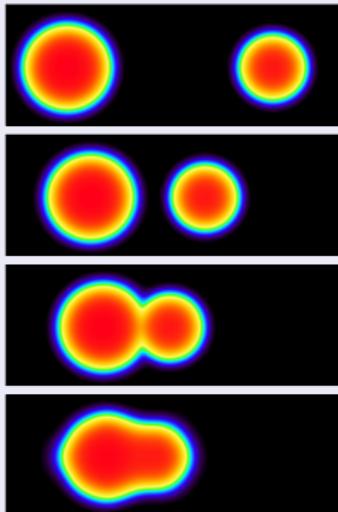




CANHP 2015

Dynamical description of fission



Guillaume SCAMPS

Tohoku University

Collaboration : K. Hagino, D. Lacroix, C. Simenel

Lack of theoretical prediction

Lack of theoretical prediction

- Error of order of magnitudes on the life-time
- Lack of prediction for the charge/mass distribution

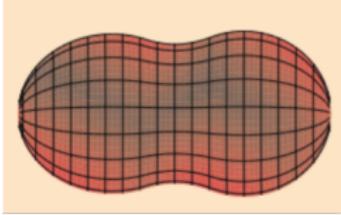
Prediction are necessary for :

- Astrophysics (r-process)
- Industrial applications, production of ions, reactors...

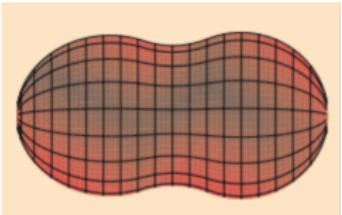
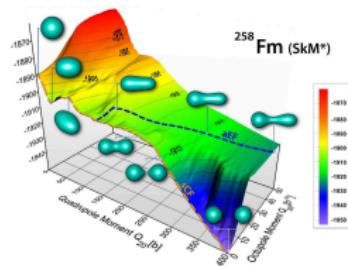
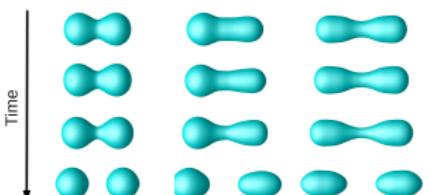
Lots of theoretical questions

- How to define the scission ?
- What are the important degrees of freedom ?
- Shell effects ?
- Effect of pairing ? Odd-even effects ?
- How the energy is split into the fragments ?
- ...

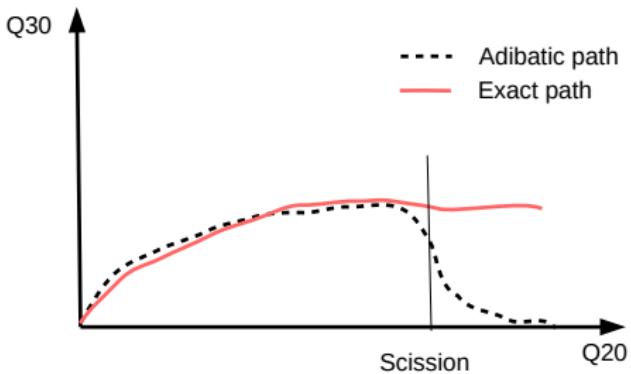
State of the art :

	Macroscopical model
Static	<p>Liquid drop with shell correction</p>  <p>P. Moller, et al., Nature 409 (2001)</p>
Dynamics	<p>Stochastic motion</p>  <p>J. Randrup, PRL 106 (2011)</p>

State of the art :

	Macroscopical model	Microscopical model
Static	<p>Liquid drop with shell correction</p> 	<p>Mean-field theory with pairing, HF+BCS or HFB</p> 
Dynamics	<p>Stochastic motion</p> 	<p>Dynamical mean-field TDHF+BCS</p> 

Adiabatic approximation



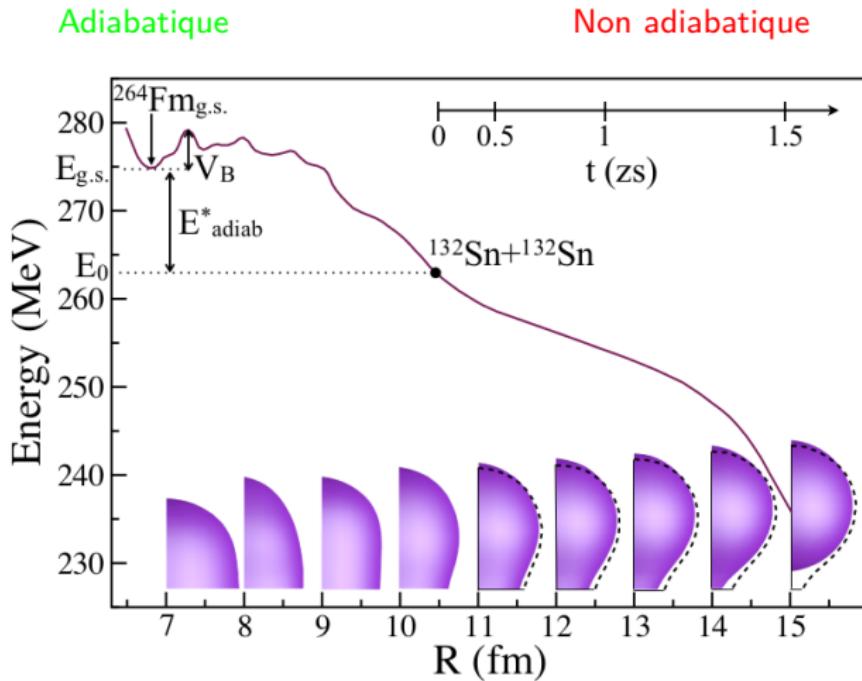
Adiabatic path

Path that minimize the energy with respect to degrees of freedom orthogonal to the elongation.

TDHF or TDHF+BCS

All the degrees of freedom are taken into account

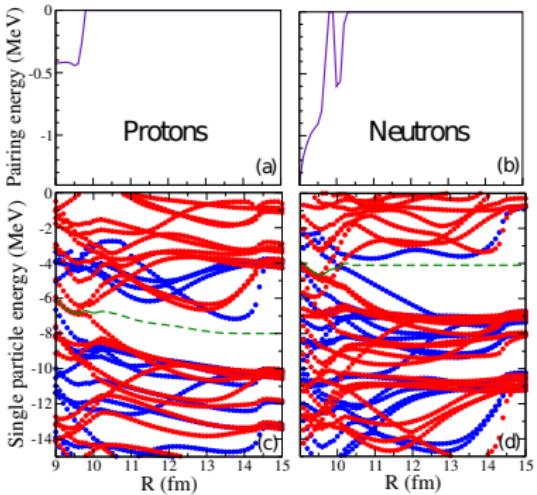
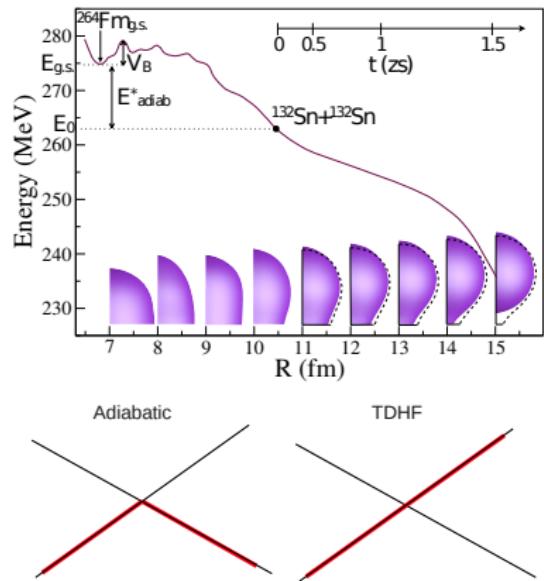
TDHF calculation, fission of ^{264}Fm



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.

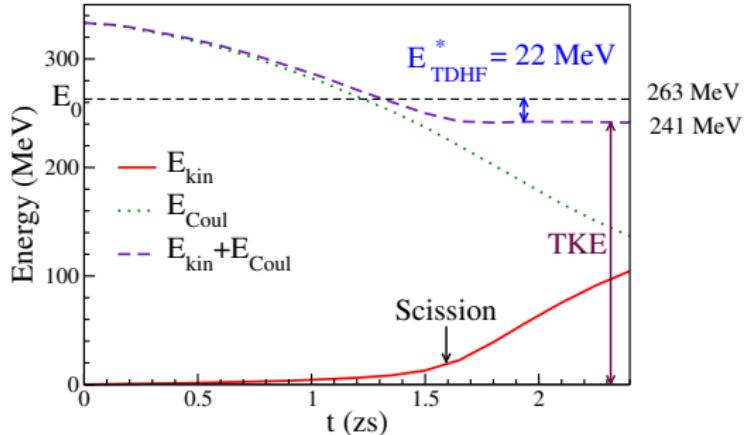
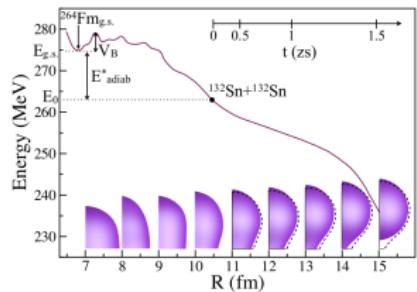
TDHF calculation, fission of ^{264}Fm



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

The adiabaticity is not assumed in the TDHF evolution

TDHF calculation, fission of ^{264}Fm



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

Conclusion

Total Kinetic energy = 241 MeV

Excitation energy = $E^*_{\text{adiabatic}} + E^*_{\text{TDHF}} = 34$ MeV

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 :
 $i\hbar \frac{d\phi_i}{dt} = (\hat{h}_{MF} - \epsilon_i)\phi_i$
 $i\hbar \frac{dn_i}{dt} = \Delta_i^* \kappa_i - \Delta_i \kappa_i^*$
 $i\hbar \frac{d\kappa_i}{dt} = \kappa_i(\epsilon_i - \epsilon_{\bar{i}}) + \Delta_i(2n_i - 1)$

TDHFB vs TDHF+BCS

Inconvenient of the BCS approximation

- gaz problem
- continuity equation

Inconvenient of the BCS approximation

- gaz problem
- continuity equation

Limitation of the TDHF+BCS and TDHFB

- no mixing of states -> classical trajectory
- no Bohr term in the evolution -> lack of dissipation
- 3 and more correlation are neglected
- Fluctuation of the number of particles > projection is needed

Inconvenient of the BCS approximation

- gaz problem
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Strategy

The computational time saved by using the BCS approximation can be used to go beyond the TDHFB approach.

Inconvenient of the BCS approximation

- gaz problem
- continuity equation

Limitation of the TDHF+BCS and TDHFB

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Strategy

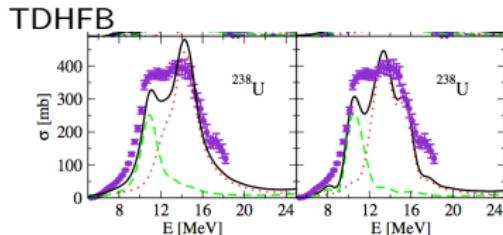
The computational time saved by using the BCS approximation can be used to go beyond the TDHFB approach.

Exemple

- Stochastic TDHF+BCS,
- Time dependent projected BCS,
- Time dependent density matrix,
- Time dependent multi-particles multi-holes,
- TDQRPA.

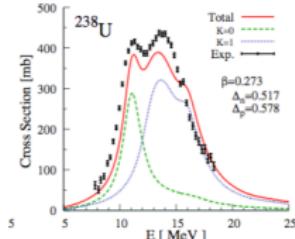
TDHFB vs TDHF+BCS

Giant Dipole resonance



Stetcu et al., PRC 84 (2011)

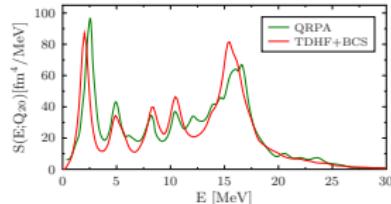
TDHF+BCS



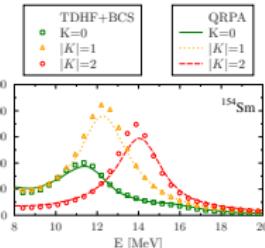
Ebata, PHD thesis (2011)

Giant Quadrupole resonance

Neutron rich nuclei : ^{34}Mg

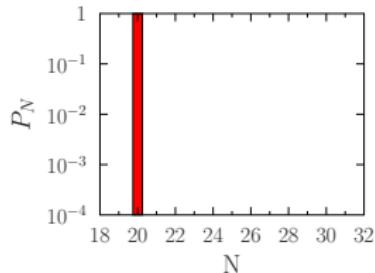
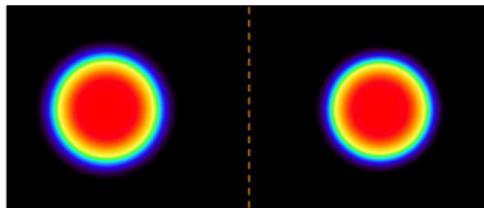
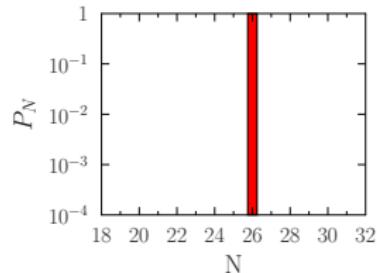


C. Losa et al. PRC 81 (2010)
G. Scamps and D. Lacroix, PRC89 (2014)

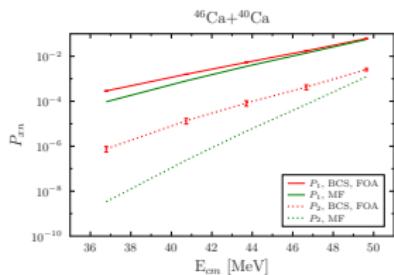


K. Yoshida and T. Nakatsukasa, Phys. Rev. C 88, 034309 (2013)

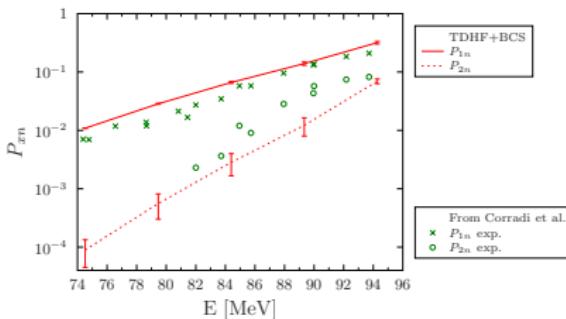
TDHF+BCS has an exploratory method : transfer reaction



Effect of pairing on P_1 and P_2



$^{40}\text{Ca} + ^{96}\text{Zr}$ (Corradi et al., PRC 84 (2011))

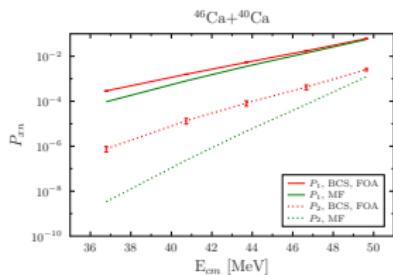


G. Scamps, D. Lacroix, PRC 87, 014605 (2013)

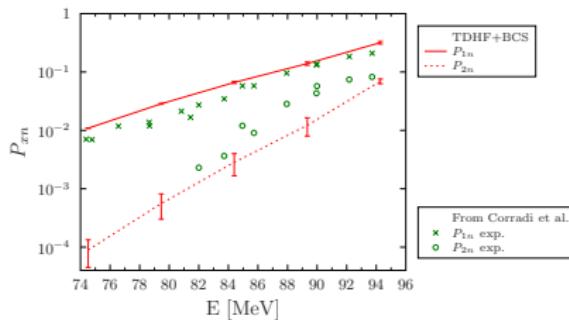
TDHF+BCS has an exploratory method : transfer reaction



Effect of pairing on P_{1n} and P_{2n}



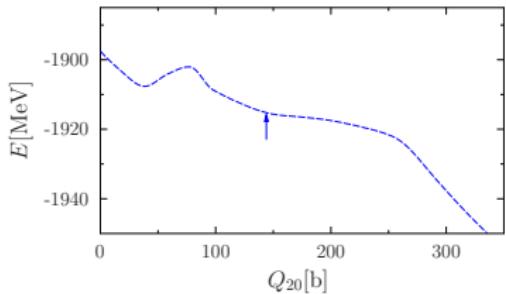
$^{40}\text{Ca} + ^{96}\text{Zr}$ (Corradi et al., PRC 84 (2011))



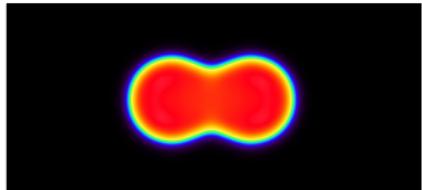
G. Scamps, D. Lacroix, PRC 87, 014605 (2013)

Why does we need pairing ?

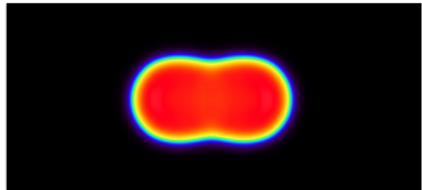
Fission barrier : ^{258}Fm



TDHF



TDHF+BCS

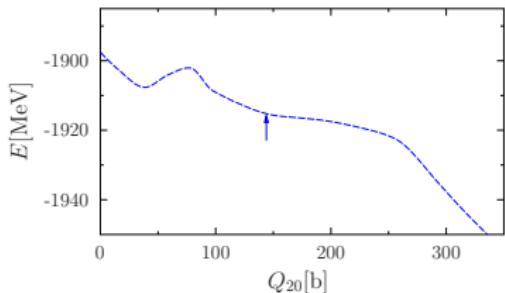


G. Scamps, C. Simenel, D. Lacroix, PRC 92 (2015)

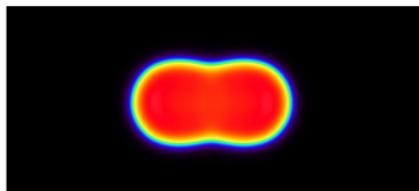
Why does we need pairing ?

TDHF

Fission barrier : ^{258}Fm



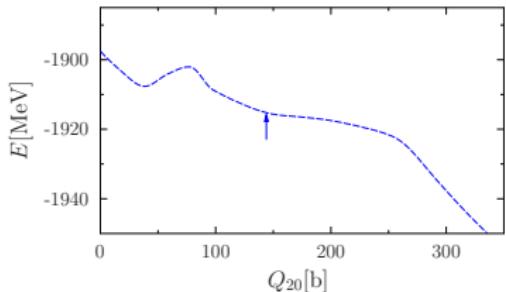
TDHF+BCS



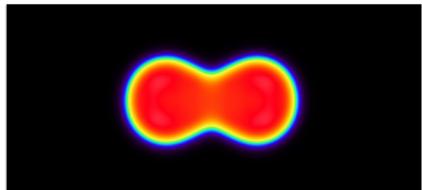
G. Scamps, C. Simenel, D. Lacroix, PRC 92 (2015)

Why does we need pairing ?

Fission barrier : ^{258}Fm



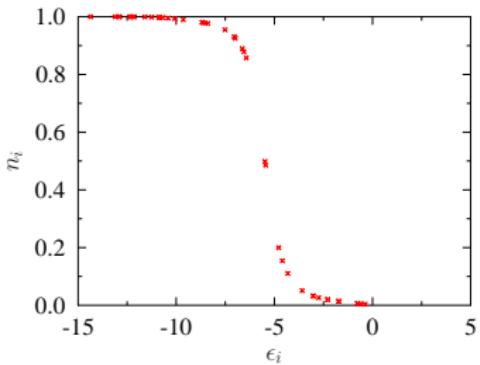
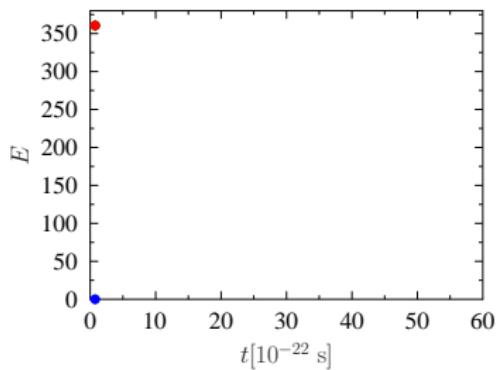
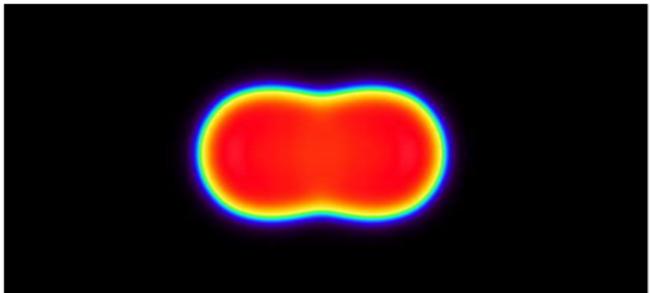
TDHF



TDHF+BCS

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

Influence of pairing on fission process



Influence of pairing on fission process

^{258}Fm : Experimental results

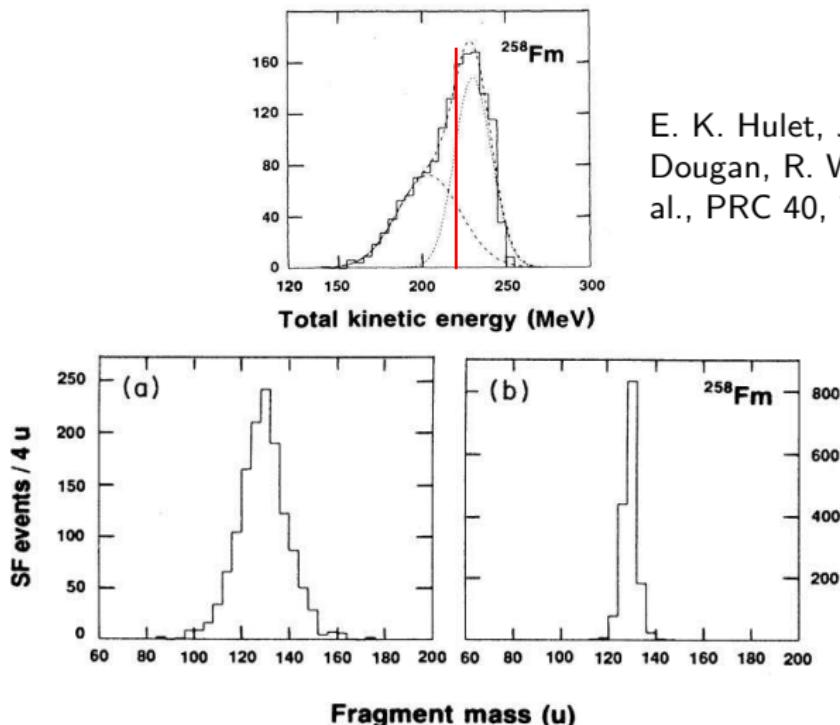


FIG. 8. Mass distributions obtained by sorting fission events according to their total kinetic energies: (a) for events with TKE's < 220 MeV and (b) for those with TKE's ≥ 220 MeV.

^{258}Fm : Bimodal or trimodal fission ?

3 possible modes

- Symmetric compact fragment



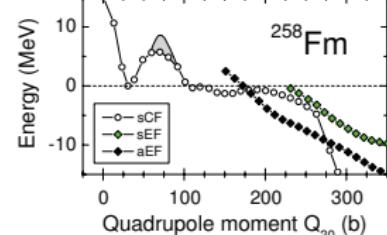
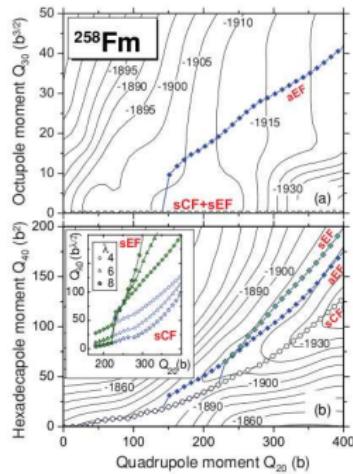
- Asymmetric elongated fragment



- Symmetric 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

3 possible modes

- Symmetric compact fragment



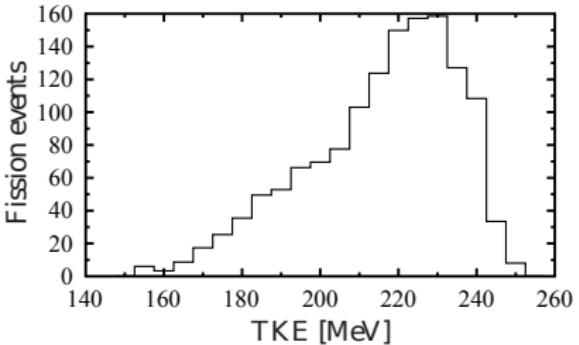
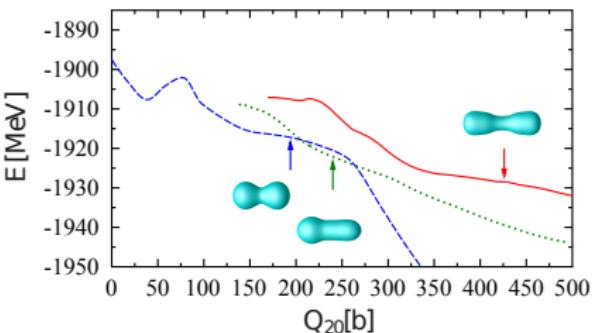
- Asymmetric elongated fragment



- Symmetric elongated fragment



Sly4d



^{258}Fm : TDHF+BCS results

3 possible modes

- Symmetric compact fragment

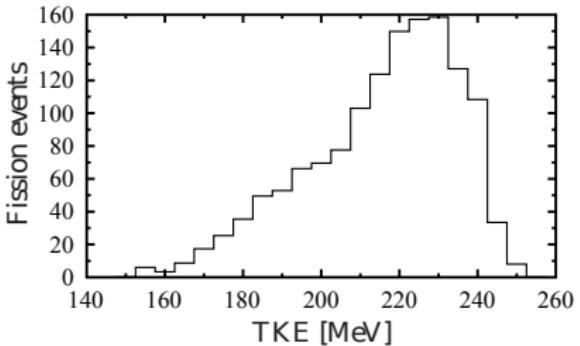
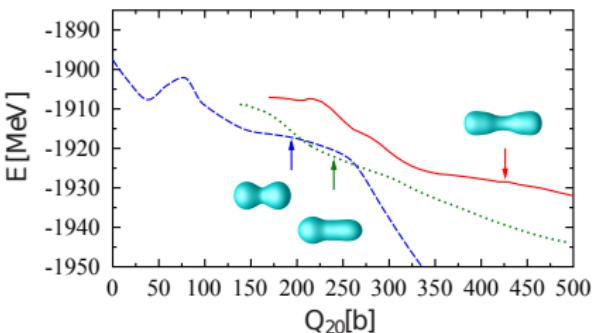


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Sly4d



^{258}Fm : TDHF+BCS results

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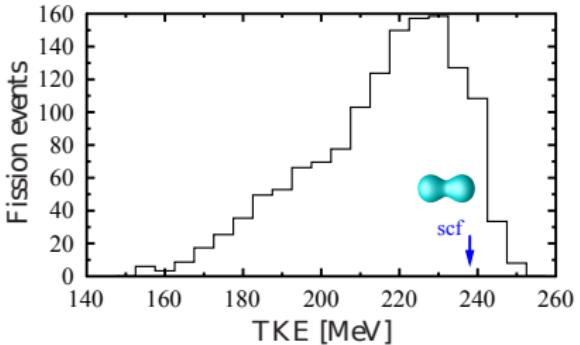
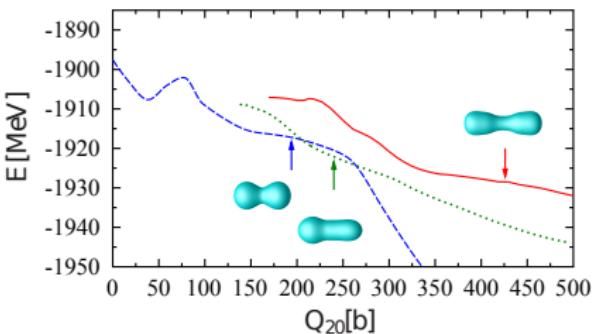
- Asymmetric elongated fragment



- Symmetric elongated fragment



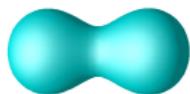
Sly4d



^{258}Fm : TDHF+BCS results

3 possible modes

- Symmetric compact fragment

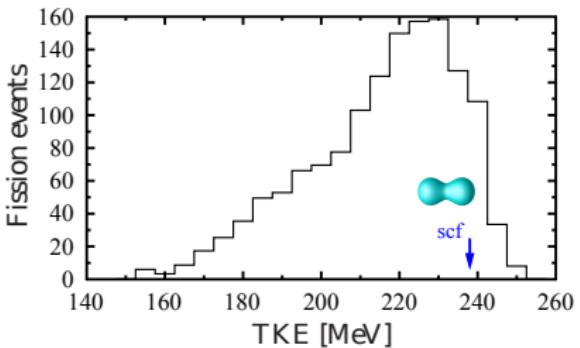
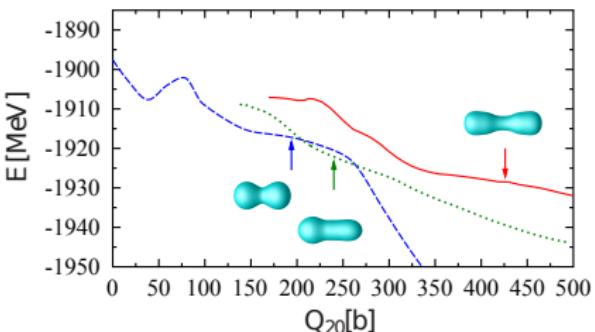


- Asymmetric elongated fragment

- Symmetric elongated fragment



Sly4d



^{258}Fm : TDHF+BCS results

3 possible modes

- Symmetric compact fragment



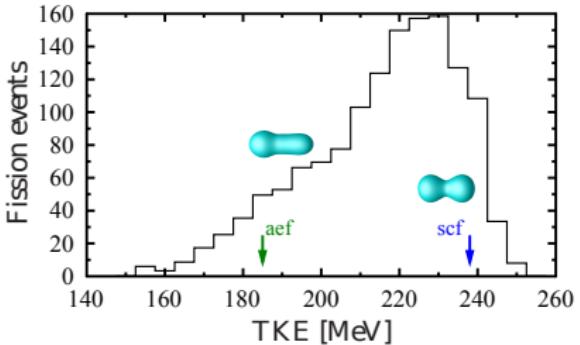
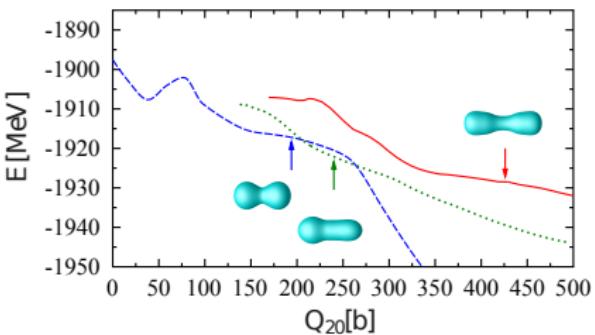
- Asymmetric elongated fragment



- Symmetric elongated fragment



Sly4d



^{258}Fm : TDHF+BCS results

3 possible modes

- Symmetric compact fragment

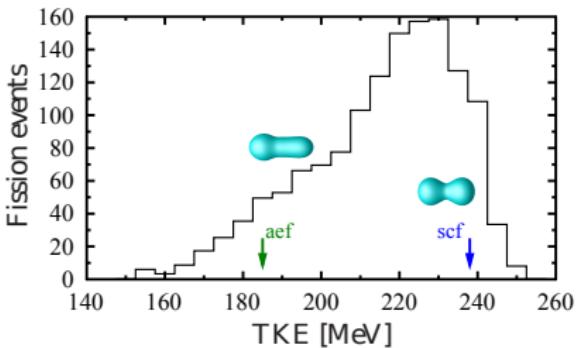
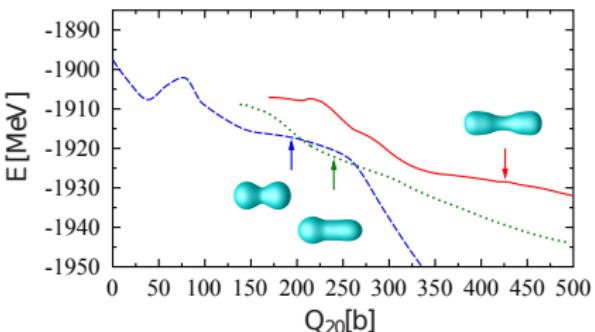


- Asymmetric elongated fragment



- Symmetric elongated fragment

Sly4d



^{258}Fm : TDHF+BCS results

3 possible modes

- Symmetric compact fragment



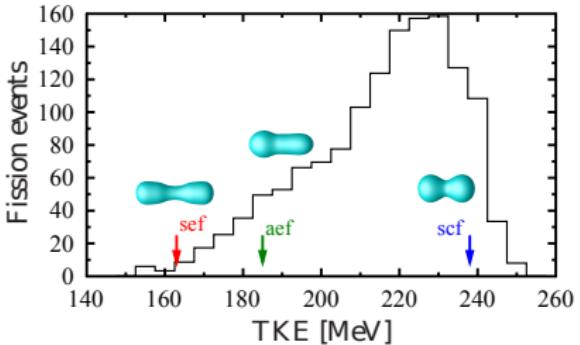
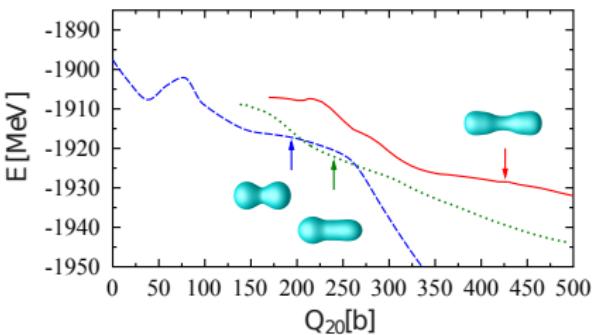
- Asymmetric elongated fragment



- Symmetric elongated fragment

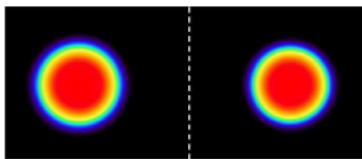


Sly4d



Distribution of number of particles

Projection technique

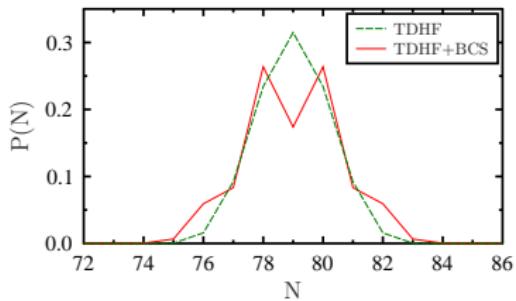


Proba (N part. on the left) = $\langle \Psi | \hat{P}_{\text{left}}(N) | \Psi \rangle$

TDHF : C. Simenel, PRL 105 (2010)

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

Results

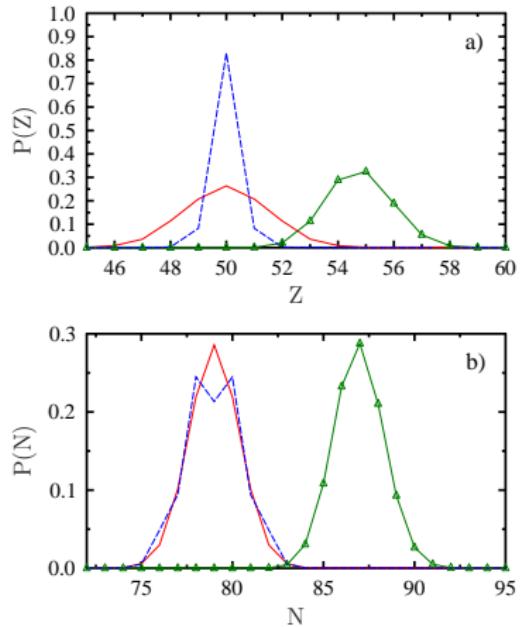


Conclusion

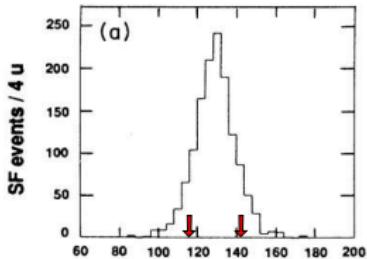
Reproduction of the odd-even effect
with TDHF+BCS

Distribution of number of particles

Results



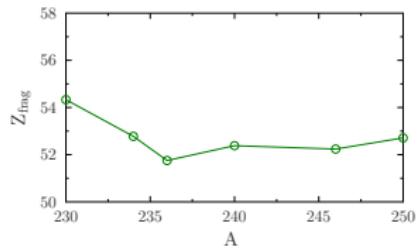
Experimental data



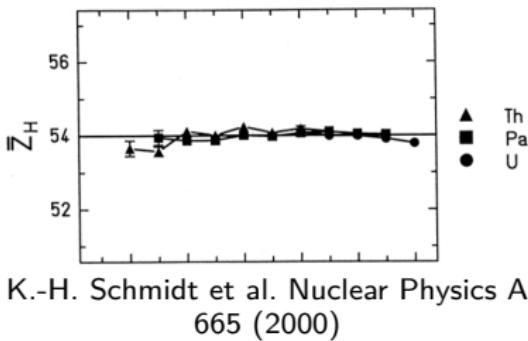
Systematic comparison for actinide

Comparison with experimental data

TDHF+BCS results for ^{230}Th , ^{234}U ,
 ^{236}U , ^{240}Pu , ^{246}Cm , ^{250}Cf



Experimental data

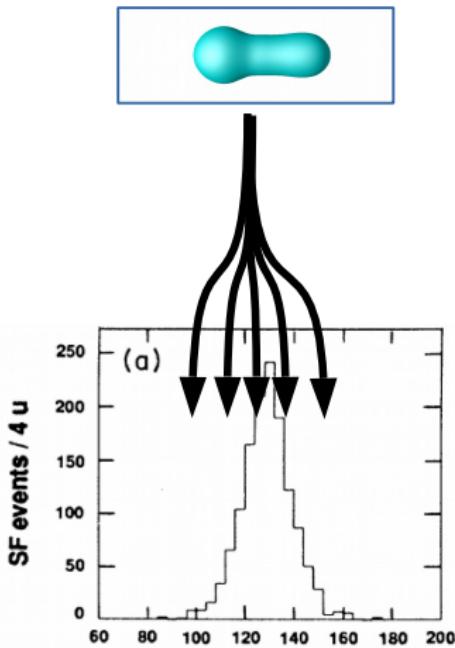
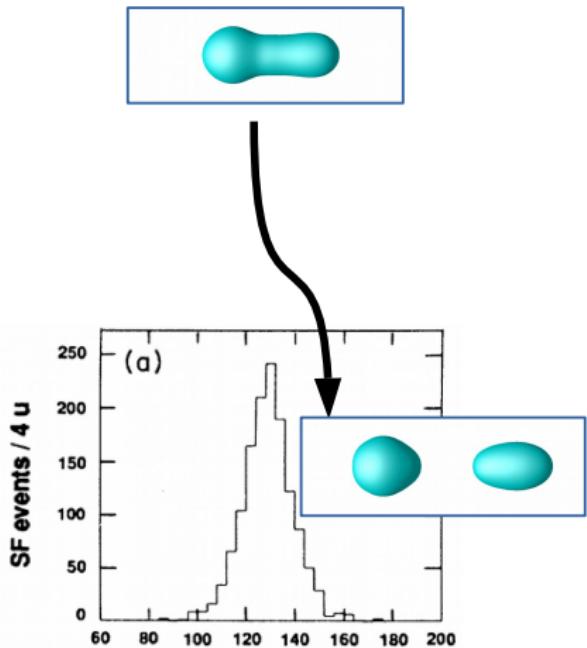


K.-H. Schmidt et al. Nuclear Physics A 665 (2000)

Conclusion

→ Good reproduction of the $Z \approx 54$ "magic" number

Lack of fluctuation with time-dependent mean field

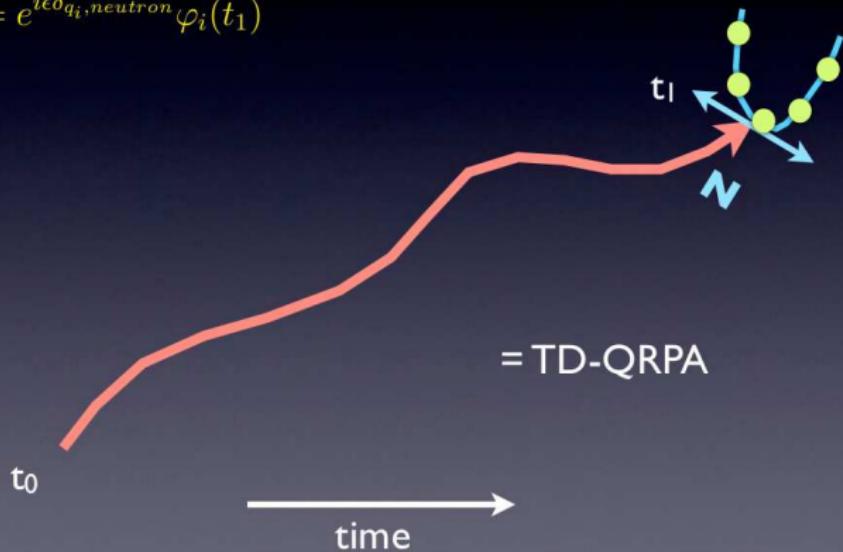


Numerical application of the BV prescription

standard forward TDHF

neutron fluctuations at t_1

$$\varphi_i(t_1, \epsilon) = e^{i\epsilon\delta_{q_i, neutron}} \varphi_i(t_1)$$



Numerical application of the BV prescription

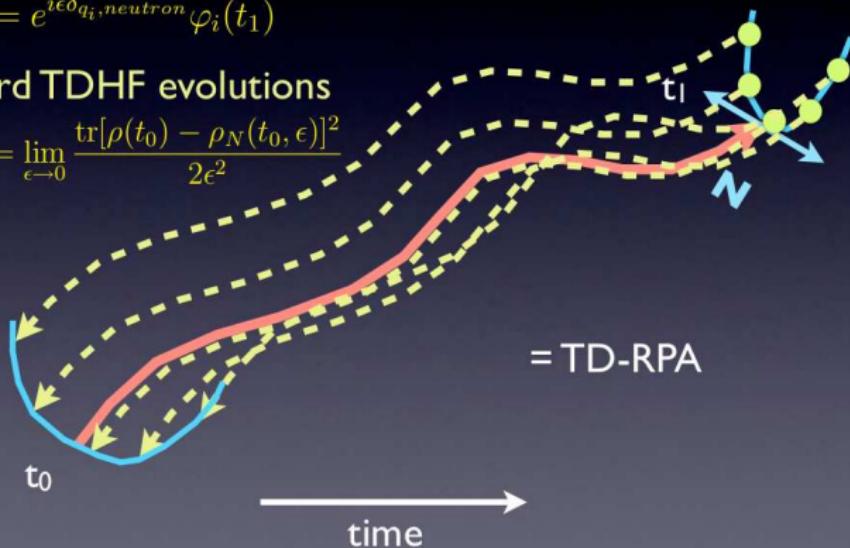
standard forward TDHF

neutron fluctuations at t_1

$$\varphi_i(t_1, \epsilon) = e^{i\epsilon\delta_{q_i, neutron}} \varphi_i(t_1)$$

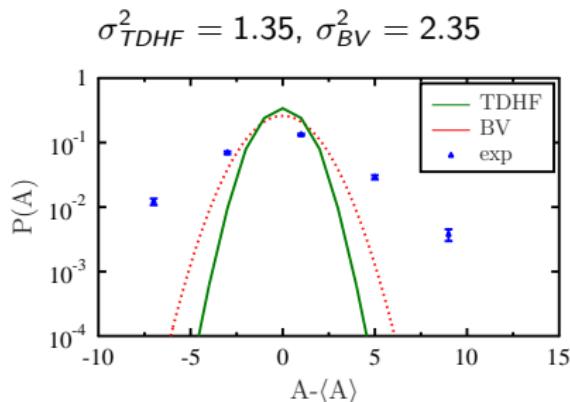
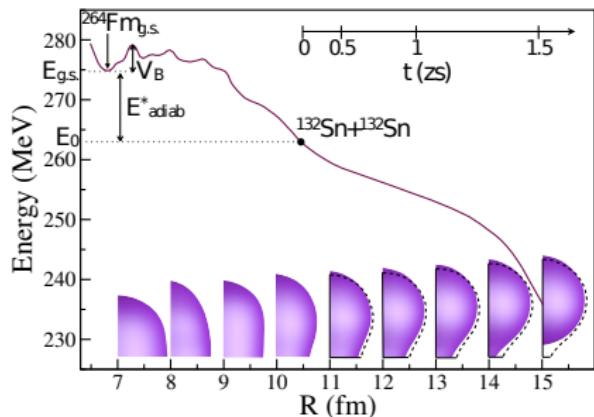
backward TDHF evolutions

$$\sigma_{NN}^2(t_1) = \lim_{\epsilon \rightarrow 0} \frac{\text{tr}[\rho(t_0) - \rho_N(t_0, \epsilon)]^2}{2\epsilon^2}$$



TDHF with Balian-Vénéroni variational principle

Results



Conclusion

BV provides the fluctuations for the scission process
Need initial fluctuations (second part of the talk)

Conclusion TDHF+BCS

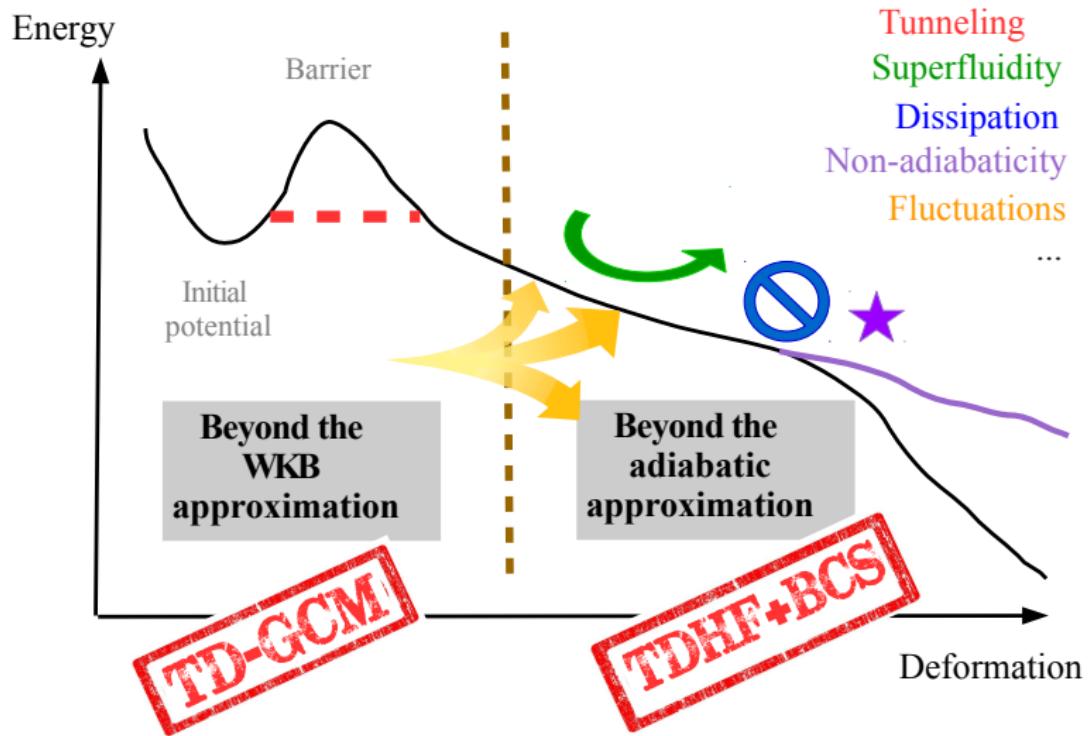
Conclusion

- Good reproduction of the total kinetic energy
- Important effect of pairing on fission process (J. W. Negele, et al. (1978))
- Reproduction of the even-odd effects
- Reproduction of the $Z \approx 54$ behavior
- Fluctuation obtained with Balian-Vénéroni method (for TDHF)

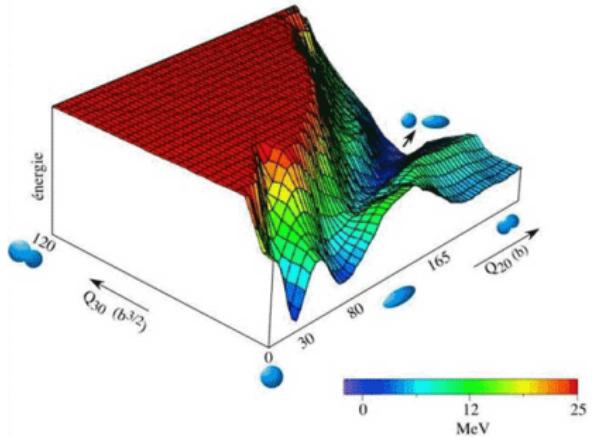
Prospects

- Finite temperature calculation
- Description of the evaporation
- Study of the collective excitation after the scission

Outlooks



Time-dependent generator coordinate method (TDGCM)

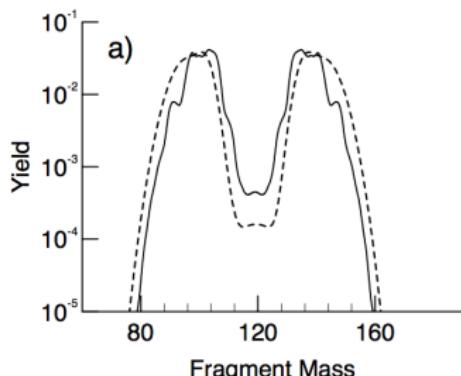


Time dependent Hill-Wheeler

$$|\Psi(t)\rangle = \int d\mathbf{q} f(\mathbf{q}, t) |\mathbf{q}\rangle$$

$$i\hbar \frac{\partial}{\partial t} g(i,j,t) = \sum_{k,l} H_{ij,kl} g(k,l,t)$$

H. Goutte Phys. Rev. C 71, 024316 (2005).



Dynamical description of tunneling effect

Aim of the study

Description of the fission dynamics under the barrier in a schematic model

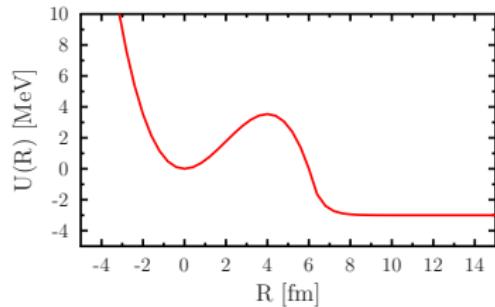
Observables of interest

- Life-time
- Fluctuations after the barrier

Can we describe the tunneling process with Time-dependent theory ?

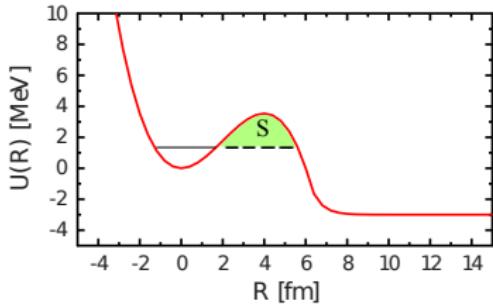
Schematic model

1D Model



$$H = -\frac{\hbar}{2M} \frac{\partial^2}{\partial R^2} + U(R)$$

WKB approximation

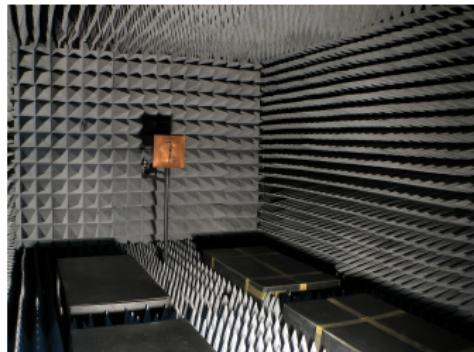


$$S = \int_{R_0}^{R_1} \sqrt{2M(U(R) - E_0)} dR$$

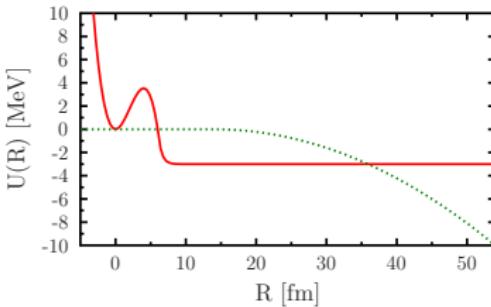
$$\tau = \frac{2\pi}{\Omega} e^{2S/\hbar}$$

CAP method

Anechoic chamber



Complex absorbing potential method



TDSE :

$$\begin{aligned} i\hbar \frac{d}{dt} |\Psi(t)\rangle &= (H + iW(R))|\Psi(t)\rangle \\ &= H'|\Psi(t)\rangle \end{aligned}$$

With

$$W(R) = W_0 \Theta(R - R_a)(R - R_a)^2$$

Numerical solution

Iterative method

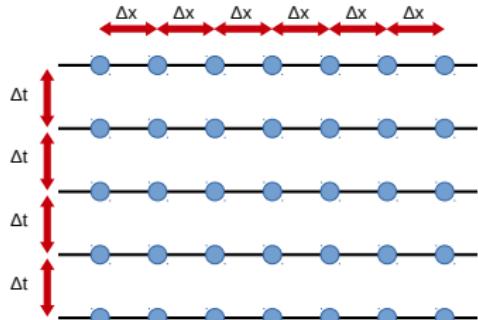
- Euler :

$$|\Psi(t + \delta t)\rangle = (1 - \frac{i\delta t}{\hbar} H') |\Psi(t)\rangle$$

- Runge-Kutta

- Crank-Nicholson :

$$|\Psi(t + \delta t)\rangle = \frac{1 - \frac{i\delta t}{2\hbar} H'}{1 + \frac{i\delta t}{2\hbar} H'} |\Psi(t)\rangle$$



Numerical solution

Iterative method

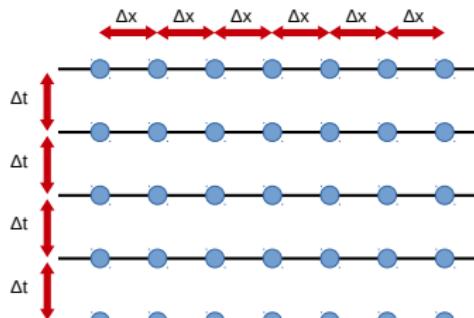
- Euler :

$$|\Psi(t + \delta t)\rangle = \left(1 - \frac{i\delta t}{\hbar} H'\right) |\Psi(t)\rangle$$

- Runge-Kutta

- Crank-Nicholson :

$$|\Psi(t + \delta t)\rangle = \frac{1 - \frac{i\delta t}{2\hbar} H'}{1 + \frac{i\delta t}{2\hbar} H'} |\Psi(t)\rangle$$



Problem

$\delta t \ll$ fission life-time

Determination of the life-time

Integration of the equation

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}tH'}|\Psi_0\rangle,$$

Hamiltonian eigenfunction basis :

$$H'|\varphi_i^r\rangle = E_i|\varphi_i^r\rangle \quad \text{and} \quad \langle\varphi_i^r|H' = E_i\langle\varphi_i^r|.$$

Closure relation :

$$|\varphi_i^r\rangle\langle\varphi_i^r| = \mathbb{1}$$

Simple evolution :

$$|\Psi(t)\rangle = \sum_i e^{-\frac{i}{\hbar}tE_i}|\varphi_i^r\rangle\langle\varphi_i^r|\Psi_0\rangle$$

Complex energy

Evolution :

$$|\Psi(t)\rangle = \sum_i e^{-\frac{i}{\hbar}tE_i}|\varphi_i^r\rangle\langle\varphi_i^r|\Psi_0\rangle$$

$$N(t) = \sum_i |\langle\varphi_i^r|\Psi_0\rangle|^2 e^{-\frac{2\text{Im}(E_i)}{\hbar}t}$$

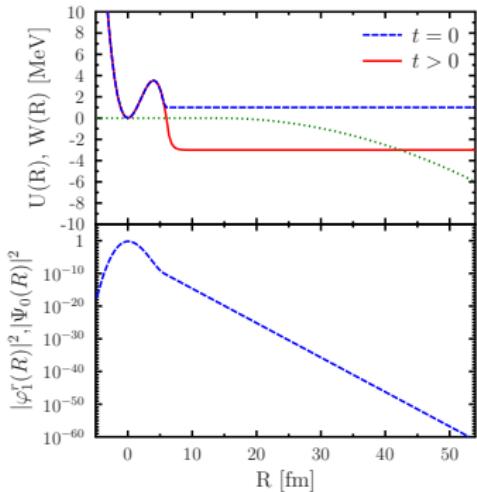
Resonance state associated with the complex energy :

$$H'|\varphi_i^r\rangle = (E_i^r + i\frac{\Gamma}{2})|\varphi_i^r\rangle$$

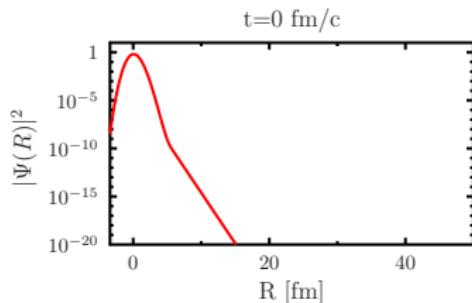
Γ : width of the resonance

1D model

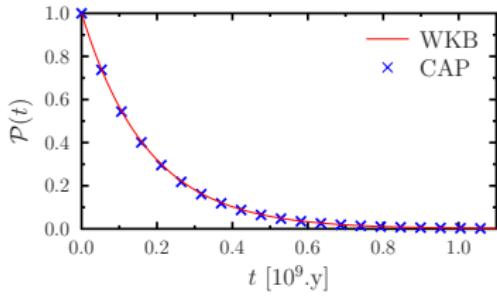
1D model



Dynamic

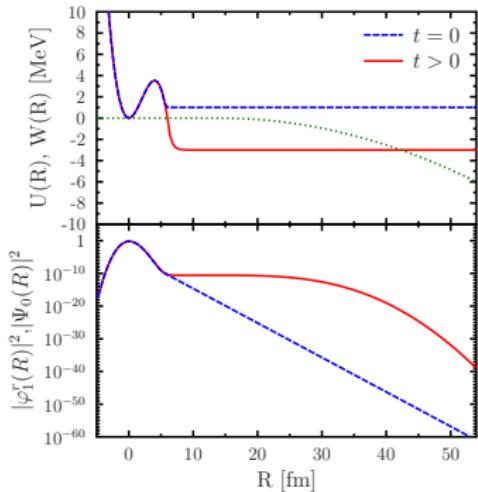


Decay

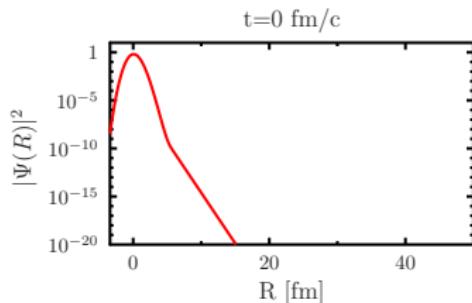


1D model

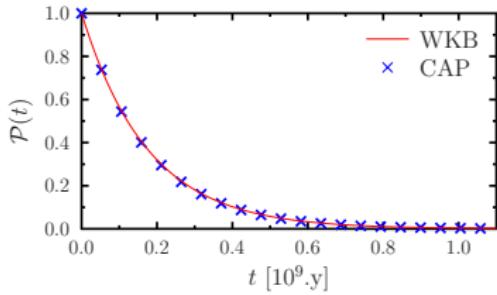
1D model



Dynamic

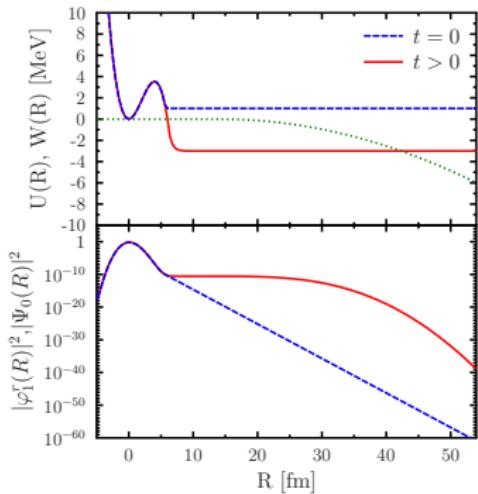


Decay



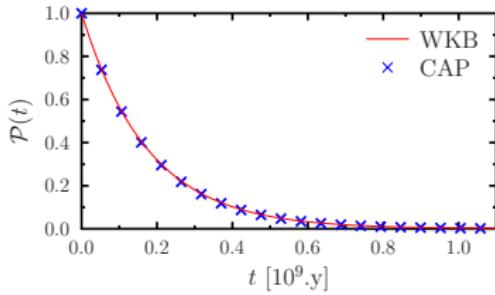
1D model

1D model



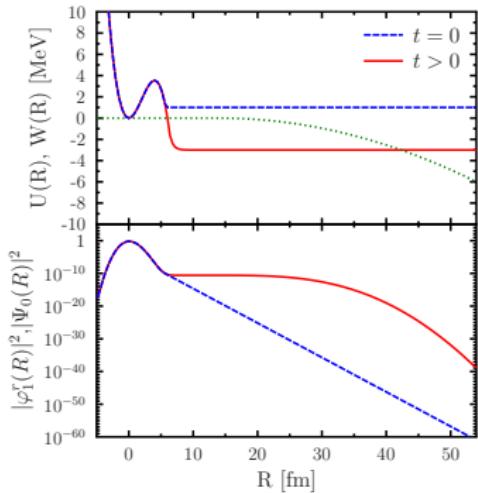
Dynamic

Decay



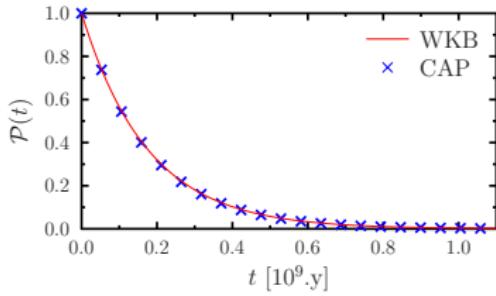
1D model

1D model



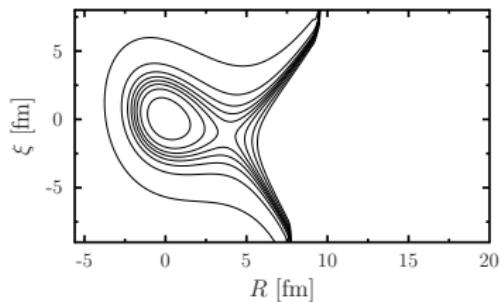
Dynamic

Decay

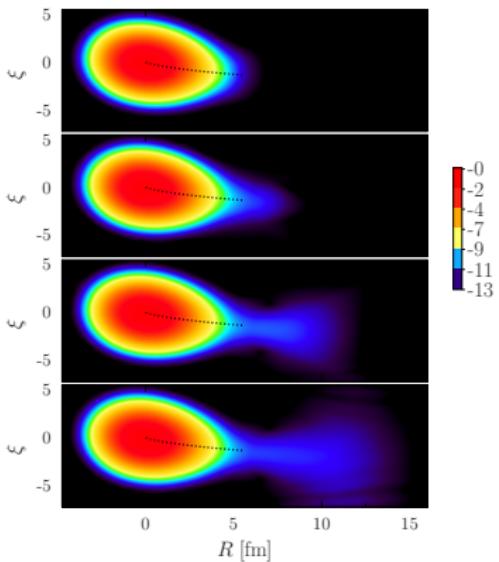


2D model

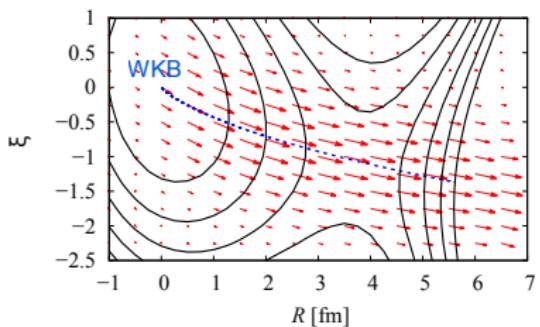
2D potential



Sub-barrier dynamics

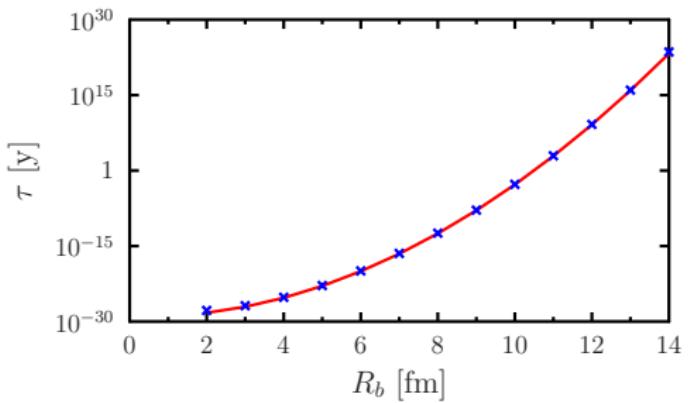


Comparaison of fission path



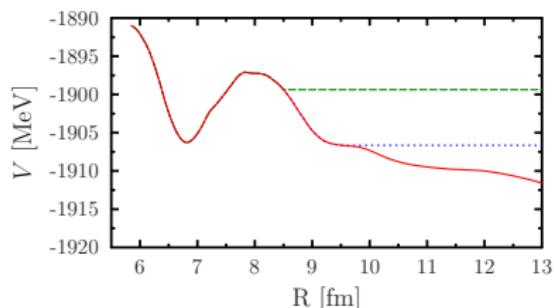
G. Scamps, K. Hagino, Phys. Rev. C 91, 044606 (2015).

Comparison with semi-classical trajectory

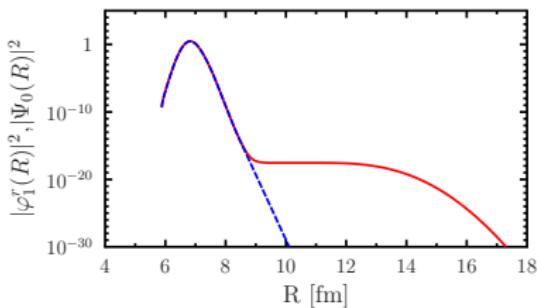


Collective hamiltonian

Static mean-field :
→ Effective mass
→ Potential $V(Q)$



Preliminary result



Difference of 20% on the life-time
between WKB and CAP method.

Conclusion

Conclusion

- Method to study very long tunneling processes
- Good agreement with the semi-classical theory

Prospect

- Application to realistic calculations

Thank you