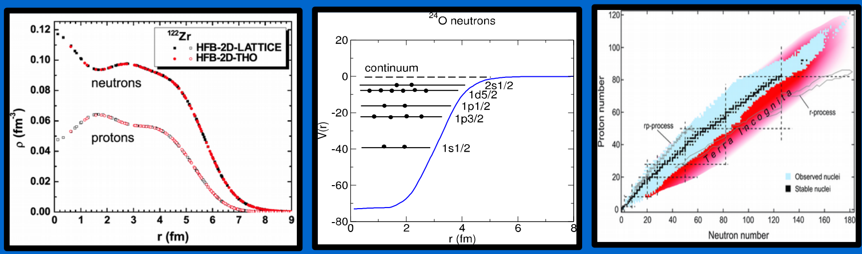
EDF in NP more complicated

$$v = v_{NN-eff} \rightarrow DFT(Hartee - Fock)$$

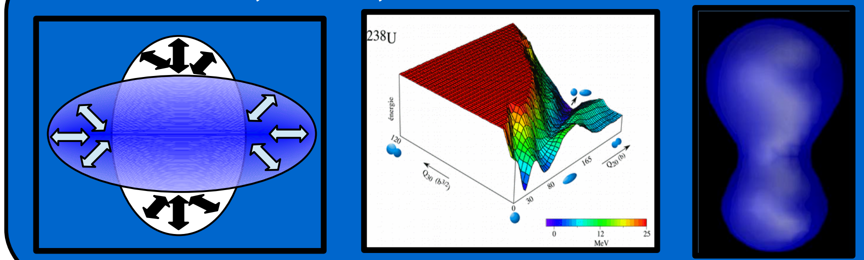
$$v \neq v_{NN-eff} \rightarrow DFT(Kohn - Sham)$$

Study Structure, Reactions, and Star Matter in Same Framework

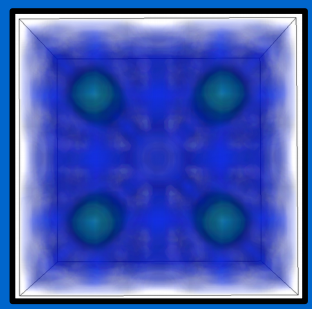
Structure



Oscillations, Fusion, Fission



Neutron Star Crust



- Time-dependent generalization TDHF or TDDFT (variational or Runge-Gross)

$$\delta S=\delta\int_{t_1}^{t_2} dt\,\langle\Phi(t)|H_{eff}-i\hbar\partial_t|\Phi(t)\rangle=0$$

$$i\frac{\partial}{\partial t}\varphi_\alpha=h(\rho,\tau,\boldsymbol{j},\boldsymbol{s},\boldsymbol{T},J_{\mu\nu}\;;\boldsymbol{r})\varphi_\alpha$$

self-consistent

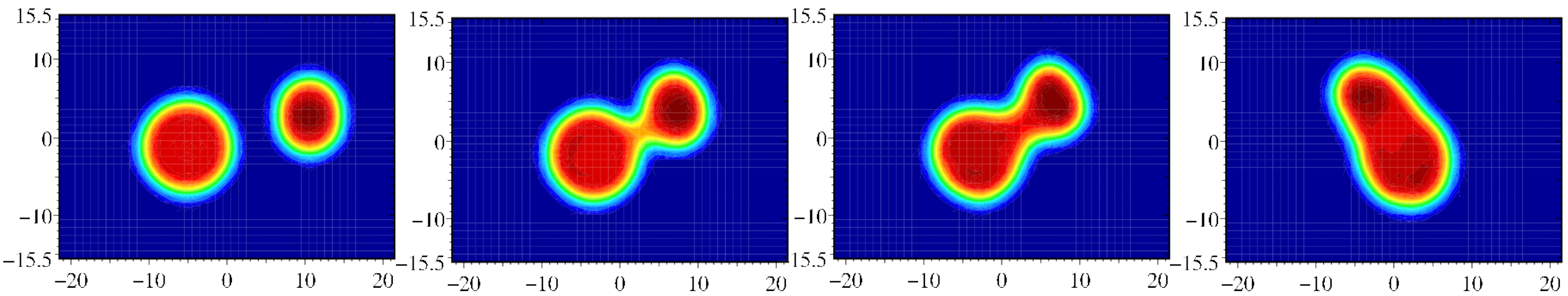
- TDHF gives the *most probable outcome* – best if *x*-section dominated by one process

Modern TDHF Codes

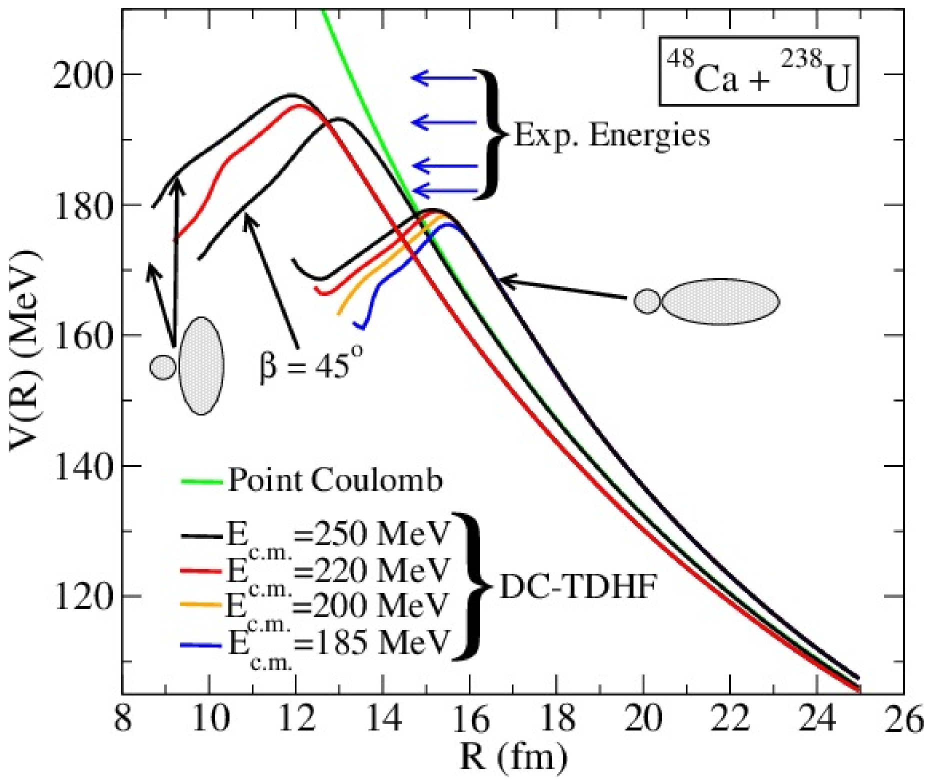
VU-TDHF Code

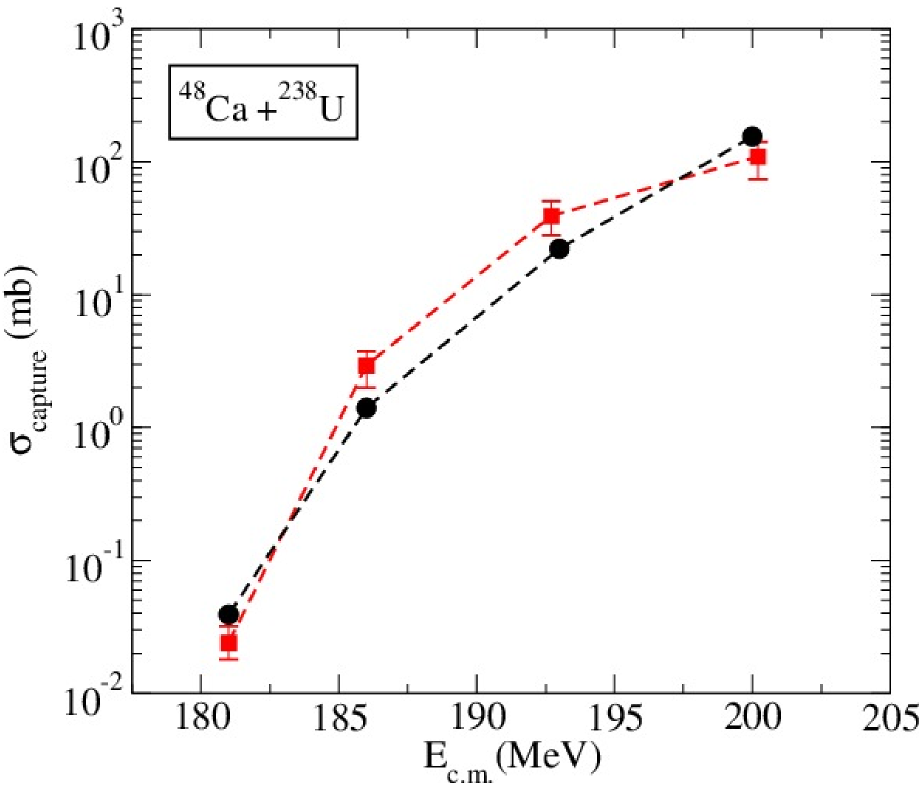
- Basis-Spline discretization for high accuracy
- 3-D Cartesian lattice – no geometrical simplification
- Complete EDF including all terms (time-even, full time-odd)
- Coded in Fortran-95 and OpenMP

1. Umar, Oberacker, VU-TDHF, Phys. Rev. C 73, 054607 (2006)
2. Maruhn, Reinhard, Stevenson, Umar, Sky3D, *Comp. Phys. Comm.* 85, 2195 (2014)



DC-TDHF Barriers – Capture





Experimental data:
1. M. G. Itkis et al., J. Nucl. Radiochem. Sci. 3, **57** (2002)
2. M. G. Itkis et al., Nucl. Phys. A **734** , 136 (2004)

Angle average ^{238}U alignment

- x-section falls rapidly for β>10°
- sin(β) multiply small angles
- P(β) is in the range 0.4-0.6

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

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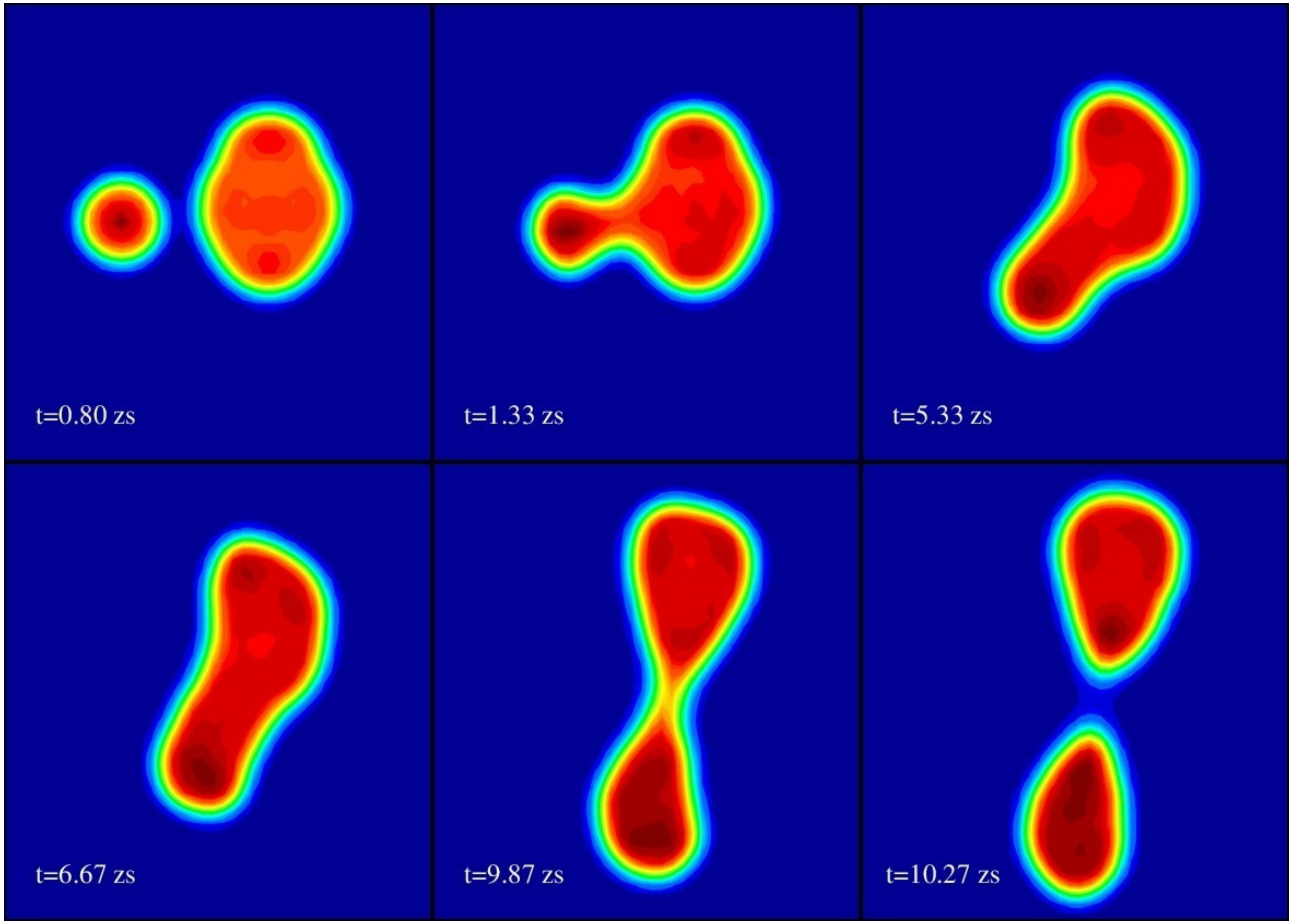
A.S. Umar, V.E. Oberacker, J.A. Maruhn, and P.-G. Reinhard, **PRC** 81, 064607 (2010).

Quasifission in TDHF – $^{40,48}Ca + ^{238}U$

Heavy Systems

$$\sigma_{capture} = \sigma_{QF} + \sigma_{fusion-fission} + \sigma_{ER}$$

- QF dominant part
- Important for studying SHE dynamics



Final masses:
$A_L = 101$, $A_R = 177$
$Z_L = 41$, $Z_R = 71$

$E_{cm} = 209$ MeV
b=1.103fm (L=20)

$^{40}Ca + ^{238}U$

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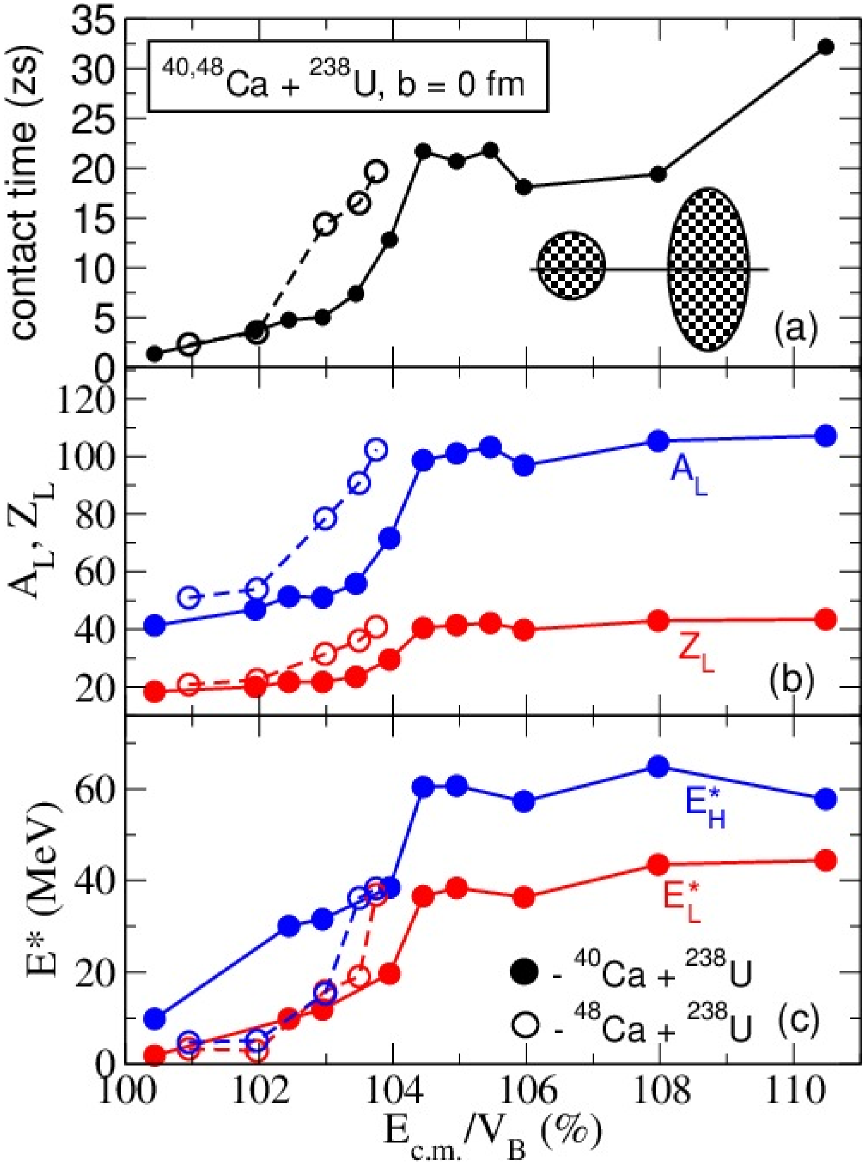
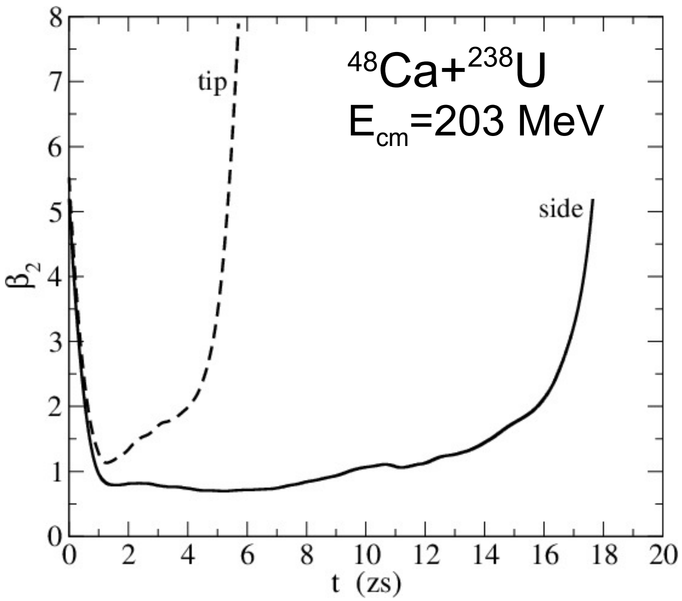
V.E. Oberacker, A.S. Umar, C. Simenel, **PRC** 90, 054605 (2014).

Quasifission – $^{40,48}Ca+^{238}U$

- Compare $^{40,48}Ca+^{238}U$ (b=0)
- **fusion** implies contact-time > 35 zs
  (plus density shows no indication of QF)
- $^{40}Ca+^{238}U$ wider energy range for QF
- E* sharing seems different
  (calculated dynamically using DC-TDHF)



Each point takes about a <u>week</u> on a 16 processor workstation

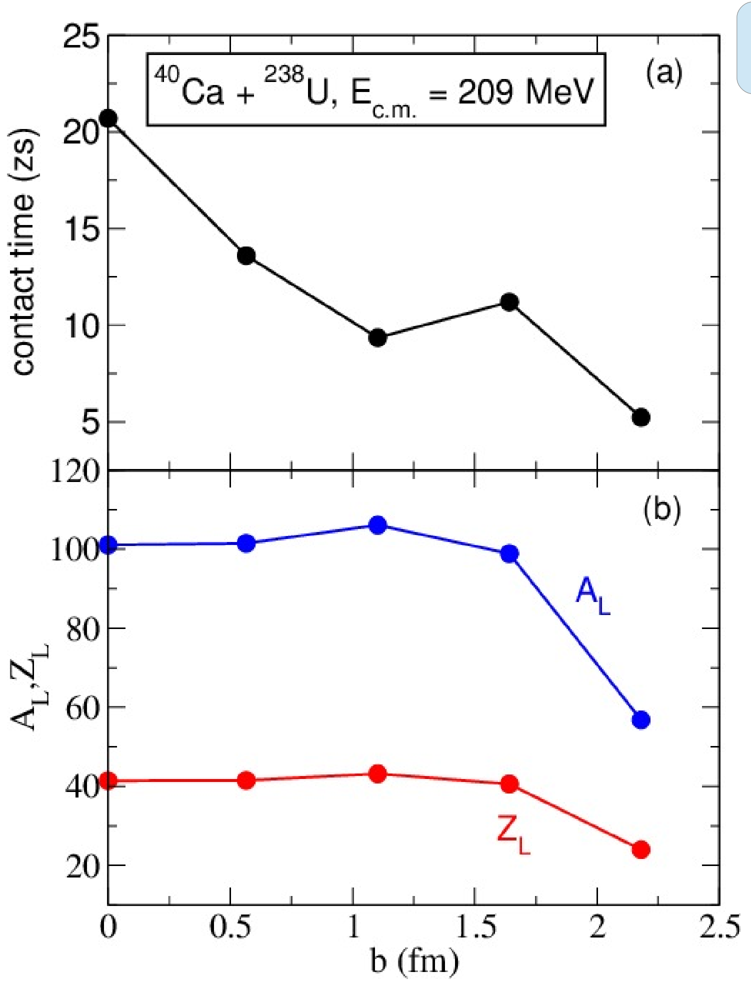


$$\beta_2 = \frac{4\pi}{3}\frac{Q_{20}}{AR_0^2}$$

The β=0° orientation of ^{238}U results in much smaller contact-times and mass transfer

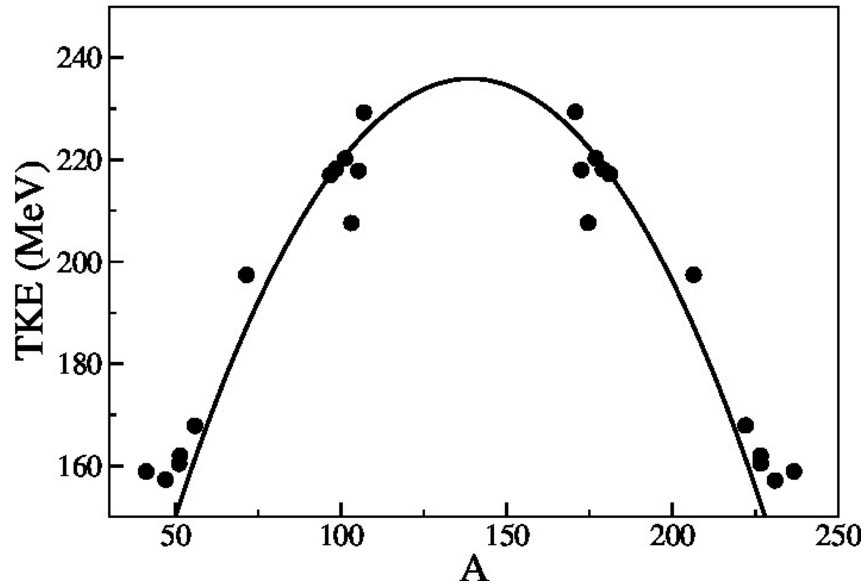
V.E. Oberacker, A.S. Umar, C. Simenel, **PRC** 90, 054605 (2014).

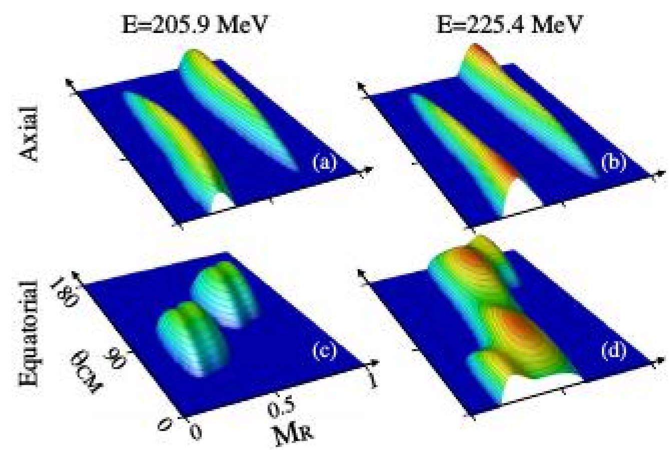
Impact Parameter Dependence – Viola Systematics



Narrow range of impact parameters at low energies

Final fragment TKE's well described by Viola systematics



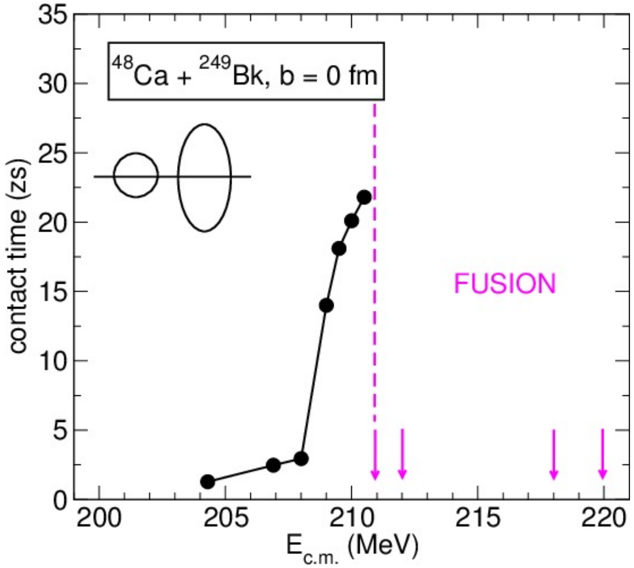


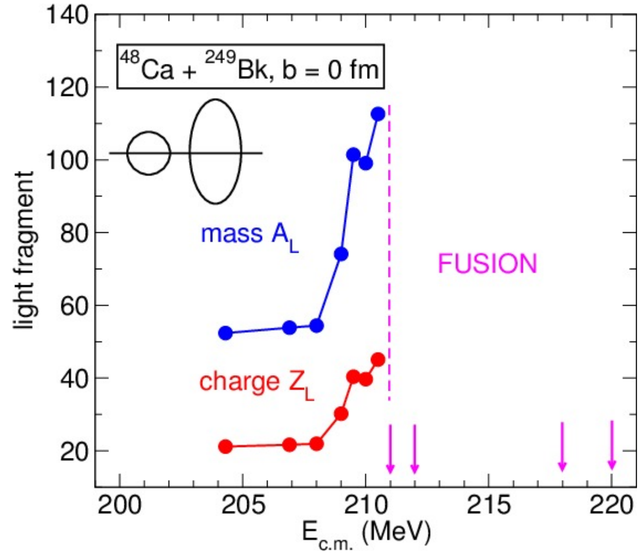
^{40}Ca + ^{238}U

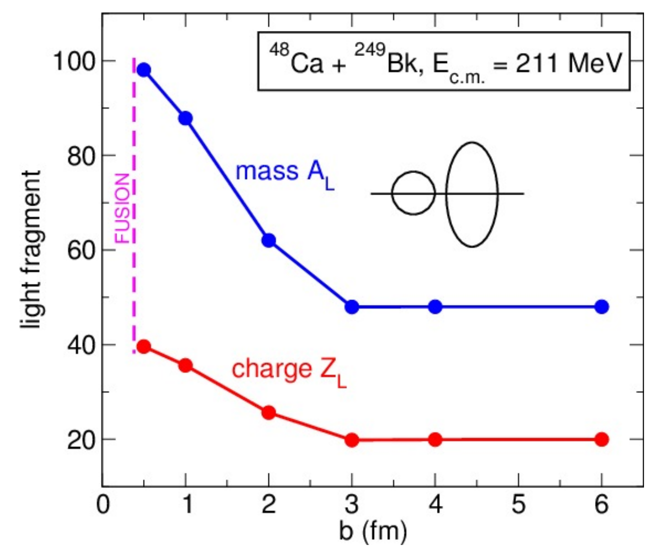
Wakhle et al., **PRL** 113, 182502 (2014).

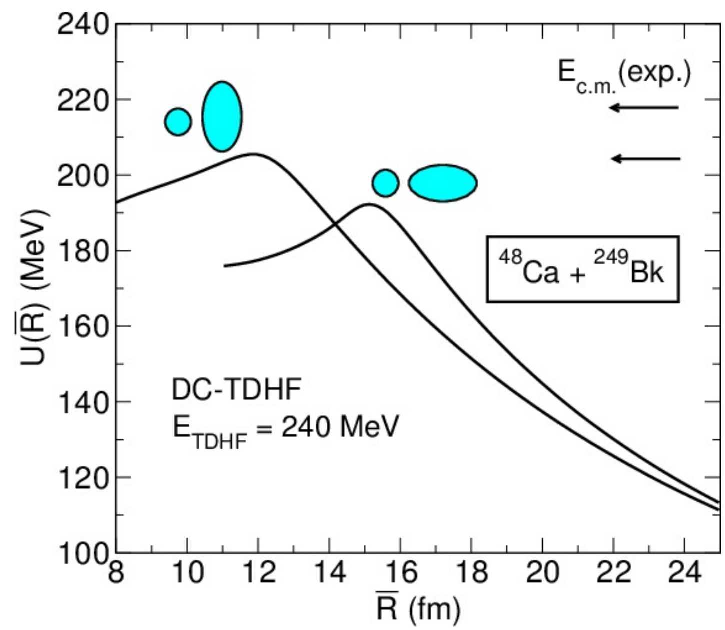
V.E. Oberacker, A.S. Umar, C. Simenel, **PRC** 90, 054605 (2014).

Quasifission in ^{48}Ca+^{249}Bk (ongoing-preliminary)



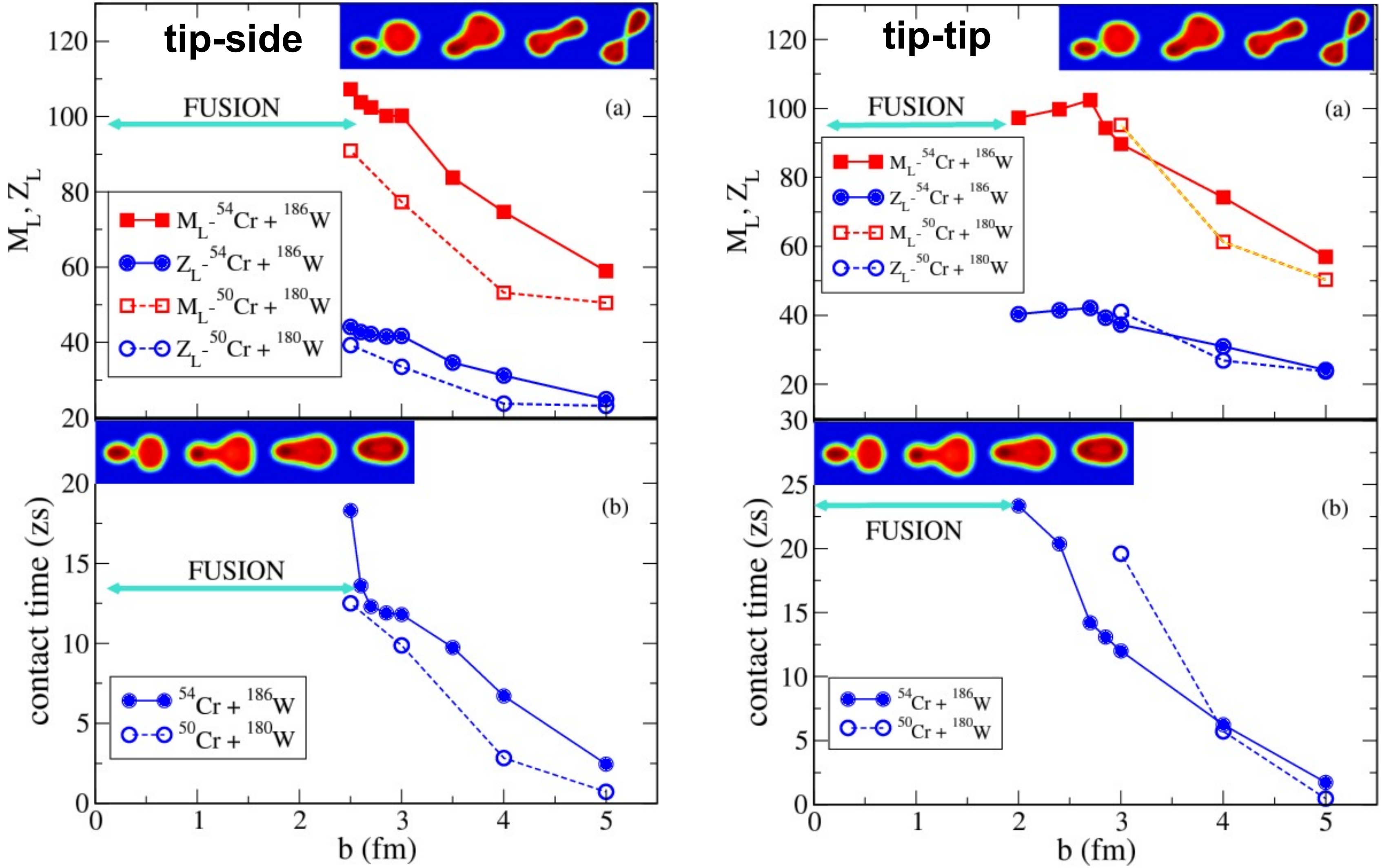






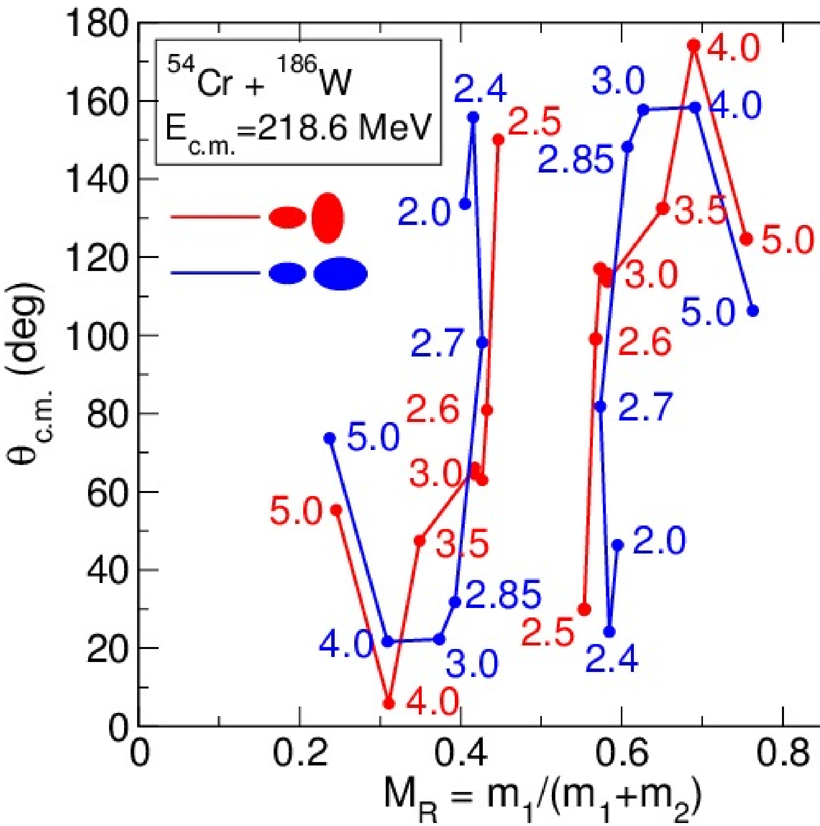
Quasifission in $^{50,54}Cr+^{180,186}W$ ($E_{c.m.}/V_B$=1.13)

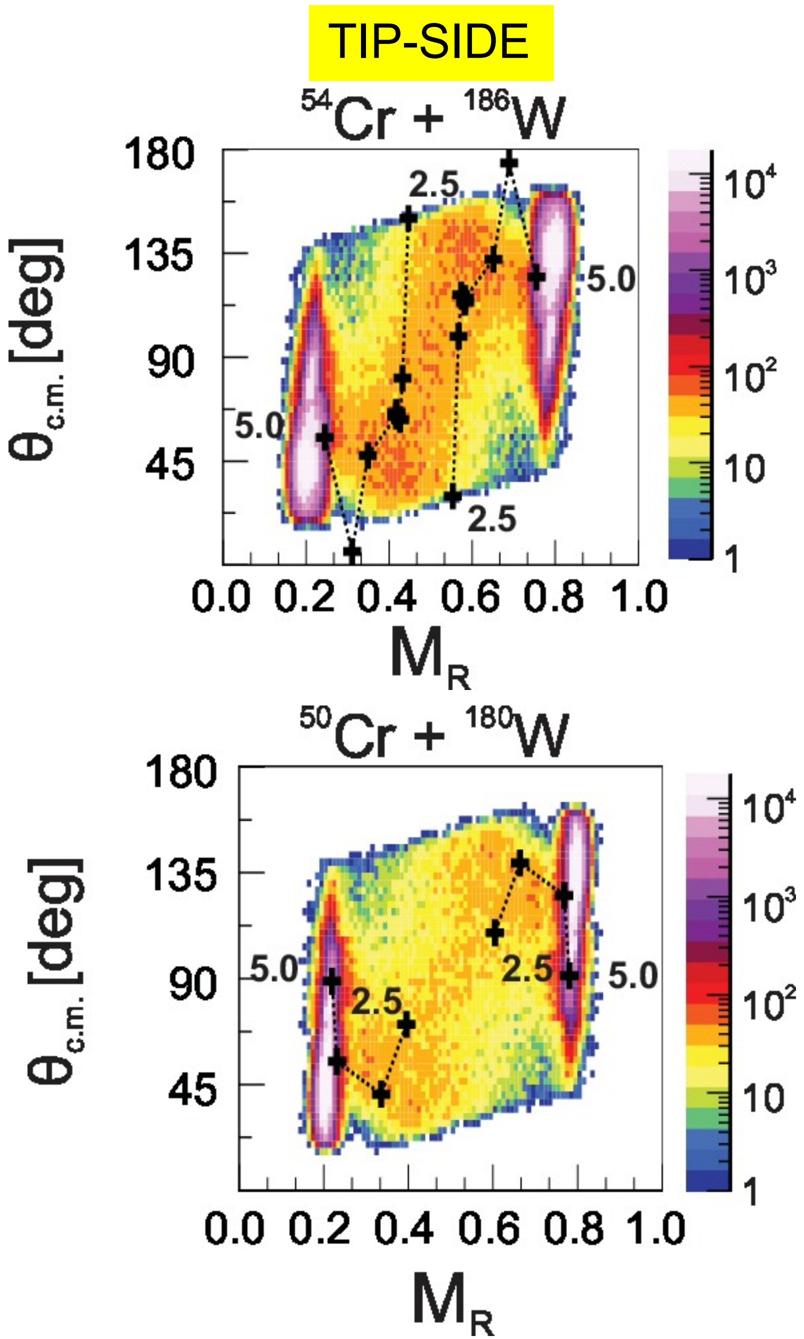
Two deformed nuclei with smaller mass/charge asymmetry than Ca+U



K. Hammerton, Z. Kohley, D. J. Hinde, M. Dasgupta, A. Wakhle, E. Williams,V. E. Oberacker, A. S. Umar, I. P. Carter, K. J. Cook, J. Greene, D. Y. Jeung, D. H. Luong, S. D. McNeil, C. S. Palshetkar, D. C. Rafferty, C. Simenel, and K. Stiefel, PRC 91, 041601(R) (2015)

Mass Angle Distributions (MAD's)





Fission Fragment Angular Distributions - P_{CN}

- Angular distribution based on TSM (see Yanez *et al.* PRC 88, 014606 (2013))

$$W(\theta) = \sum_{J=0}^{J_{CN}} \frac{(2J+1)^2 exp[-(J+1/2)^2 sin^2\theta/4K_0^2(FF)] J_0[i(J+1/2)^2 sin^2\theta/4K_0^2(FF)]}{erf[(J+1/2)/(2K_0^2(FF))^{1/2}]}$$
$$+ \sum_{J=J_{CN}}^{J_{\max}} \frac{(2J+1)^2 exp[-(J+1/2)^2 sin^2\theta/4K_0^2(QF)] J_0[i(J+1/2)^2 sin^2\theta/4K_0^2(QF)]}{erf[(J+1/2)/(2K_0^2(QF))^{1/2}]}$$

QF angular distribution

$$P_{CN} \approx \frac{\sigma_{FF}}{\sigma_{QF} + \sigma_{FF}}$$

- Parameter K_0 involves shape and temperature

$$K_0^2 = T\Im_{eff}/\hbar^2$$

- Need parallel/perpendicular moment of inertia

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\parallel}} - \frac{1}{\Im_{\perp}}$$

- Assumption!

$$\Im_0/\Im_{eff} = 1.5$$

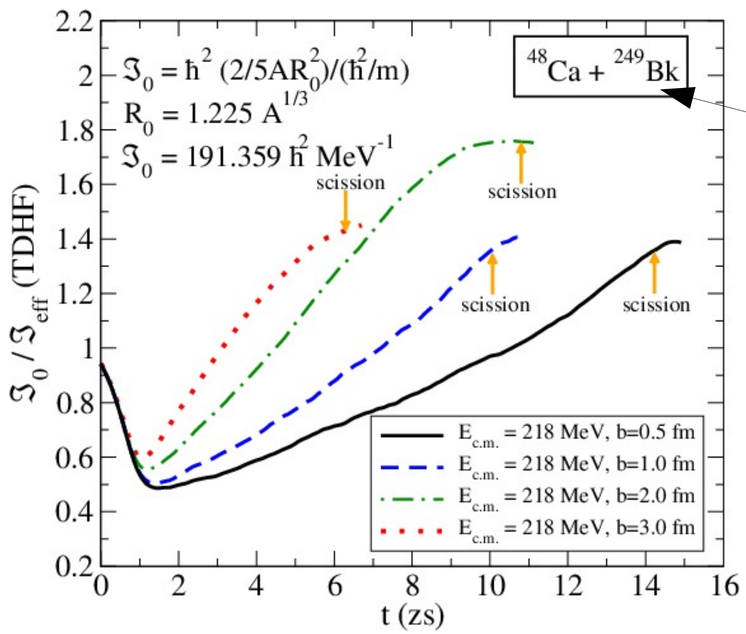
- Temperature at the saddle point ?

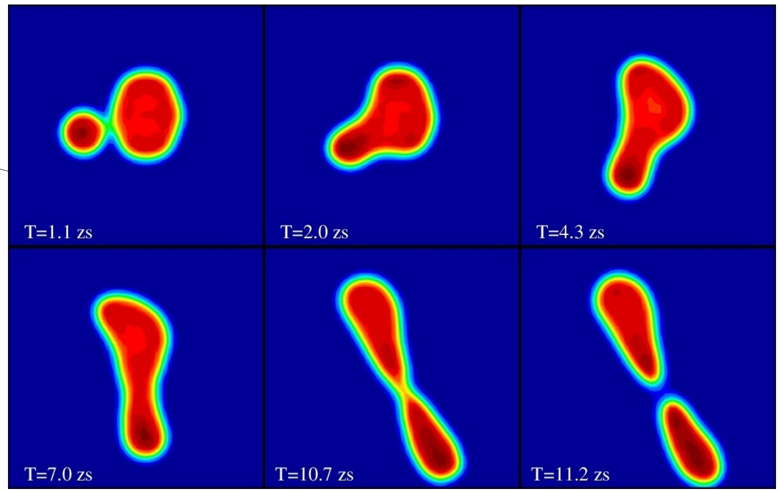
$$\mathcal{T} = \left[\frac{E^* - B_f - E_{rot} - E_\nu}{A/8.5}\right]^{1/2}$$

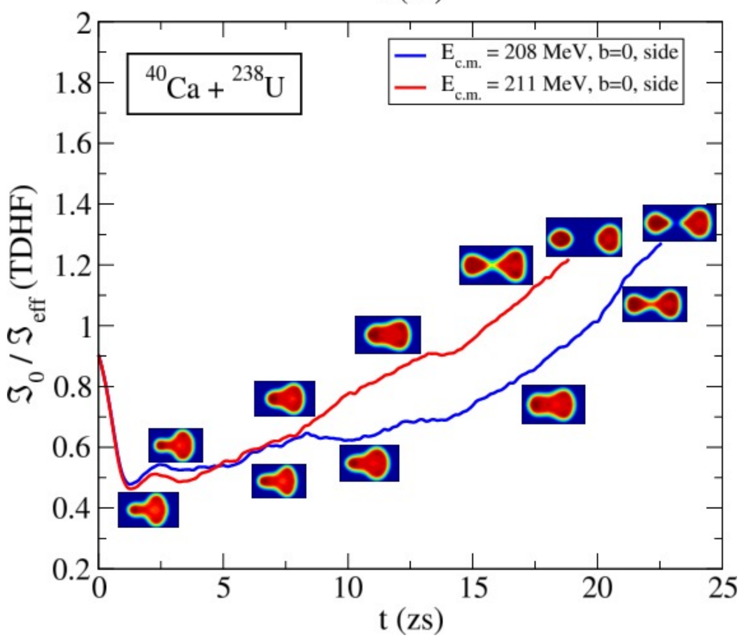
- Can obtain from dynamical E* using DC-TDHF

$$\mathcal{T} = \left[\frac{E^*_{TDHF}}{A/8.5}\right]^{1/2}$$

Moment of Inertia from TDHF







- Diagonalize the moment of inertia tensor

$$\Im_{ij}/m = \int d^3r\ \rho_{TDHF}(\mathbf{r},t)(r^2\delta_{ij} - x_i x_j)$$

- Eigenvalues give the parallel/perpendicular moment of inertia

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\parallel}} - \frac{1}{\Im_{\perp}}$$

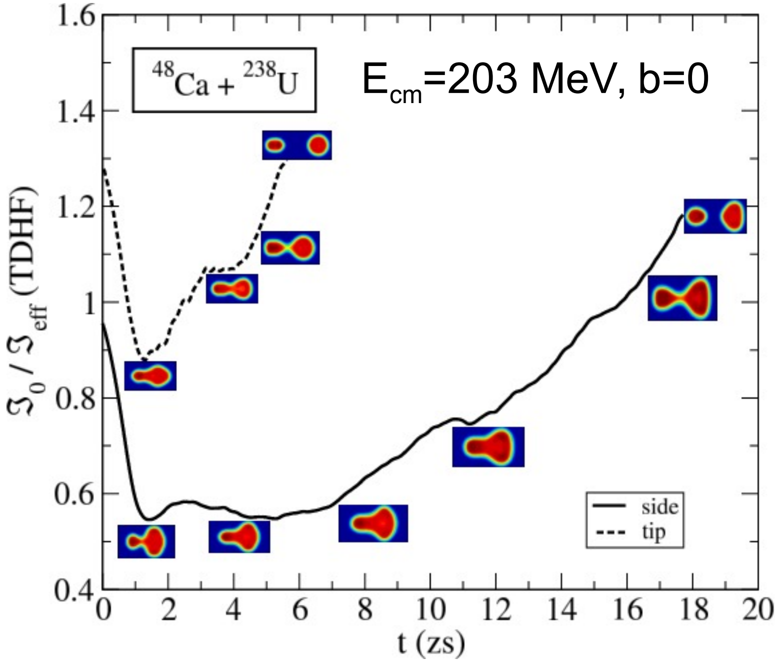
- Ratio $\Im_0/\Im_{eff}$

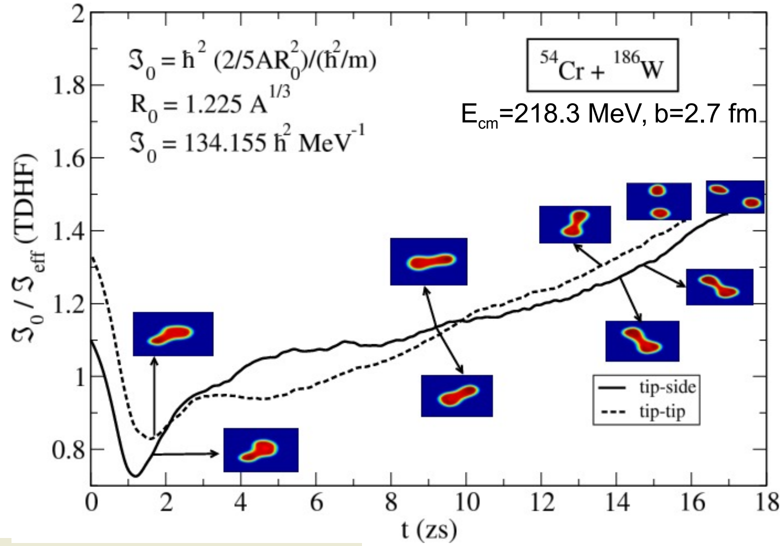
$$\Im_0 = \hbar^2(2/5AR_0^2)/(\hbar^2/m)$$

Equivalent sphere

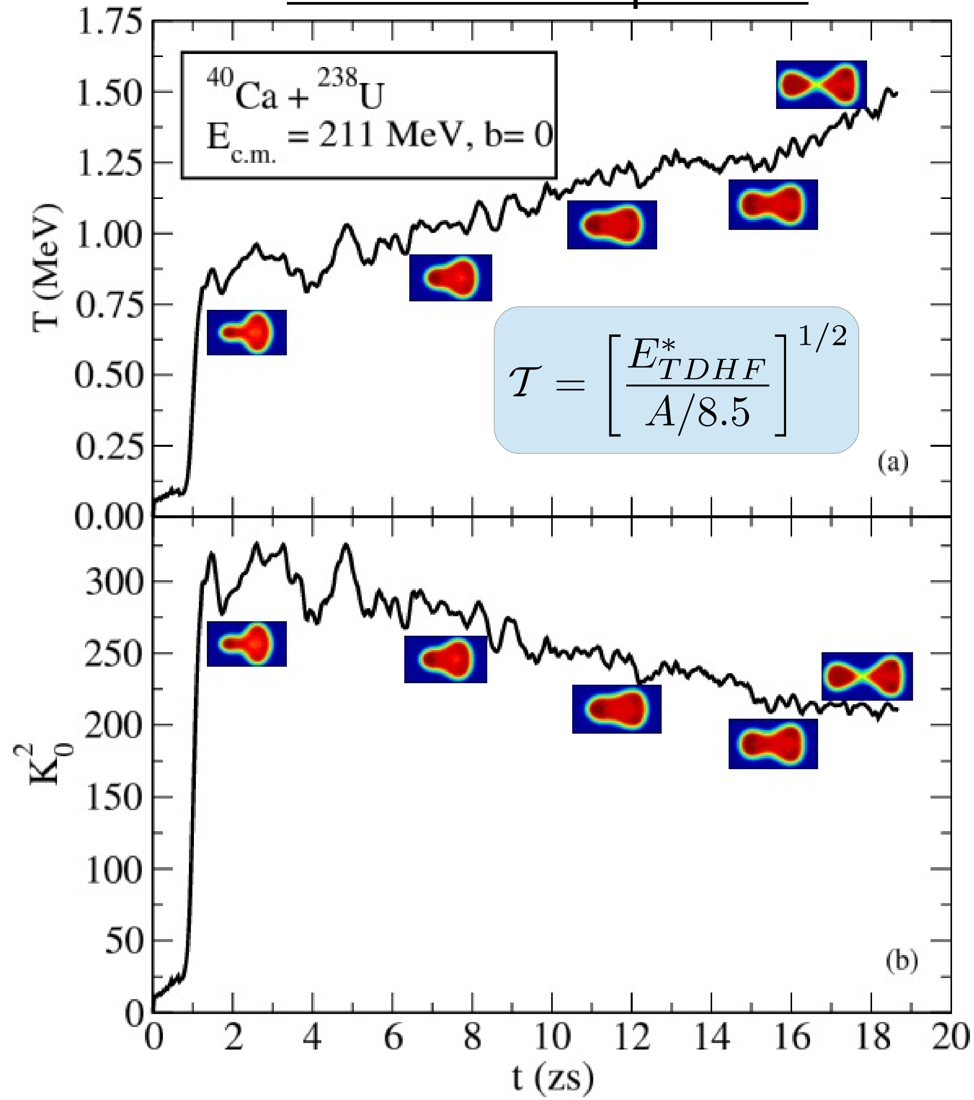
Moment of Inertia Cont'd

Dependence on alignment



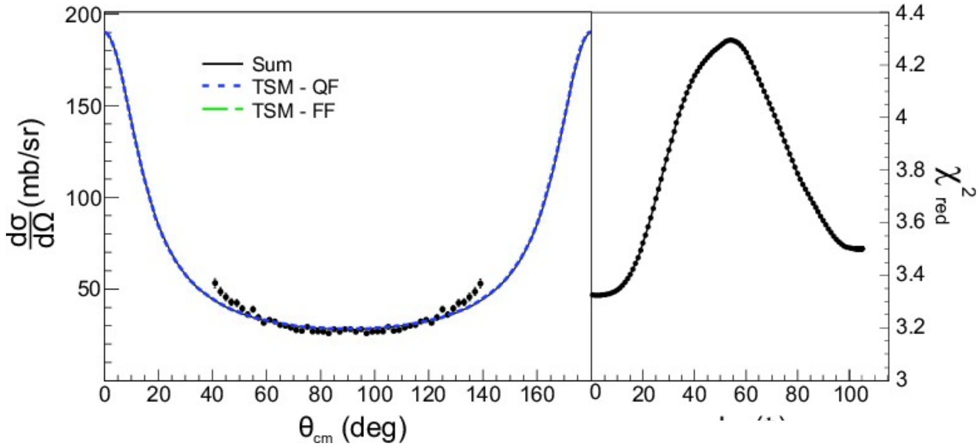


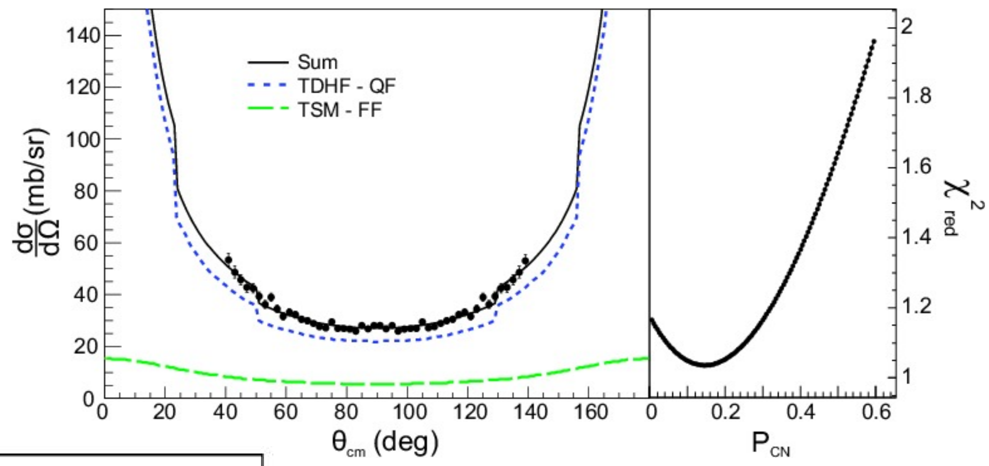
Evolution of temperature

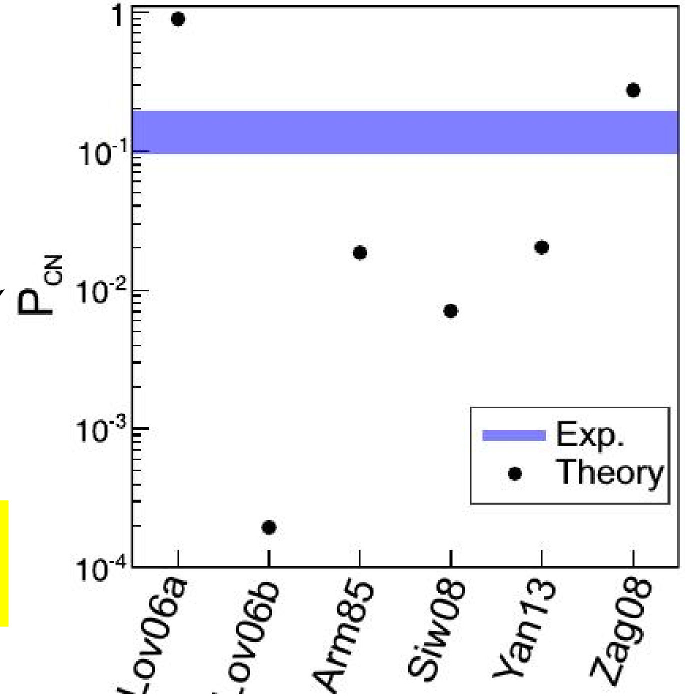


2 months of computing time!
Don't need full time-dependence in practice

P_{CN} from TDHF Angular Distributions $^{54}Cr+^{186}W$





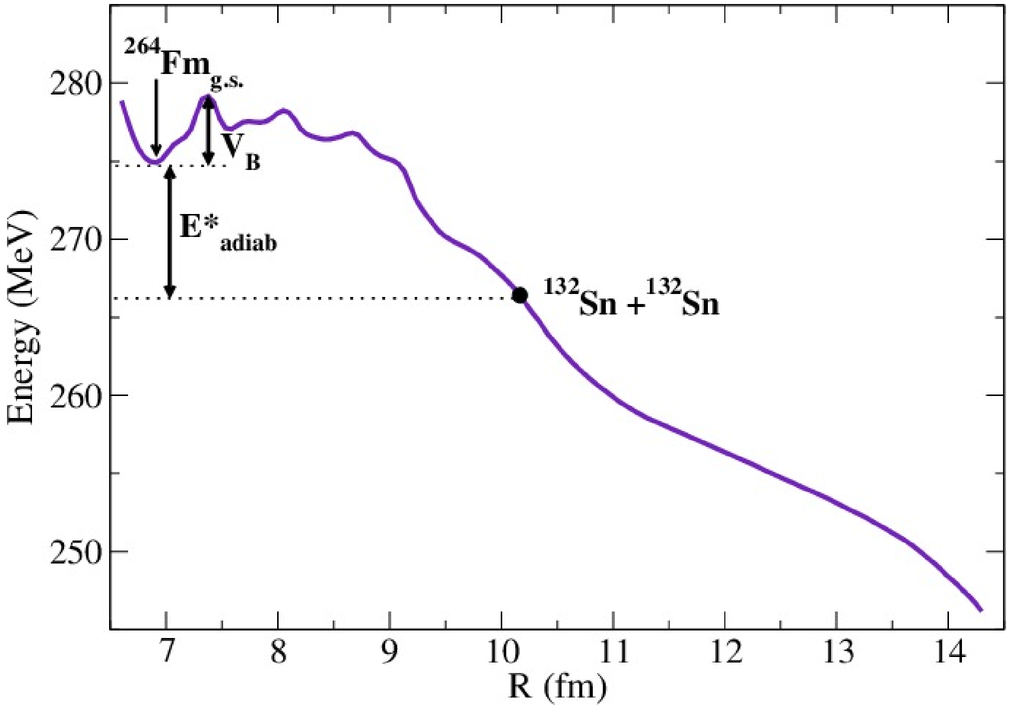


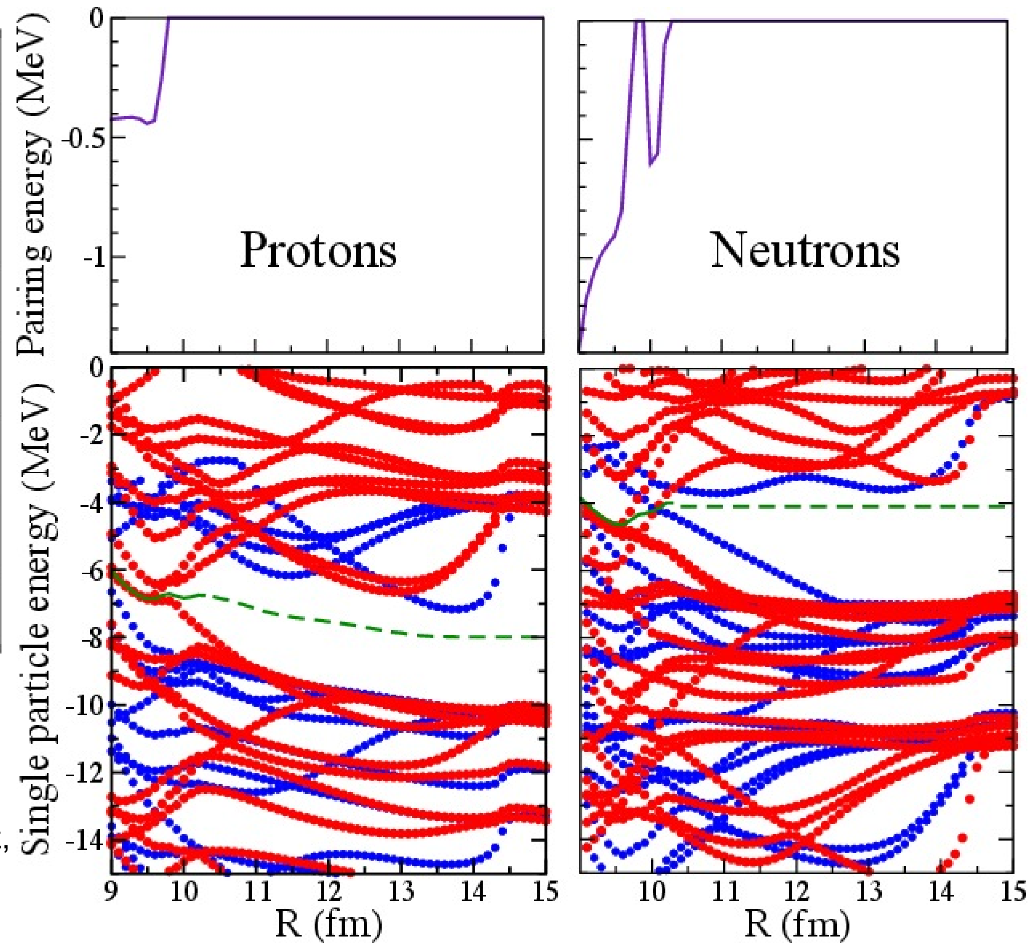
Comparison with different models

Z. Kohley, private communication

Scission Dynamics Using TDHF – Fragment Pre-Formation

- Transition from adiabatic motion to non-adiabatic motion of scission
- Follow the single-particle states as a function of deformation, look for the last level crossing.



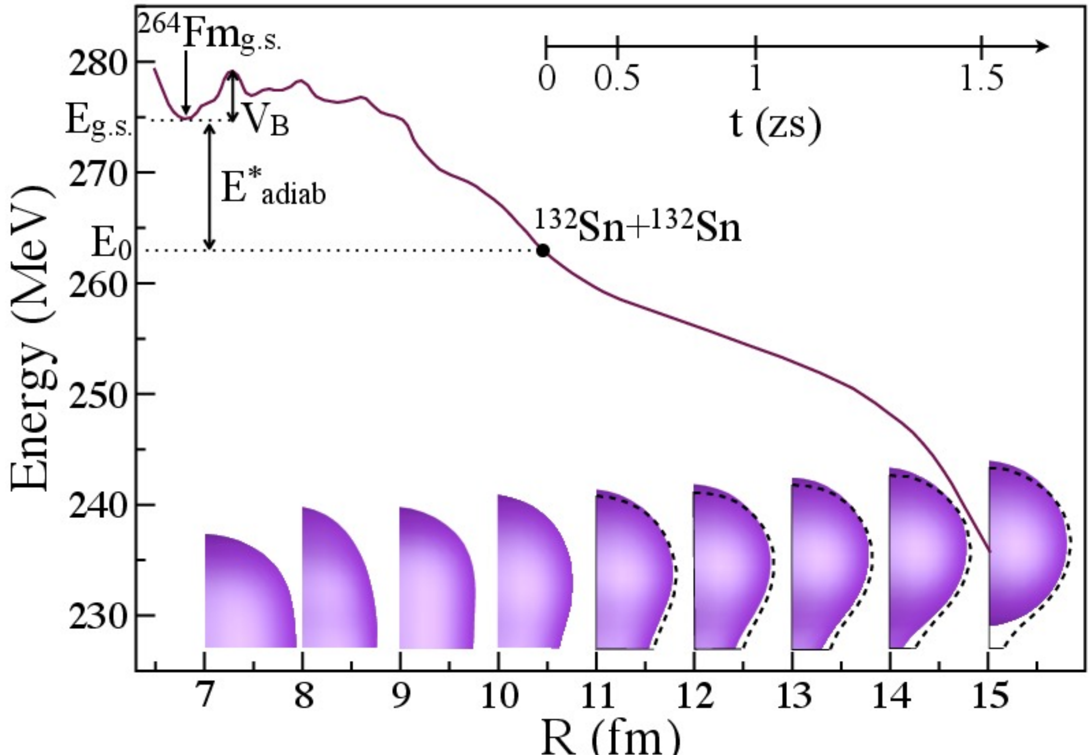


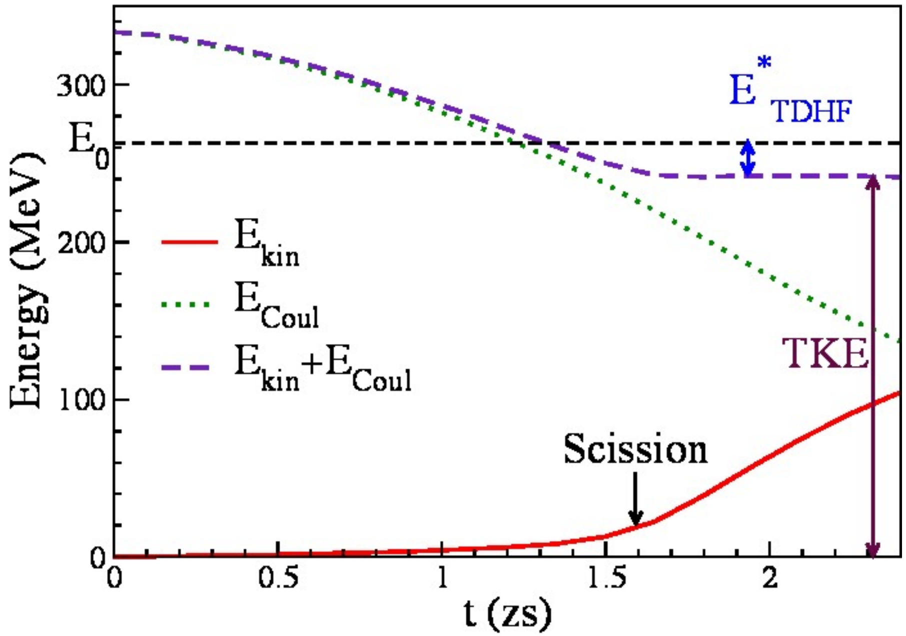
C. Simenel and A.S. Umar, **PRC** 89 (R), 031601 (2014)

J. Sadhukhan, K. Mazurek, A. Baran, J. Dobaczewski, W. Nazarewicz, and J. A. Sheikh, **PRC** 88, 064314 (2013).

Scission Dynamics Using TDHF - Dynamics

- Start TDHF evolution at the point of fragment formation
- Compare results to adiabatic scission, can calculate TKE, E* etc.





- Asymptotic TKE is around 241 MeV
- Adiabatic E* is about 12 MeV
- Dynamic TDHF E* is about 22 MeV leading to a total of 34 MeV excitation
- Also done 258Fm, TKE is 238-241 MeV (exp. Value 235 MeV).

(exp: E.K. Hulet et al. **PRL** 56, 313 (1986))

Summary

TDDFT have a strong place among the theories needed for future challenges of low-energy nuclear physics

Numerical issues are resolved – limitations only due to theoretical approximations (effective interactions, mean-field theory, etc.)

Quasifission and deep-inelastic reactions are well suited for TDDFT

We may be able to calculate P_{CN} directly from TDHF without MAD's!

$$P_{CN} \approx \frac{\sigma_{Capture} - \sigma_{QF}}{\sigma_{Capture}}$$

We now have a reasonable handle on above- and sub-barrier fusion employing the DC-TDHF approach

One major and difficult area that needs attention is the dynamics of fission