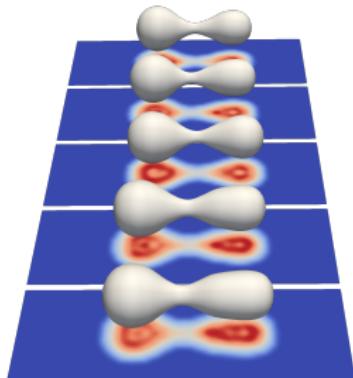


ECT*

"Spontaneous and induced fission of very heavy and super-heavy nuclei"



Dynamical effects of superfluidity on fusion and fission

Guillaume SCAMPS

Tsukuba University

March 9-13, 2018



Collaboration : Y. Hashimoto, T. Nakatsukasa,
C. Simenel, D. Lacroix

Mean-field theory with pairing

TDHF

- Independent particle
- Initialisation : $\hat{h}_{MF} |\phi_i\rangle = \epsilon_i |\phi_i\rangle$
- Evolution :
 $i\hbar \frac{d\rho}{dt} = [h_{MF}, \rho]$

TDHFB

- Pairing correlation
- Quasi-particles : $|\omega_\alpha\rangle = \begin{pmatrix} u_\alpha \\ v_\alpha \end{pmatrix}$
- Evolution :
 $i\hbar \frac{d|\omega_\alpha\rangle}{dt} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} |\omega_\alpha\rangle$

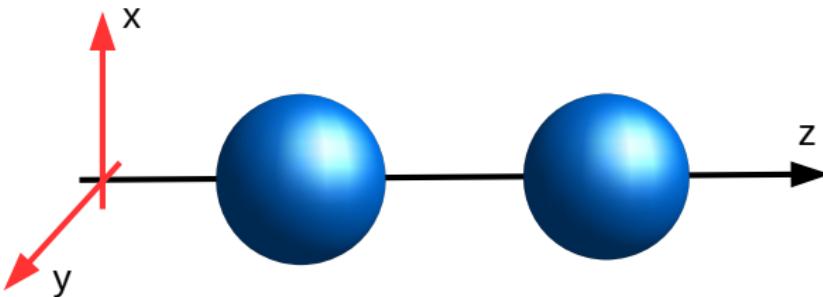
TDHF+BCS

- Based on TDHFB with the approximation : $\Delta_{ij} = \delta_{ij}\Delta_i$
- Evolution :
 $i\hbar \frac{d\phi_i}{dt} = (\hat{h}_{MF} - \epsilon_i)\phi_i$
 $i\hbar \frac{dn_i}{dt} = \Delta_i^* \kappa_i - \Delta_i \kappa_i^*$
 $i\hbar \frac{d\kappa_i}{dt} = \kappa_i(\epsilon_i - \epsilon_{\bar{i}}) + \Delta_i(2n_i - 1)$

Fusion

Y. Hashimoto, G. Scamps, PRC **94**, 014610 (2016).
G. Scamps, arXiv :1801.01250 (2017).

TDHFB with Gogny D1S interaction



- x and y direction : Harmonic oscillator basis $n_x + n_y \leq 4$
- z direction : Lagrange mesh
 $n_z = 46$
- $N_{\text{base}} = 2760$
- full cartesian mesh about 100 000 degrees of freedom

Cost of the calculation : one collision done in one day with 20 CPUs

Y. Hashimoto, G. Scamps, Phys. Rev. C 94, 014610 (2016)



Multidisciplinary Cooperative Research

筑波大学計算科学研究センター 学際共同利用

COMA (PACS-IX) System

Computation node	CPU	Intel E5-2670v2 (Ivy Bridge-EP) 2.5GHz x2
	# of cores	20 (10 cores / CPU)
	MIC	Intel Xeon Phi 7110P 61 core x2
	Main memory	64 GB (DDR3 1866MHz x 8 channel, 119.4GB/s)
	MIC memory	16 GB (8GB/MIC, 352GB/s/MIC)
	Peak performance	400 GFLOPS (CPU) + 2147 GFLOPS (MIC)
	Network HCA	InfiniBand FDR
	Peak network b/w	7 GB/s
Number of nodes	393	
Interconnection configuration	Fat-Tree with full bisection b/w	
Peak performance	1.001 PFLOPS (CPU: 157 TFLOPS, MIC:844 TFLOPS)	
Network bisection b/w	2.75 TB/s	
Shared file system	Lustre file system	
File system capacity	1.5 PB (user space)	

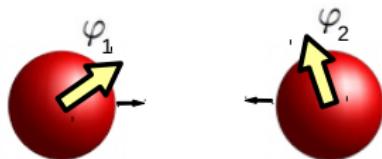


共同利用・共同研究拠点

「先端学際計算科学共同研究拠点」(文部科学省)

Advanced Interdisciplinary Computational Science Collaboration Initiative (the MEXT of Japan)

Effect of the relative gauge angle in reactions between superfluid heavy nuclei



Main questions :

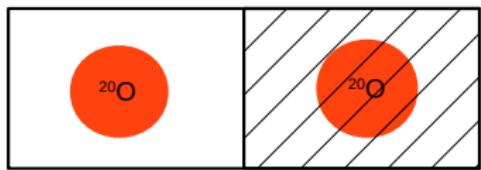
- What are the effects predicted by TDHFB ?
- How to interpret the gauge angle in small systems ?
- How can we restore the symmetry of the gauge angle ?
- Can we find experimental evidence ?

Ideal test case : Reaction of superfluid nuclei

Gauge angle dependence of the fusion reaction

In collision between two superfluid nuclei, the relative gauge angle have a strong influence

$^{20}\text{O} + ^{20}\text{O}$

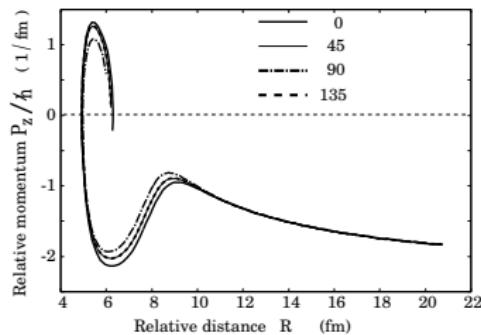


at $t=0$

$$U \rightarrow e^{i\varphi} U \theta(z)$$

$$V \rightarrow e^{-i\varphi} V \theta(z)$$

Results :

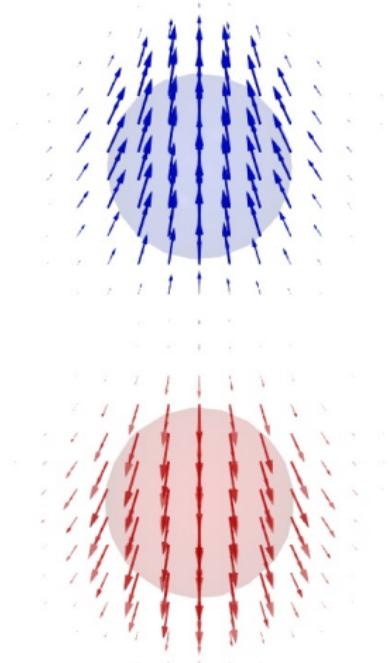


$E_{\text{cm}} = 11.41 \text{ MeV}$

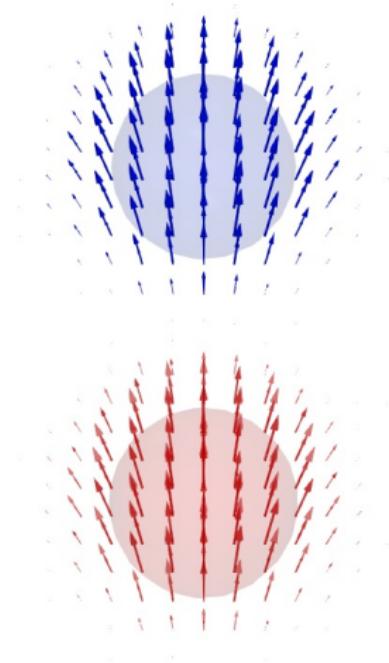
Y. Hashimoto, G. Scamps, Phys. Rev. C 94, 014610 (2016).

Effect of gauge angle on trajectories

Evolution of two TDHFB calculation at the vicinity of the barrier



$$\kappa(r, \uparrow, r, \downarrow) = |\kappa(r, \uparrow, r, \downarrow)| e^{2i\varphi}$$



Effect of gauge angle on trajectories

Evolution of two TDHFB calculation at the vicinity of the barrier

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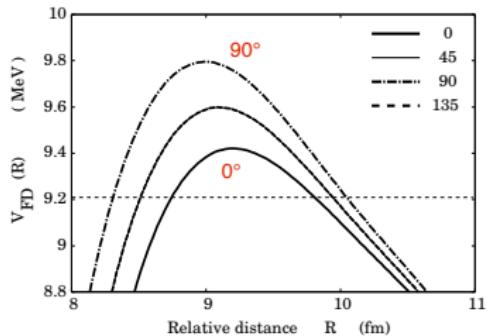
Effect of gauge angle on trajectories

Evolution of two TDHFB calculation at the vicinity of the barrier

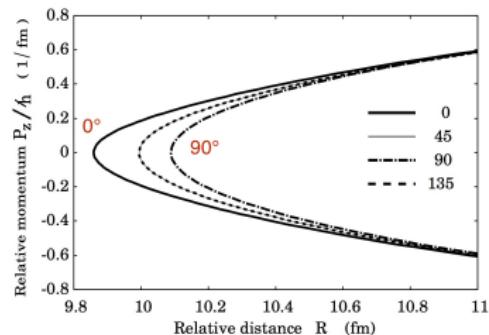
$$\kappa(r, \uparrow, r, \downarrow) = |\kappa(r, \uparrow, r, \downarrow)| e^{2i\varphi}$$

Nucleus-Nucleus potential

Frozen potential



Trajectory



$$U \rightarrow e^{i\varphi} U \theta(z)$$

$$V \rightarrow e^{-i\varphi} V \theta(z)$$

$$\rho = V^* V^t \rightarrow \rho$$

$$\kappa = V^* U^t \rightarrow \kappa e^{2i\varphi}$$

$$\kappa = \kappa^{(l)} + \kappa^{(r)} e^{2i\varphi}$$

$$E_{\text{pair}} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \kappa_{\alpha\beta}^* \kappa_{\gamma\delta}$$

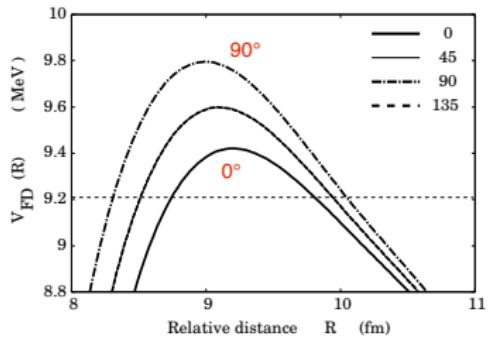
$$\Delta E \propto \sin(\varphi)^2$$

Important point

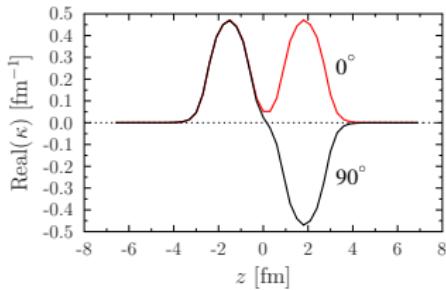
The Nucleus-nucleus potential depends on the relative gauge angle

Nucleus-Nucleus potential

Frozen potential



κ density



$$U \rightarrow e^{i\varphi} U \theta(z)$$

$$V \rightarrow e^{-i\varphi} V \theta(z)$$

$$\rho = V^* V^t \rightarrow \rho$$

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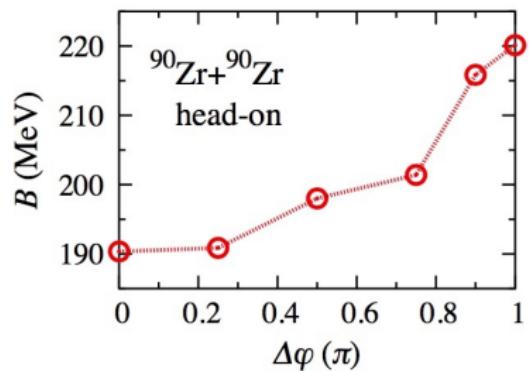
$$\Delta E \propto \sin(\varphi)^2$$

Important point

The Nucleus-nucleus potential depends on the relative gauge angle

Heavy ion collisions

TDHFB with Fayans functionnal,
without spin-orbit



Magierski, Sekizawa, Wlalowski, PRL
119, 042501 (2017).

Amplitude of the barrier fluctuations

Interaction	System	ΔB
Gogny	$^{20}\text{O} + ^{20}\text{O}$	0.4 MeV
Fayans	$^{44}\text{Ca} + ^{44}\text{Ca}$	2.3 MeV
Fayans	$^{90}\text{Zr} + ^{90}\text{Zr}$	30 MeV

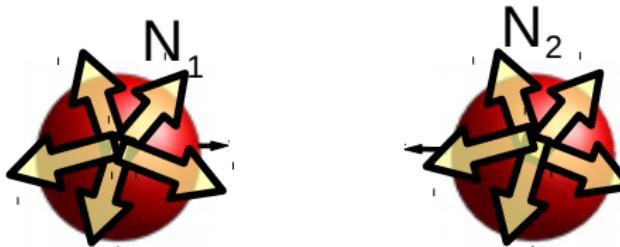
Problem

The relative gauge angle is not a parameter of the reaction. We should restore the symmetry of the relative gauge angle

Projection method

$$|\Psi(t=0)\rangle = \hat{P}_{N_L - N_R}(N_L - N_R)|\phi\rangle,$$
$$\hat{P}_{N_L - N_R}(N_L - N_R) = \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi[(\hat{N}_L - \hat{N}_R) - (N_L - N_R)]} d\varphi$$

We have to consider an evolution of a superposition of HFB states



Two possibilities

Classical restoration

We consider the gauge angle as a parameter of the reaction. We look at the average and the fluctuations of the observables.

Projection method

We first project on the good number of particles in both fragments and then we make the evolution.

Toy model

$$\sum_{i \neq j} V(t) a_i^\dagger a_i^\dagger a_j a_j$$



$$\sum_{i \neq j} G a_i^\dagger a_i^\dagger a_j a_j$$

$$\sum_{i \neq j} G a_i^\dagger a_i^\dagger a_j a_j$$

Simple model

$$V(t) = V_0 \exp(-\alpha t^2)$$

Exact solution

Time-dependent
Multi-configuration method

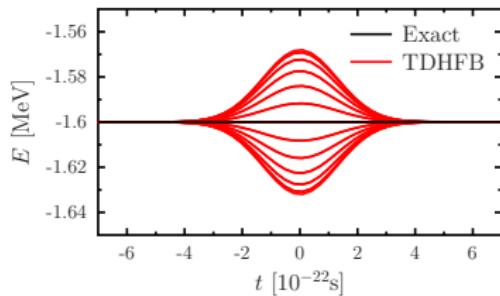
K. Dietrich, Phys. Let. B 32, 6 (1970).

Fluctuations of the energy

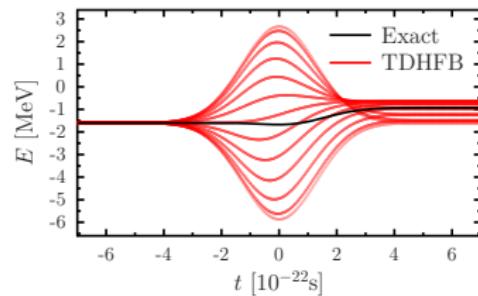
Does the fluctuations of the Nucleus-Nucleus potential is physical in TDHFB ?

Exact solution : good initial number of particles, no gauge angle dependence.

Weak interaction



Strong interaction

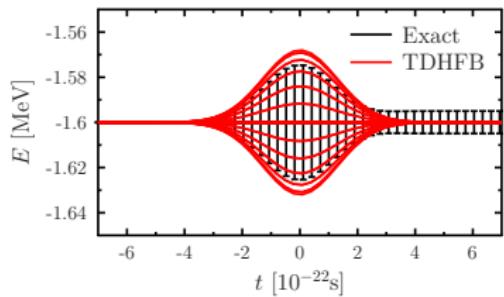


Fluctuations of the energy

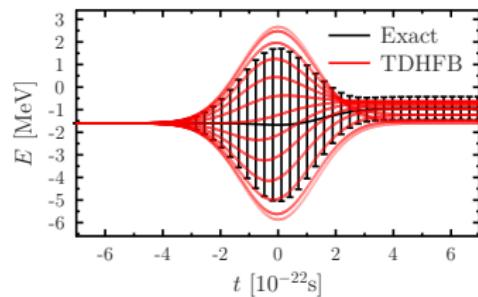
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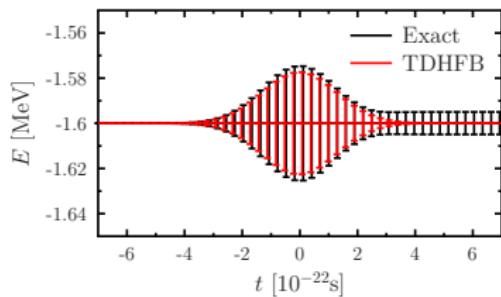
$$\sigma = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$$

Fluctuations of the energy

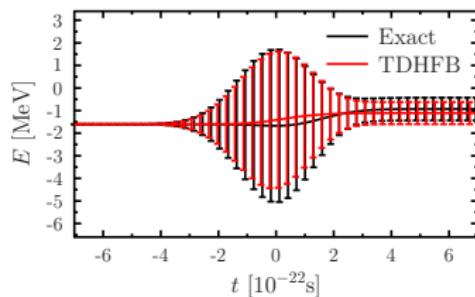
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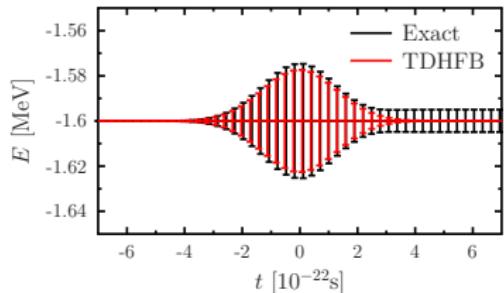
$$\sigma_{\text{clas.}} = \sqrt{\bar{E}^2 - \bar{E}^2}$$

Fluctuations of the energy

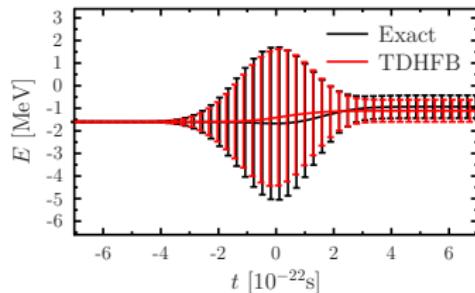
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G. Scamps, Y. Hashimoto, EPJ Web Conf. 163, 00049 (2017)

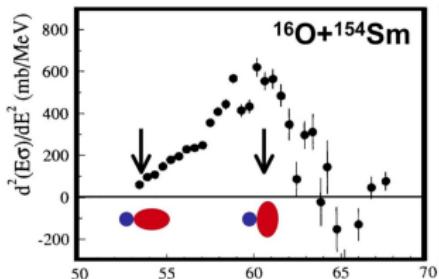
D. Regnier, D. Lacroix, G. Scamps, Y. Hashimoto, Phys. Rev. C 97, 034627 (2018).

Research of experimental evidences

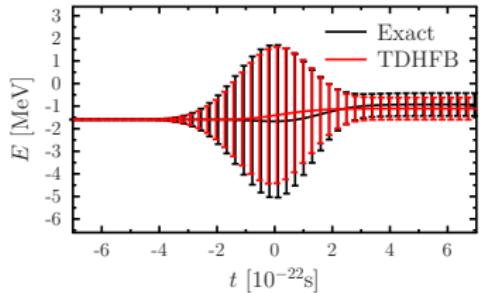
TDHFB calculations

Interaction	System	ΔB
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Effect of deformation



Toy model



Goal of this study

Can we find experimental evidence of this phenomena ?

Statistical approach

Strategy

- Compilation of experimental fusion cross section data
- Determination of a method to extract the fluctuations of the barrier
- Correlations with the superfluidity ?

Experimental barrier distribution

Three points formulae :

Distribution barrier

$$D(B) = \frac{1}{\pi R_\sigma^2} \frac{d^2[E\sigma_{\text{fus}}(E)]}{dE^2}$$

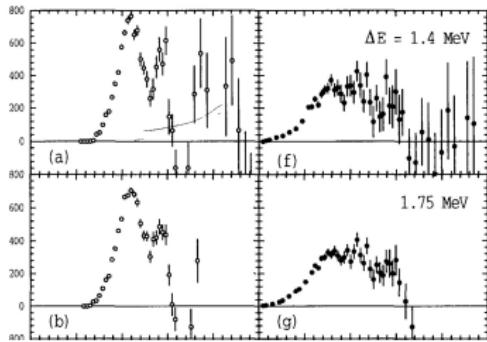
$$\frac{d^2(E\sigma)}{dE^2} \simeq \frac{E_1\sigma(E_1) - 2E_2\sigma(E_2) + E_3\sigma(E_3)}{(\Delta E)^2}$$

$$E_1 = E - \Delta E; E_2 = E; E_3 = E + \Delta E$$

Problem :

$$\delta_c \text{ uncertainty of } \frac{d^2(E\sigma)}{dE^2}$$

$$\delta_c E \propto \frac{\sigma(E)}{(\Delta E)^2}$$



Alternative method

Direct computation of standard deviation

$$\sigma_B^2 = \frac{1}{N} \int_0^{E_M} E^2 \frac{d^2}{dE^2} (E\sigma(E)) dE - \langle B \rangle^2$$

Integration by parts :

$$\begin{aligned} & \int_0^{E_M} E^2 \frac{d^2}{dE^2} (E\sigma(E)) dE \\ &= E_M^2 \left. \frac{d}{dE} (E\sigma(E)) \right|_{E=E_M} - E_M^2 2\sigma(E_M) + 2 \int_0^{E_M} E\sigma(E) dE \end{aligned}$$

$$\begin{aligned} & \int_0^{E_M} E \frac{d^2}{dE^2} (E\sigma(E)) dE = E_M \left. \frac{d}{dE} (E\sigma(E)) \right|_{E=E_M} - \sigma(E_M) \\ & \int_0^{E_M} \frac{d^2}{dE^2} (E\sigma(E)) dE = \left. \frac{d}{dE} (E\sigma(E)) \right|_{E=E_M} \end{aligned}$$

Direct method

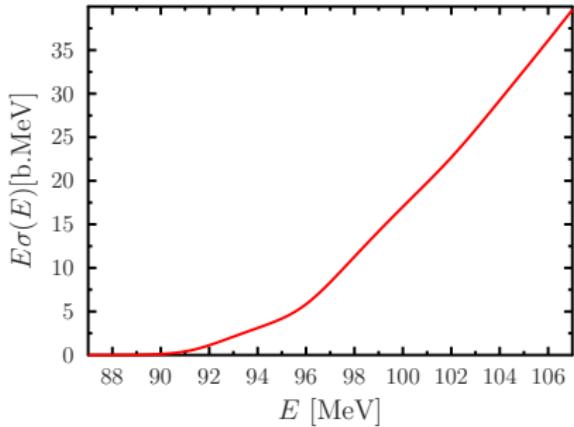
Integration method

$$R_\sigma^2 = \frac{1}{\pi} \left. \frac{d}{dE} \left(E\sigma(E) \right) \right|_{E=E_M}$$

$$B_0 = E_M \left(1 - \frac{\sigma(E_M)}{\pi R_B^2} \right)$$

$$\sigma_B^2 = \frac{2}{\pi R_\sigma^2} \int_0^{E_M} (E\sigma(E) - g(E)) dE$$

Integration method



Direct method

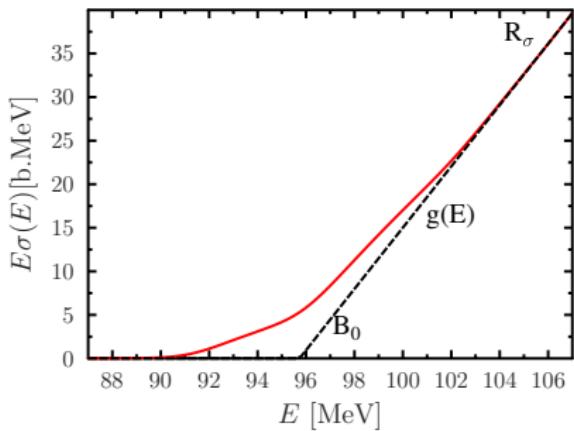
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Integration method



Direct method

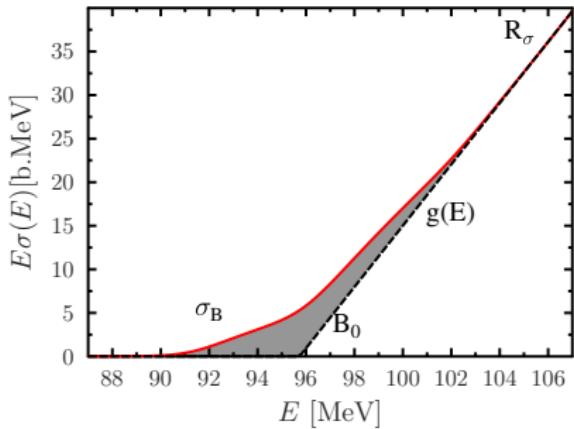
Integration method

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Integration method



Direct method

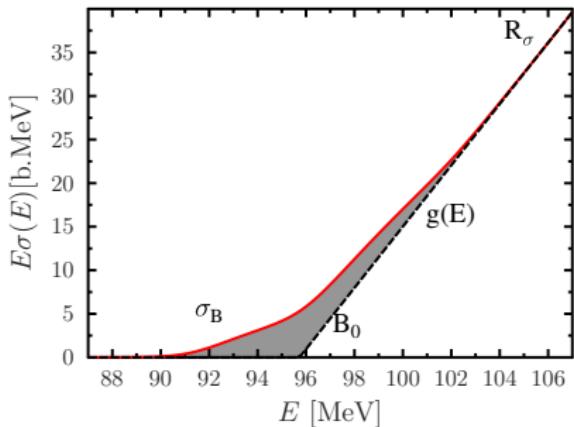
Integration method

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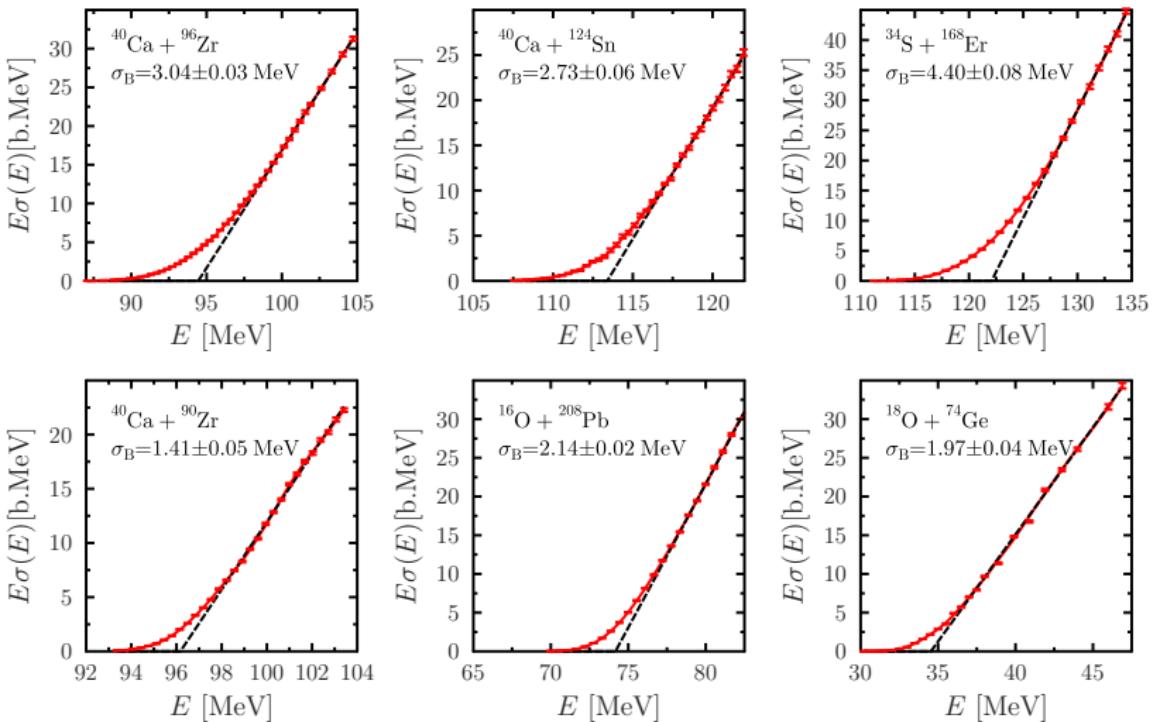
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Integration method

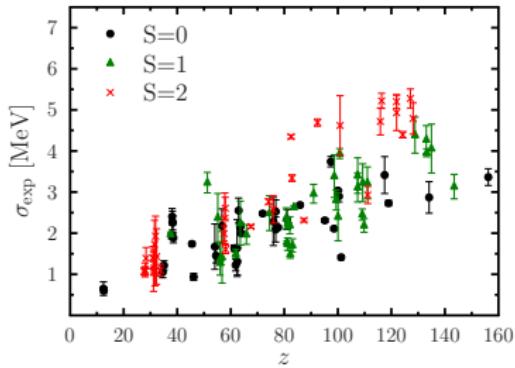


Similar method to compute the centroid : M. Dasgupta, P. R. S. Gomes, D. J. Hinde, S. B. Moraes, R. M. Anjos, A. C. Berriman, R. D. Butt, N. Carlin, J. Lubian, C. R. Morton, J. O. Newton, and A. Szanto de Toledo, Phys. Rev. C **70**, 024606 (2004).



Results

Effect of the superfluidity



$$z = \frac{Z_1 Z_2}{A_1^{1/3} + A_2^{1/3}}$$

Superfluidity variable :

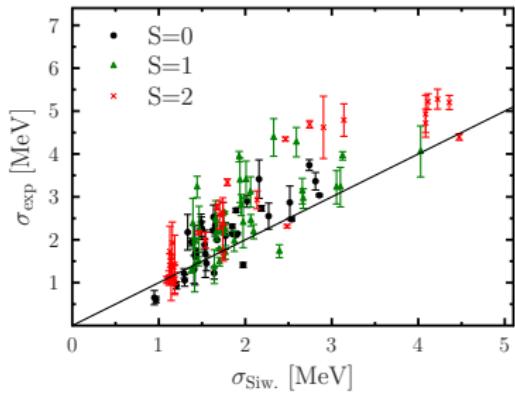
S=0

N1 and N2 non magic : S=S+1

Z1 and Z2 non magic : S=S+1

Results

Comparison theory-experiment



Superfluidity variable :

$S=0$

$N1$ and $N2$ non magic : $S=S+1$

$Z1$ and $Z2$ non magic : $S=S+1$

G. Scamps, arXiv :1801.01250
(2017).

From Ref : K. Siwek-Wilczynska, J. Wilczynski, PRC 69, 024611 (2004) (without effect of gauge angle) :

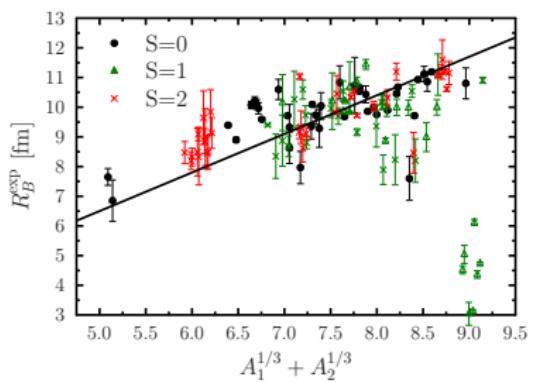
$$w = \sqrt{w_{\text{tunnel}}^2 + w_{\text{stat}}^2(1) + w_{\text{stat}}^2(2) + w_{\text{vibr}}^2(1) + w_{\text{vibr}}^2(2)}, \quad (27)$$

Conclusion

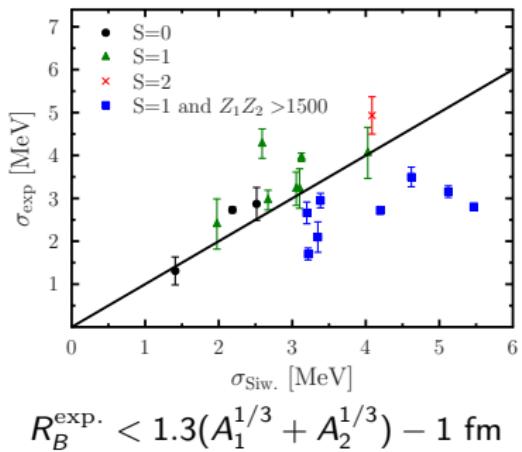
Evidence of an enhancement of the barrier fluctuations with the superfluidity

Experimental method

Fusion radius



System with small radii



$$R_B^{\text{exp.}} < 1.3(A_1^{1/3} + A_2^{1/3}) - 1 \text{ fm}$$

Possible effect of the experimental method.

Conclusion

- TDHFB calculation predict an enhancement of the fluctuations of the barrier.
- A toy-Model confirm that it's not a spurious effect of the mean-field approximation.
- We find experimental evidence of this effect.

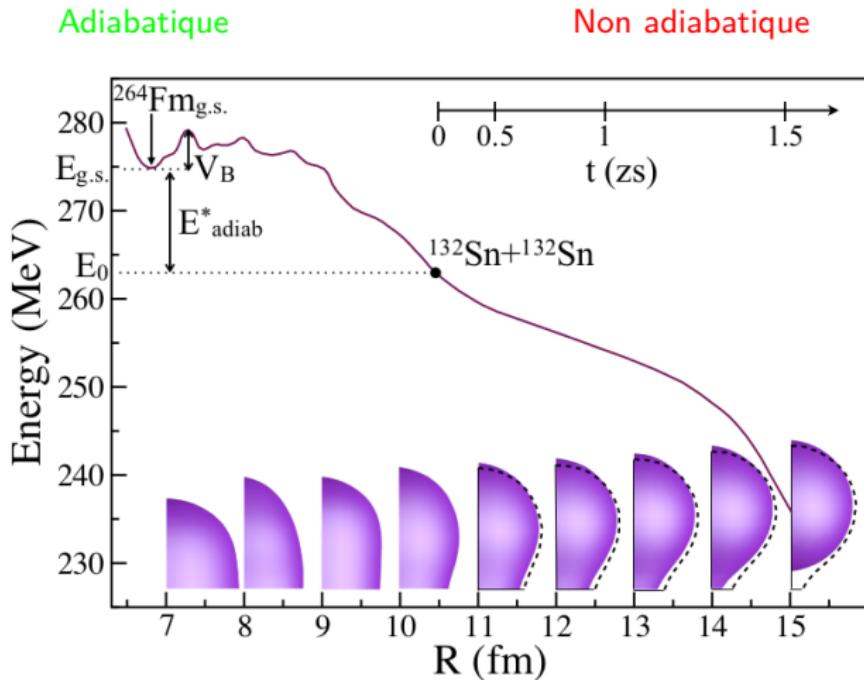
Outlooks :

- Direct comparison from TDHFB with experimental data
- Need of more experimental data
- Density-constraint Time-dependent Hartree-Fock-Bogoliubov calculation

Fission

G. Scamps, C. Simenel, D. Lacroix,
PRC **92**, 011602(R) (2015).

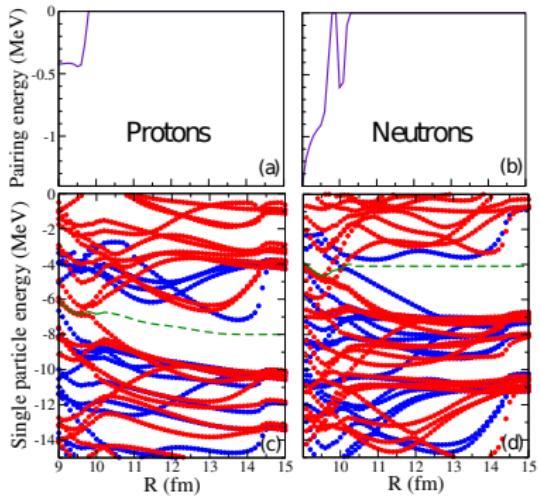
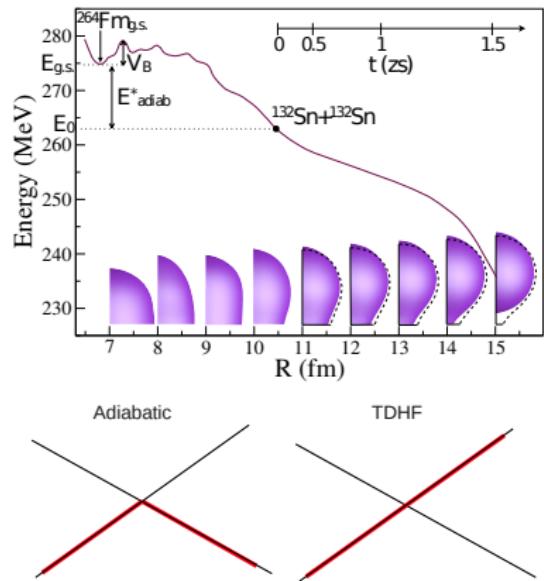
TDHF calculation, fission of ^{264}Fm



C. Simenel and A. S. Umar, Phys. Rev. C 89, 031601(R), 2014

The adiabaticity approximation is assumed for the barrier crossing but is known to break down before scission.

TDHF calculation, fission of ^{264}Fm

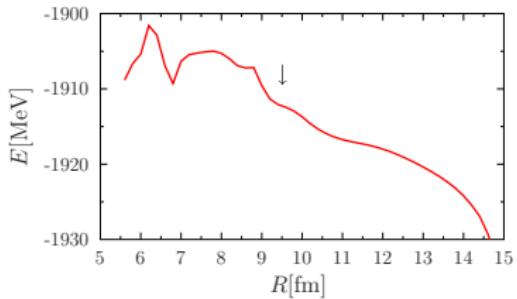


C. Simenel and A. S. Umar, Phys. Rev. C 89, 031601(R), 2014

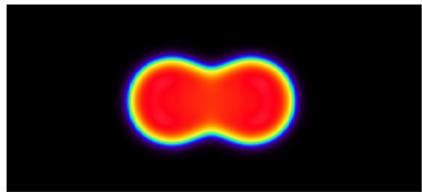
The adiabaticity is not assumed in the TDHF evolution

Why does we need pairing ?

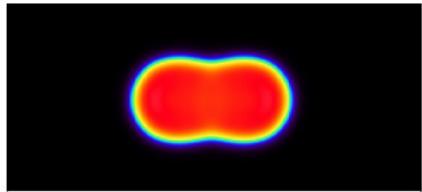
Fission barrier : ^{258}Fm



TDHF



TDHF+BCS

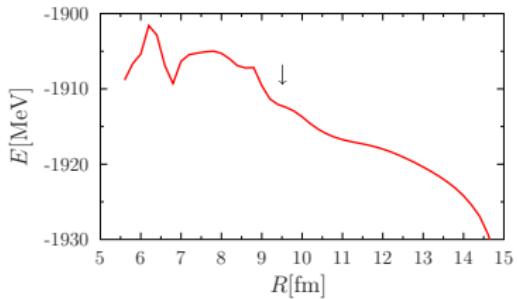


G. Scamps, C. Simenel, D. Lacroix, PRC **92**, 011602(R) (2015).

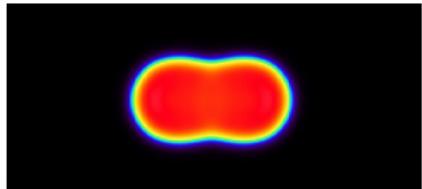
Why does we need pairing ?

TDHF

Fission barrier : ^{258}Fm



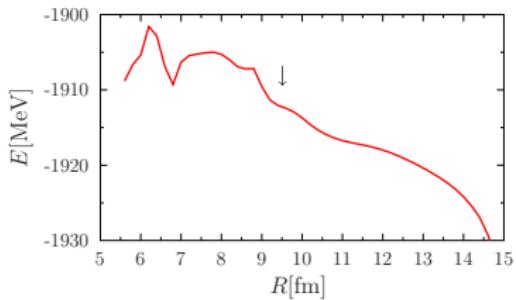
TDHF+BCS



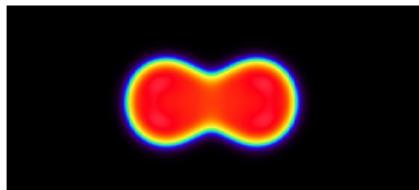
G. Scamps, C. Simenel, D. Lacroix, PRC **92**, 011602(R) (2015).

Why does we need pairing ?

Fission barrier : ^{258}Fm



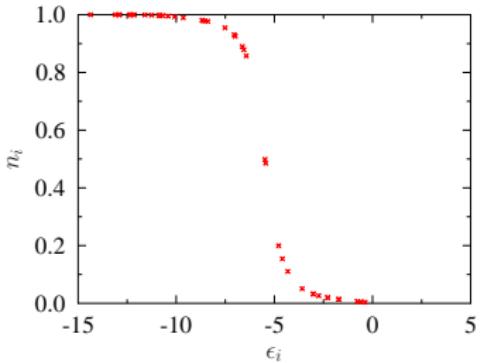
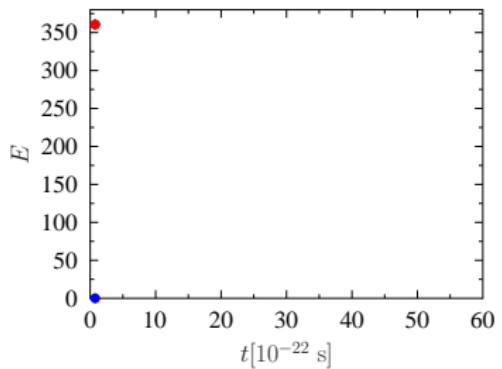
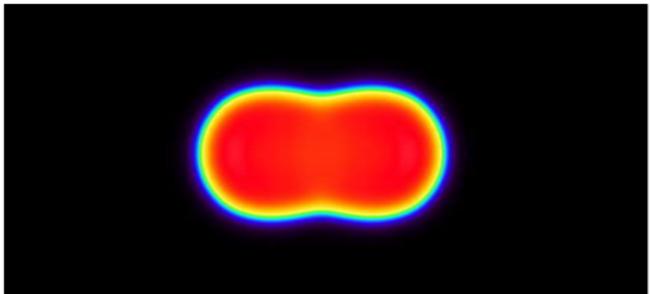
TDHF



TDHF+BCS

G. Scamps, C. Simenel, D. Lacroix, PRC **92**, 011602(R) (2015).

Influence of pairing on fission process



Influence of pairing on fission process

^{258}Fm : experimental results

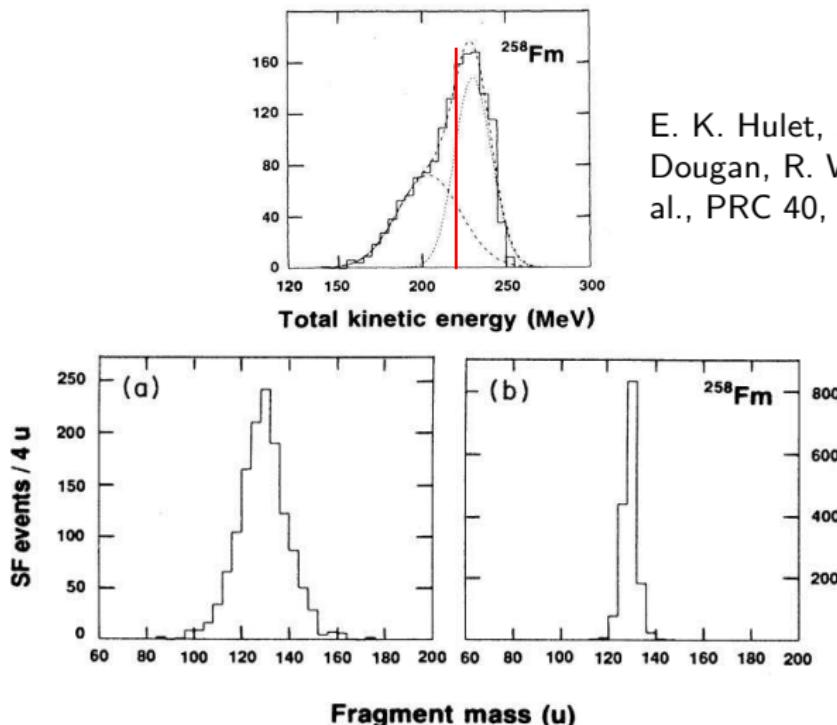


FIG. 8. Mass distributions obtained by sorting fission events according to their total kinetic energies: (a) for events with TKE's < 220 MeV and (b) for those with TKE's ≥ 220 MeV.

^{258}Fm : Bimodal or trimodal fission ?

3 possible modes

- Symmetric compact fragment



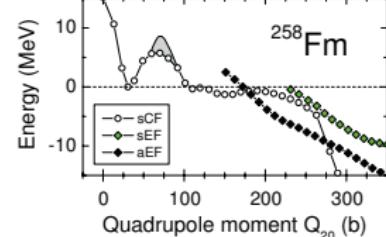
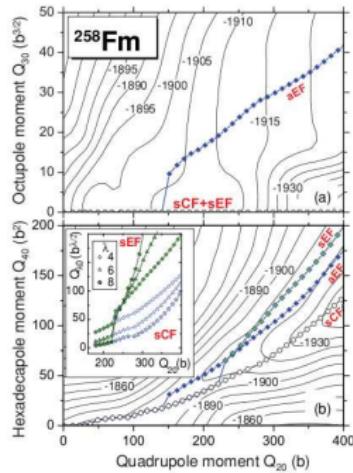
- Symmetric elongated fragment



- Asymmetric elongated fragment



Constraint HF+BCS calculations (SkM*)



A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, PRC 80, 014309 (2009)

^{258}Fm : Bimodal or trimodal fission ?

3 possible modes

- Symmetric compact fragment

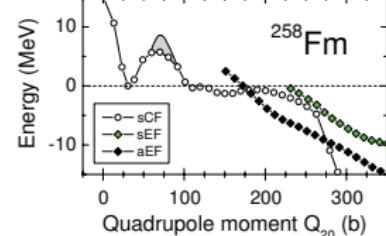
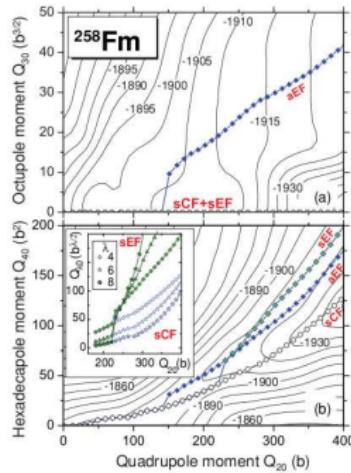


- Symmetric elongated fragment



- Asymmetric elongated fragment

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- Symmetric compact fragment

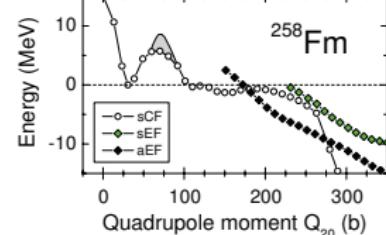
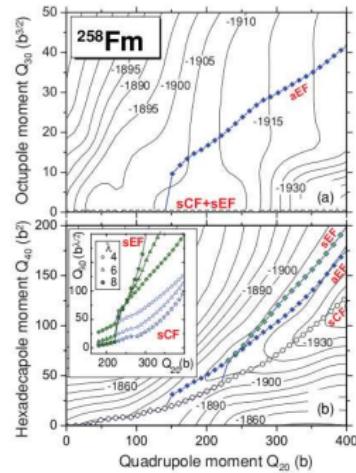


- Symmetric elongated fragment



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^{258}Fm : Bimodal or trimodal fission ?

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- Symmetric compact fragment

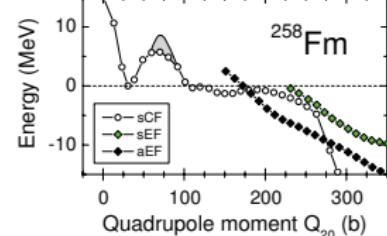
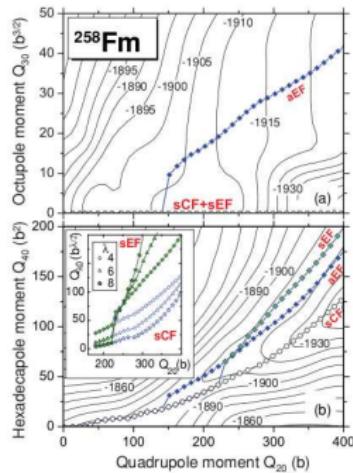


- Symmetric elongated fragment



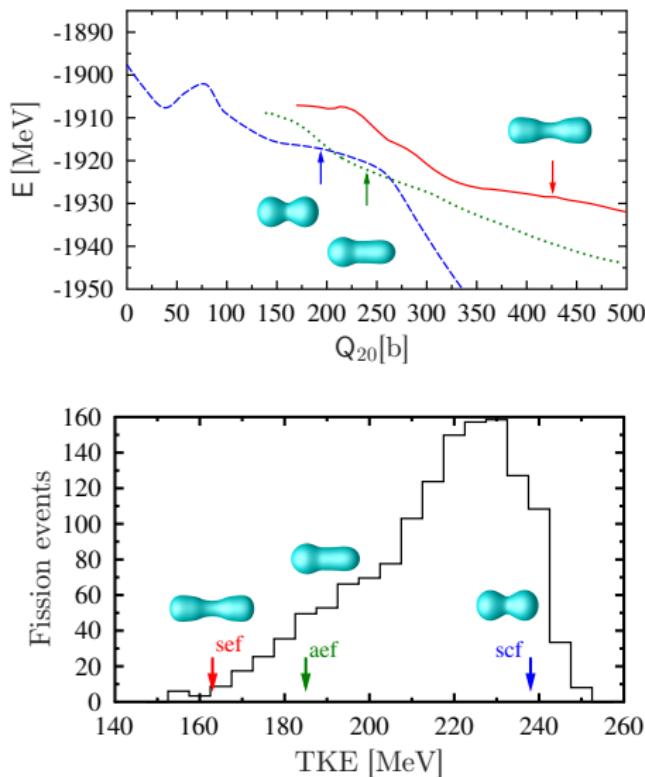
- Asymmetric elongated fragment

Constraint HF+BCS calculations (SkM*)



A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, PRC 80, 014309 (2009)

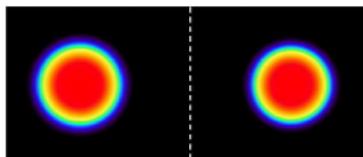
^{258}Fm : TDHF+BCS results



G. Scamps, C. Simenel, D. Lacroix, PRC **92**, 011602(R) (2015).

Distribution of number of particles

Projection technique

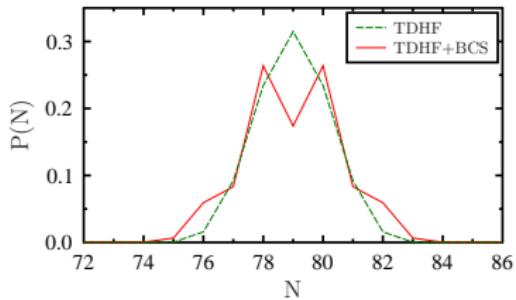


Proba (N part. on the left) = $\langle \Psi | \hat{P}_{\text{left}}(N) | \Psi \rangle$

TDHF : C. Simenel, PRL 105 (2010)

TDHF+BCS : G. Scamps and D. Lacroix, PRC 87, 014605 (2013)

Results

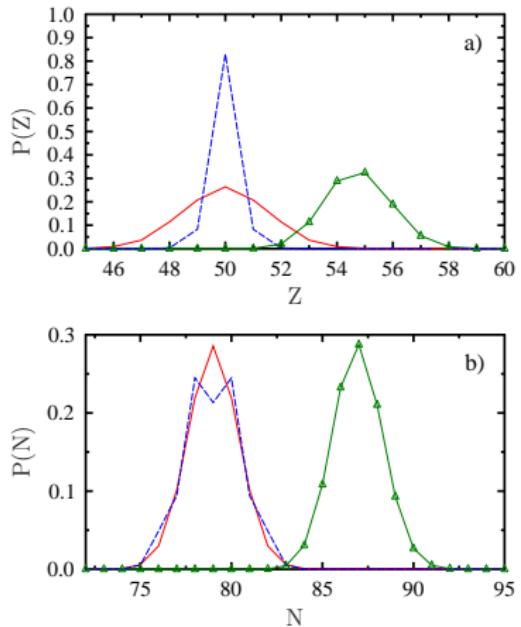


Conclusion

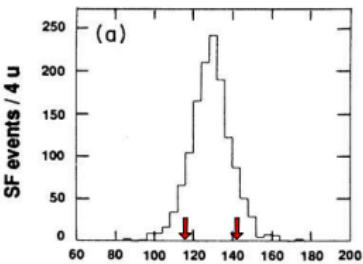
Reproduction of the odd-even effect
with TDHF+BCS

Distribution of number of particles

Results



experimental data



G. Scamps, C. Simenel, and D. Lacroix, Phys. Rev C **92**, 011602(R) (2015)

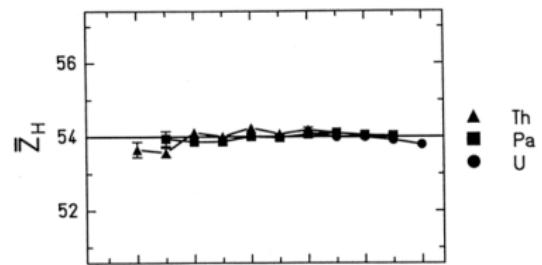
How can we explain microscopically the $Z=54$ behavior in actinide ?

G. Scamps, C. Simenel, in Arxiv tomorrow.

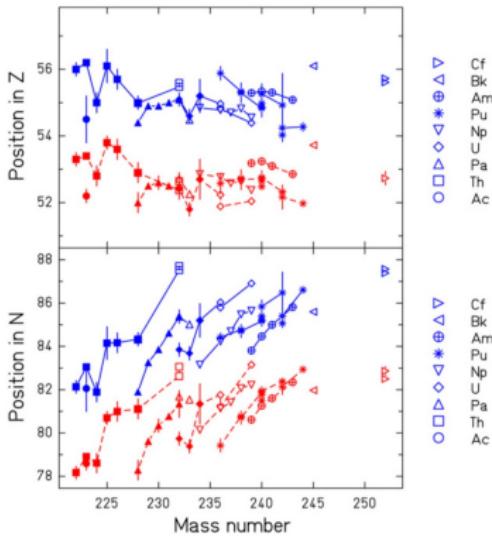
Systematic comparison for actinide

Empirical behavior of actinide nuclei

C. Böckstiegel et al. / Nuclear Physics A 802 (2008) 12–25



K.-H. Schmidt et al. Nuclear Physics A
665 (2000)

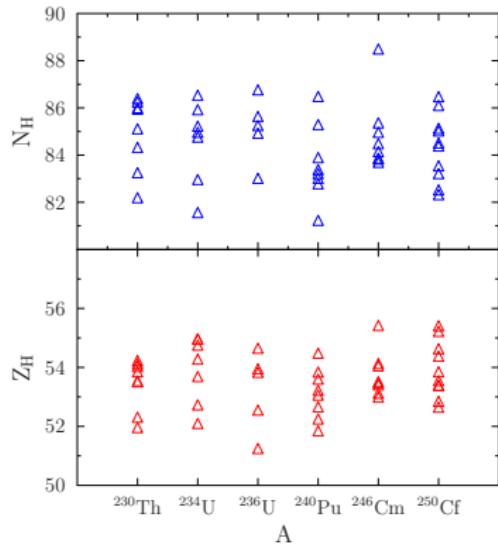


Motivation

How can we understand the $Z \approx 54$ behavior?

TDHF+BCS systematics results

TDHF+BCS



Details

- Sly4d
- Surface type of pairing
- Initialization on the adiabatic path
- Different value of Q_2 after the barrier around $E^*=0$

Nucleon localization function

Fermion localization function

$$\mathcal{C}_{q\sigma}(\mathbf{r}) = \left[1 + \left(\frac{\tau_{q\sigma}\rho_{q\sigma} - \frac{1}{4}|\nabla\rho_{q\sigma}|^2 - \mathbf{j}_{q\sigma}^2}{\rho_{q\sigma}\tau_{q\sigma}^{TF}} \right)^2 \right]^{-1}$$

A. D. Becke and K. E. Edgecombe, J. Chem. Phys. 92, 5397 (1990).

Physical meaning :

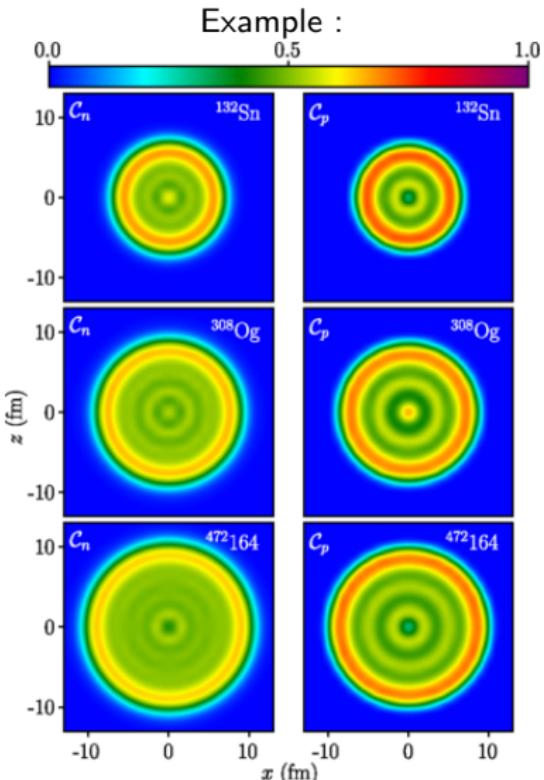
$$\mathcal{C} \in [0 : 1]$$

$\mathcal{C}_{q\sigma}(\mathbf{r}) = 1$ Probability to find another particle with the same q and σ very low.

$\mathcal{C}_{q\sigma}(\mathbf{r}) = 0.5$ Limit of uniform-density Fermi gas.

Mask function :

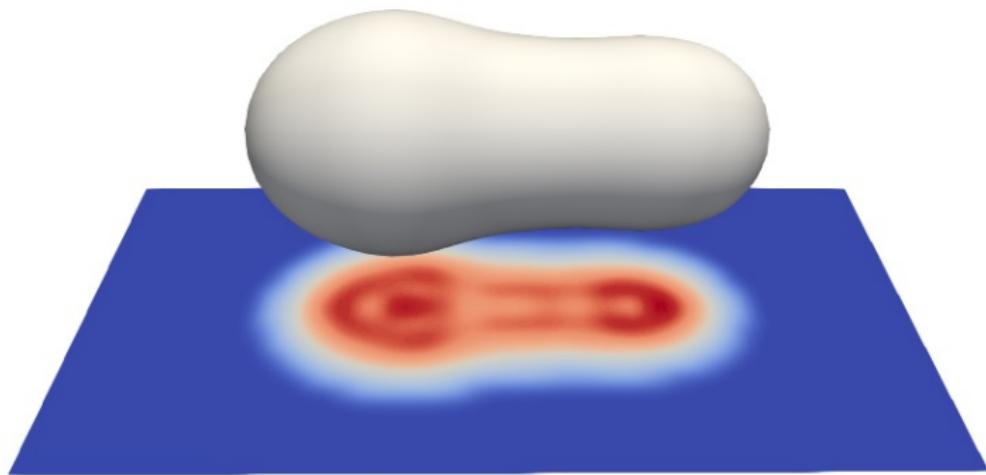
$$\rightarrow \frac{\mathcal{C}_{q\sigma}(\mathbf{r})\rho_{q\sigma}}{\rho_{q\sigma}^{\max}}$$



P. Jerabek, B. Schuettrumpf, P. Schwerdtfeger, and W. Nazarewicz, Phys. Rev. Lett. **120**, 053001 (2018).

Example of ^{240}Pu

^{240}Pu

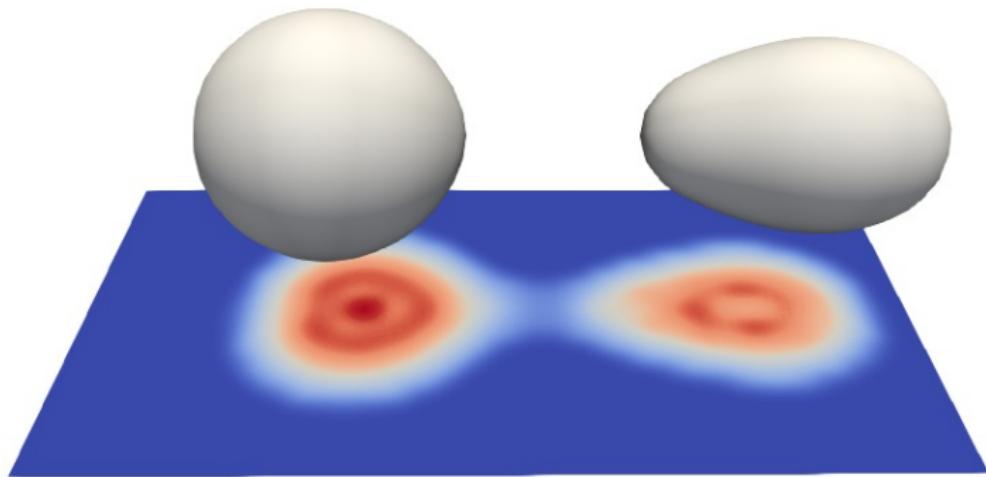


Example of ^{240}Pu

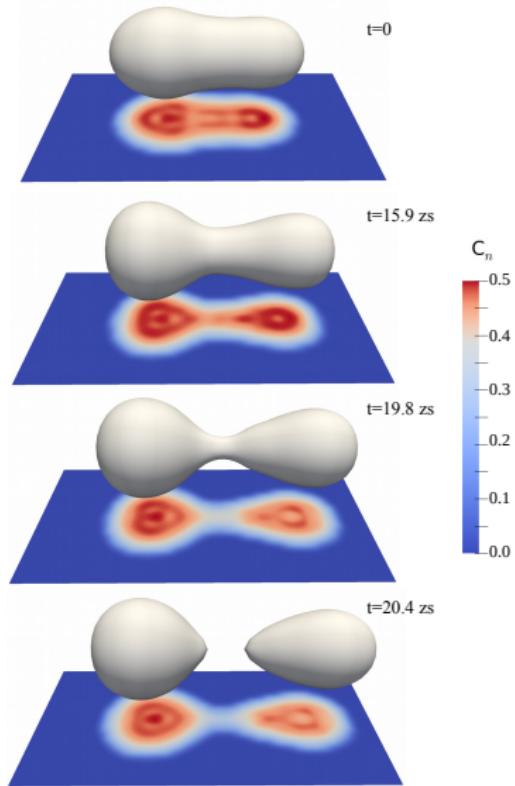
^{240}Pu

Example of ^{240}Pu

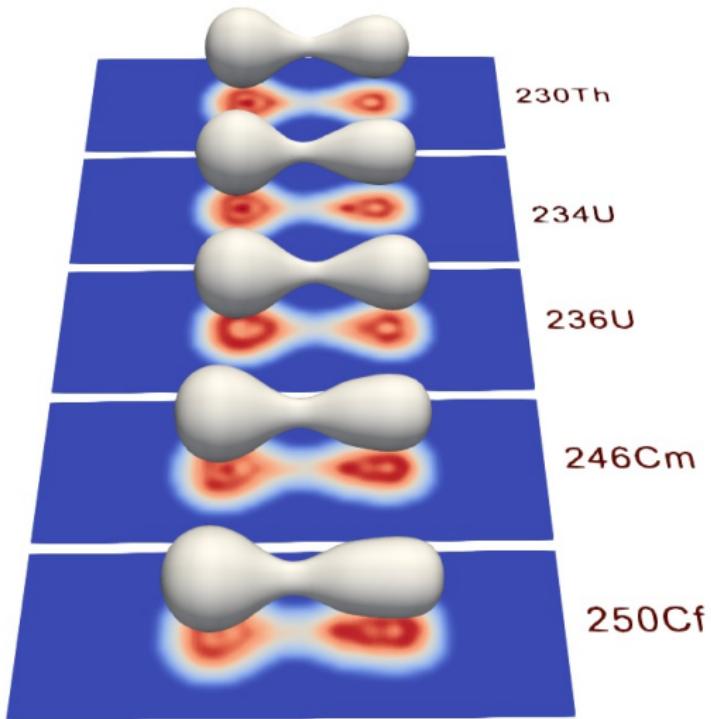
^{240}Pu



Example of ^{240}Pu

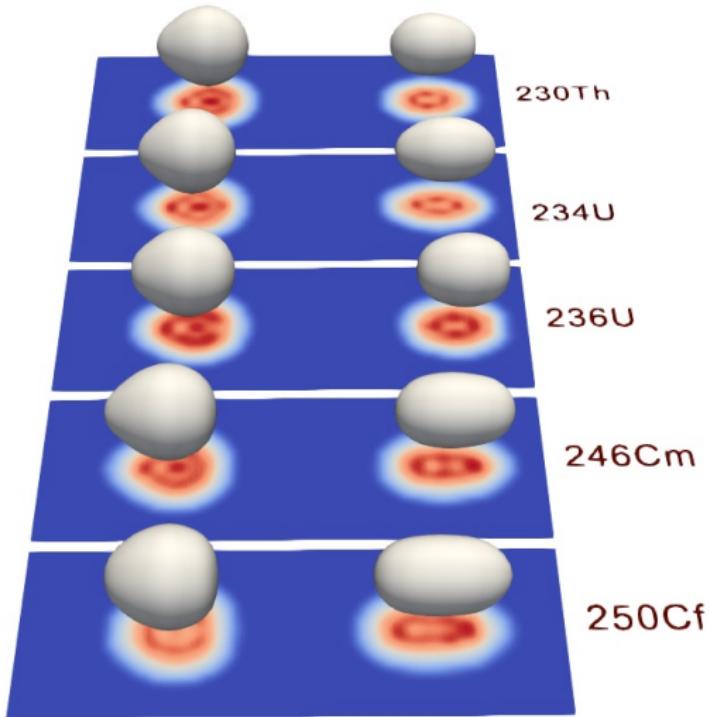


Other systems

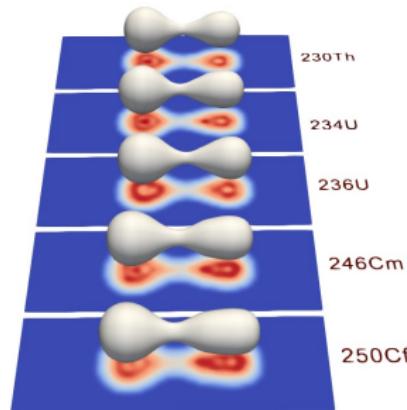
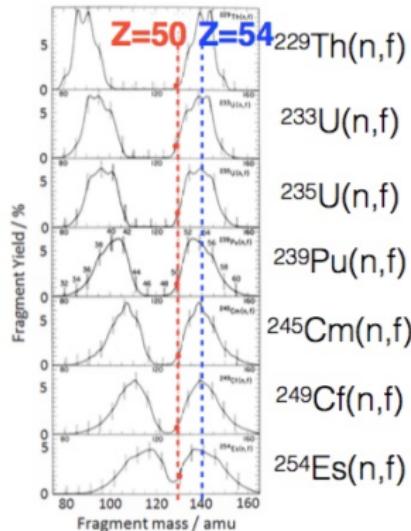


Other systems

Other systems



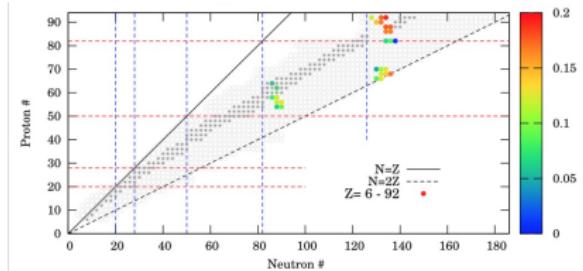
Other systems



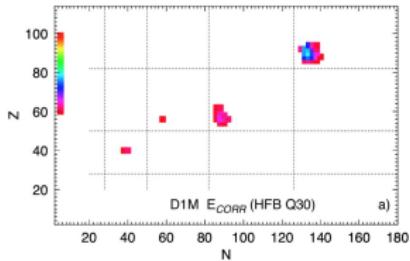
J.P. Unik, J.E. Gindler, J.E. Glendenin
et al. : Proc. "Phys. and Chem. of
Fission" IAEA Vienna , Vol II, 20 (1974)

Octupole deformation systematics

Skyrme Skm*



Gogny D1S



S. Ebata, and T. Nakatsukasa, Phys. Scr. 92 (2017) 064005

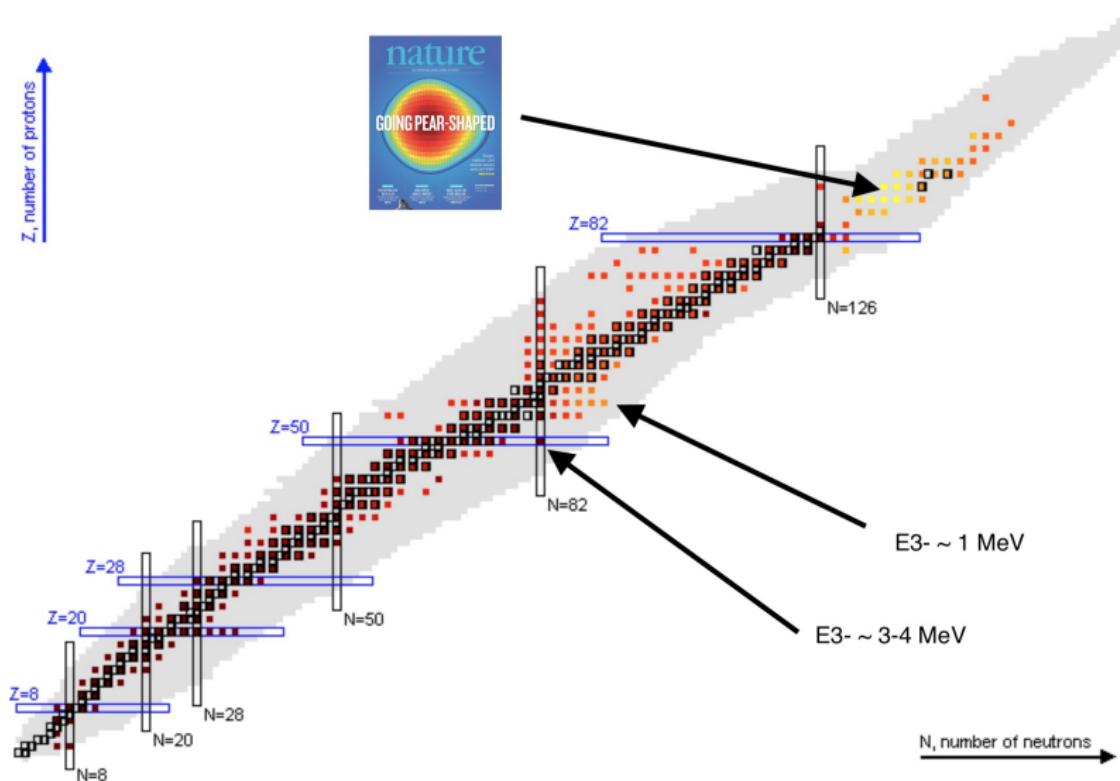
LM Robledo - J. phys. G : Nucl. and Particle Physics, 2015

Result from systematic

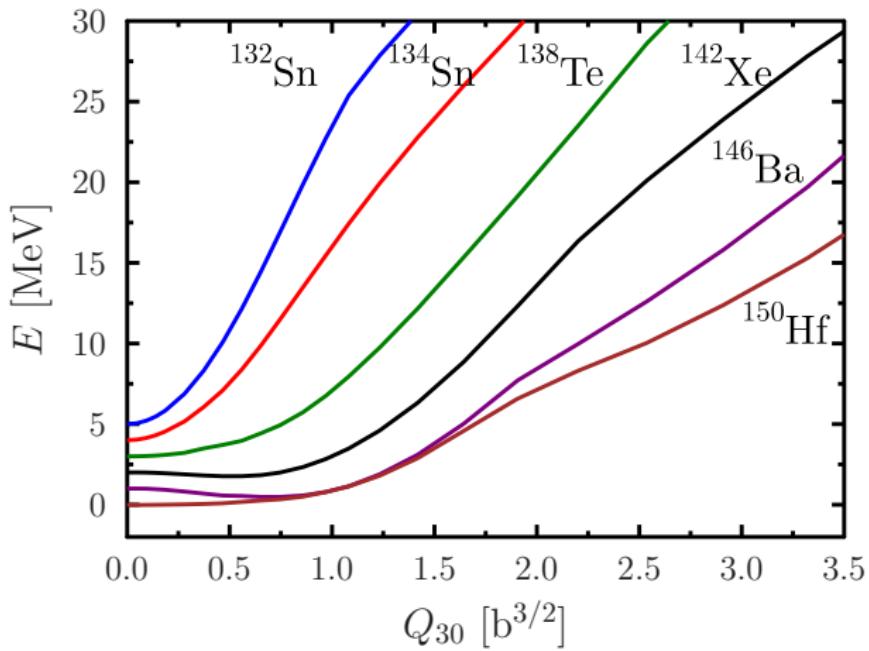
In both calculations, the region $Z \simeq 54$, $N \simeq 88$ is favorable for octupole deformation .

Octupole excitation

Energy of the first 3^-



Constraint HF+BCS octupole deformation with Sly4d

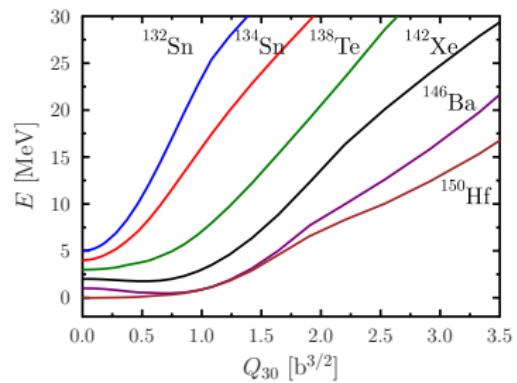


Result from constraint calculation of the heavy fragment

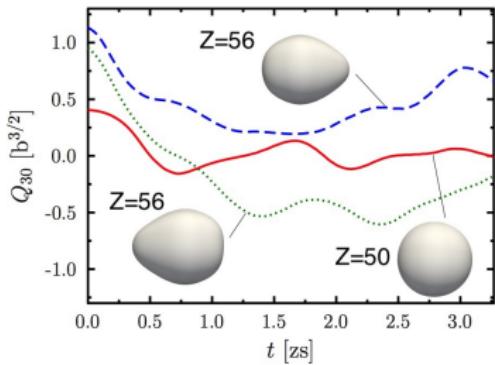
The gain in energy due to the octupole softness drive the fission to the $Z \approx 54$

Post-scission excitation

Octupole deformation energy

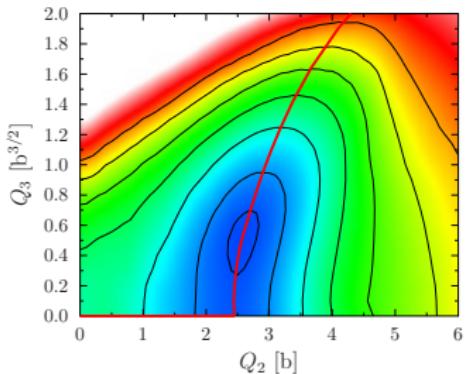


Octupole vibration for 2 mode of ^{258}Fm

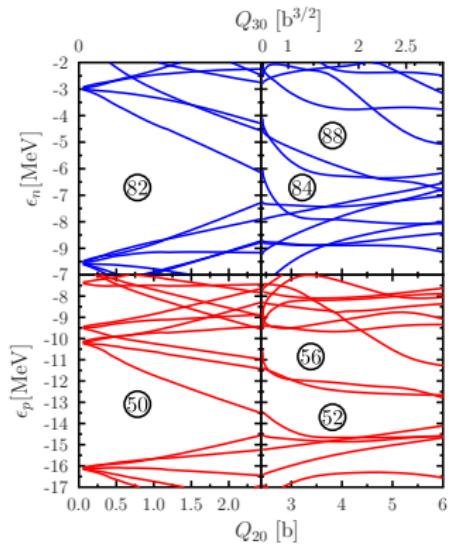


Structure, ^{142}Xe , Z=54, N=88

$Q_2 - Q_3$ potential energy surface

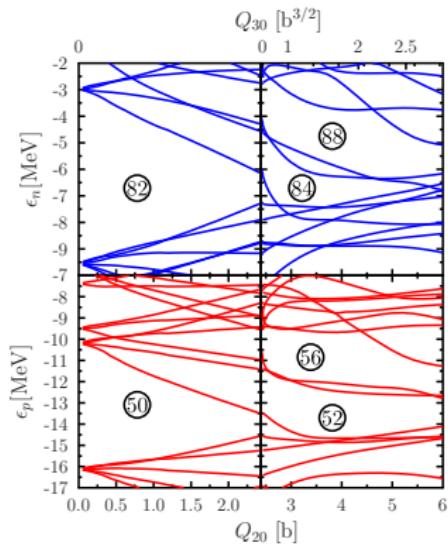


Single particle energy



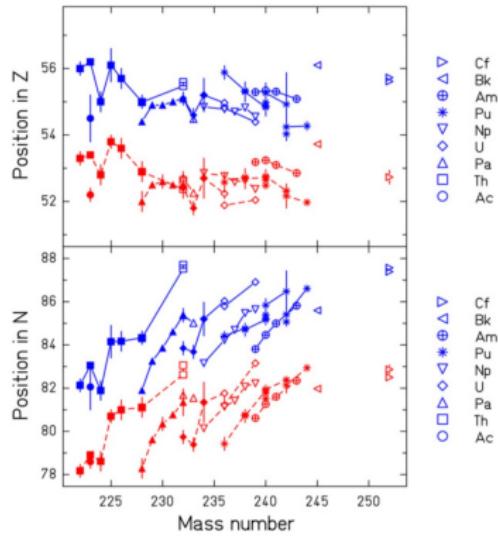
Structure

Single particle energies



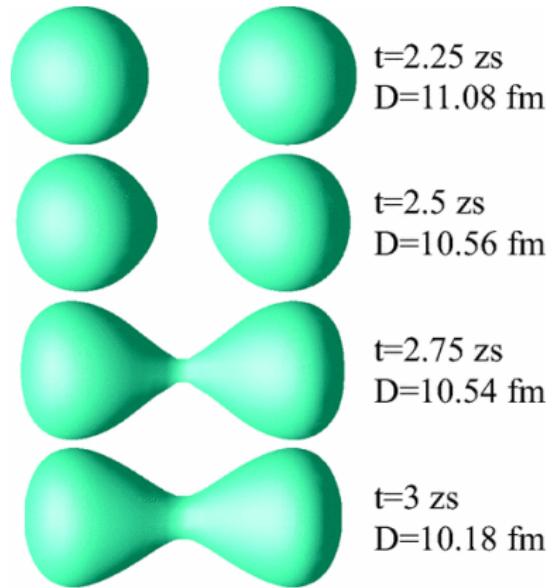
Experimental results

C. Böckstiegel et al. / Nuclear Physics A 802 (2008) 12–25

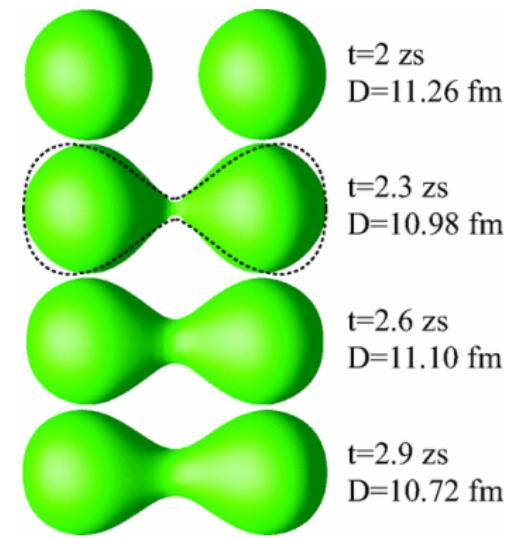


Similar effect on fusion reaction

$^{40}\text{Ca} + ^{40}\text{Ca}, E3^- = 3.7 \text{ MeV}$



$^{56}\text{Ni} + ^{56}\text{Ni}, E3^- = 7.5 \text{ MeV}$



C. Simenel, M. Dasgupta, D. J. Hinde, and E. Williams, Phys. Rev. C 88, 064604 (2013).

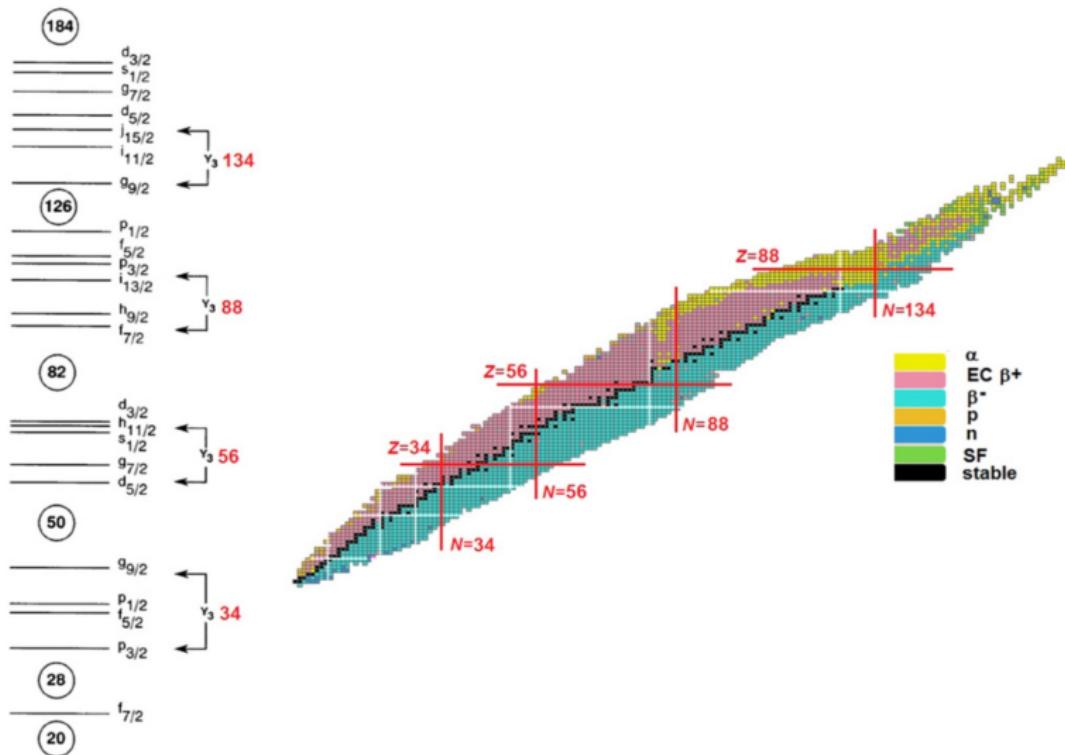
Conclusion and Outlook

Conclusion

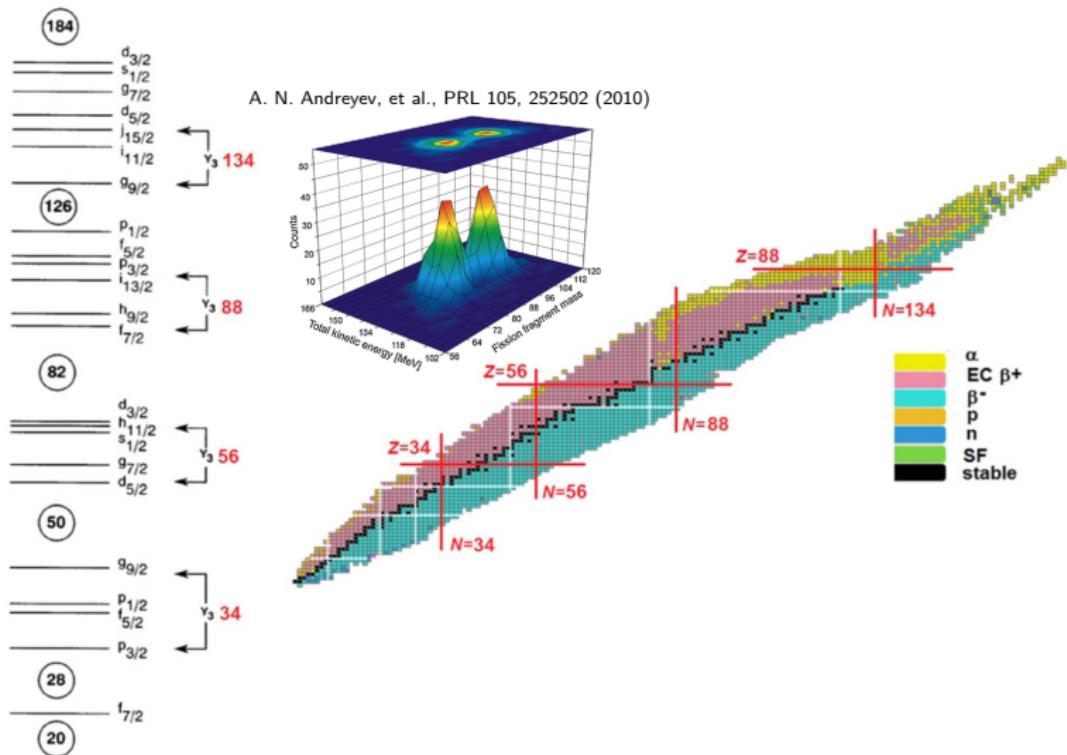
- Shell structure favors octupole shape in the region $Z \simeq 56, N \simeq 88$
- nucleus-Nucleus interaction favors the octupole shape
- Actinide fission fragments are driven in the region $Z \simeq 54, N \simeq 88$

G. Scamps, C. Simenel, in Arxiv tomorrow.

Outlook



Outlook



Thank you

Transfer Reactions

G. Scamps, and Y. Hashimoto ,
PRC **96**, 031602(R) (2017).