

# Current trends in the microscopic description of fission

Denis Lacroix



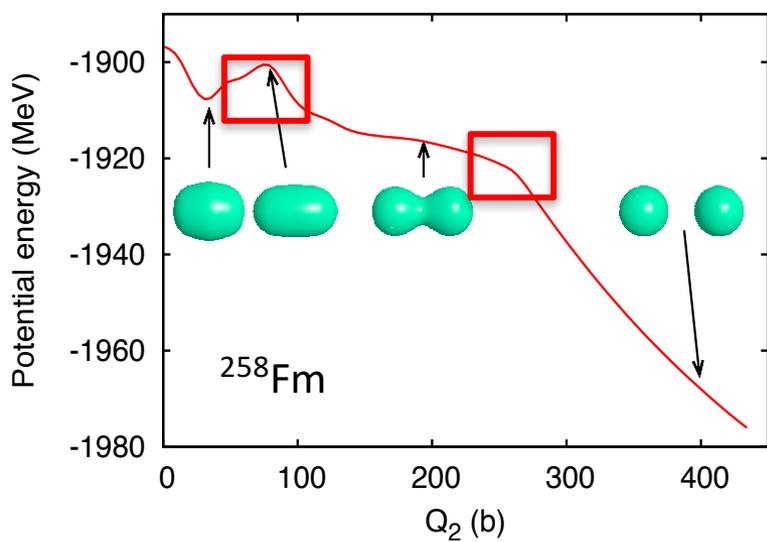
Ultimate goal:

Provide a fully microscopic description of fission from compound nucleus to separated fragments

Outline:

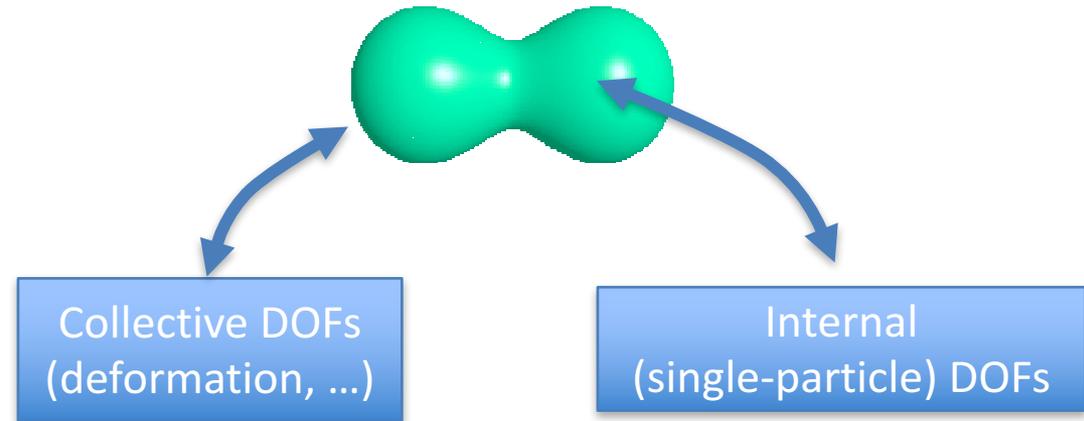
- Challenges in the description of fission
- Generalities on time-dependent approaches with pairing
- Recent application to fission
- Beyond quantum Mean-Field Theories: *deterministic vs stochastic* theories
- Applications and perspectives

Coll: S. Ayik, B. Yilmaz, C. Simenel,  
D. Regnier, G. Scamps, Y. Tanimura

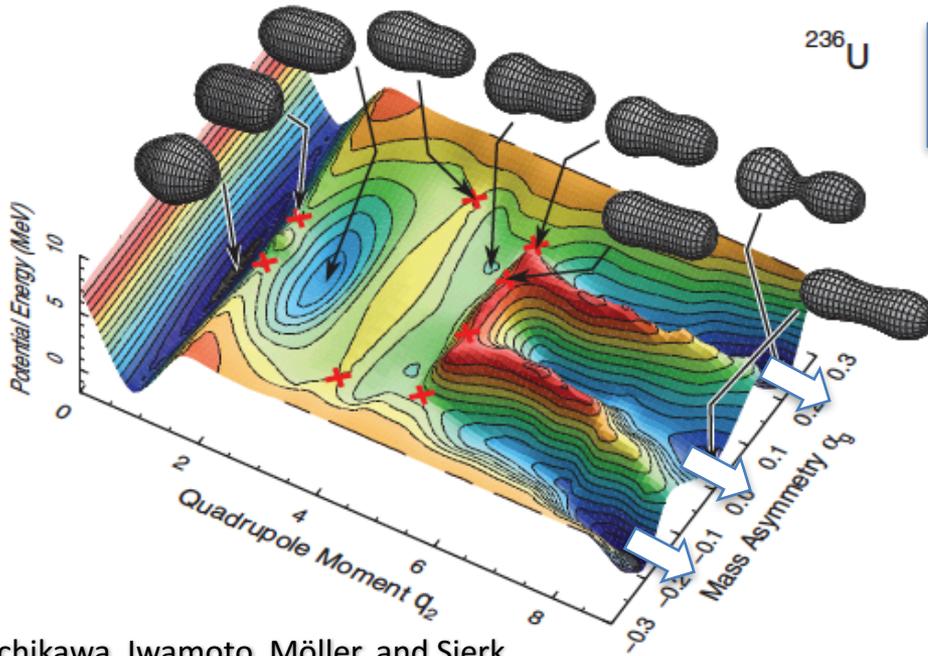


## Challenges in the fully microscopic description of fission

- Describe a large variety of degrees of freedom (DOFs) with different time-scales



- Quantum effect is important (both for collective and intrinsic): quantum tunneling, ...
- The process is not slow enough to be fully adiabatic in collective space (@scission).
- Superfluidity impact both quasi-static and dynamical effects (see later).
- Systems are big and the global time-scale can be very long (up to million of years)
- The number of DOFs might be very large.



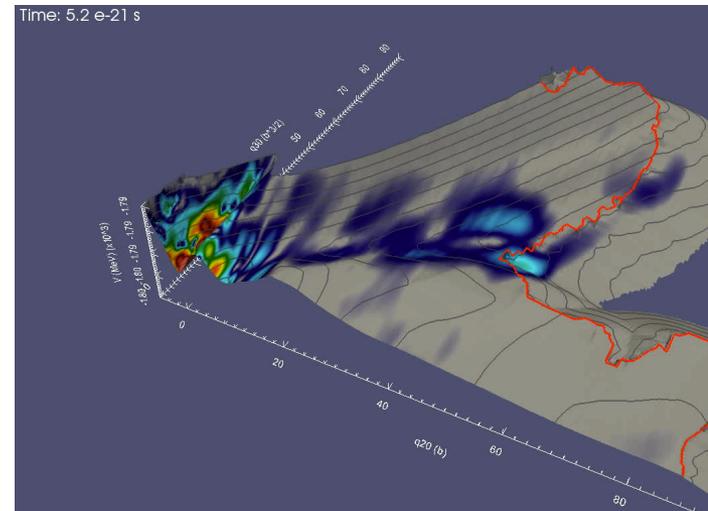
Ichikawa, Iwamoto, Möller, and Sierk,  
Phys. Rev. C 86 (2012)

Solve quantum motion in collective space

$$|\Psi(t)\rangle = \int_{\mathbf{q}} g(\mathbf{q}, t) |\xi(\mathbf{q})\rangle d\mathbf{q}$$



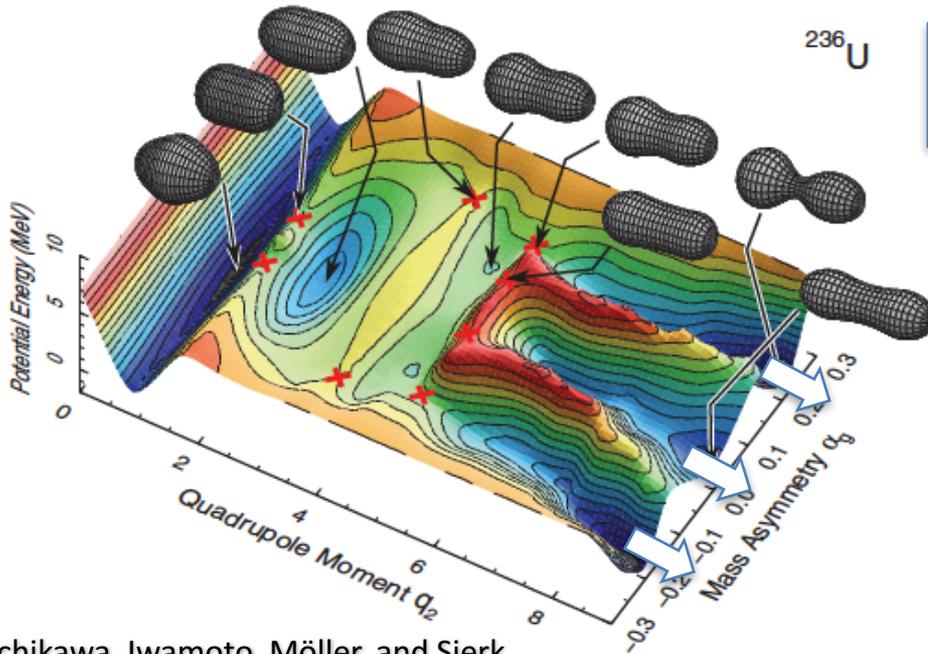
$$i\hbar \frac{\partial g(\mathbf{q}, t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q}) g(\mathbf{q}, t).$$



(Courtesy D. Regnier)

## Advantages

- ➔ Treat quantum effects in collective space: (quantum tunneling, interferences)
- ➔ As its counterpart in nuclear structure (static GCM)
- ➔ Works quite well for mass yields



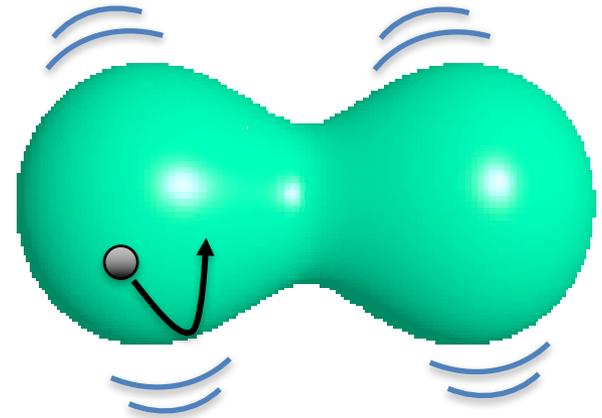
Ichikawa, Iwamoto, Möller, and Sierk, Phys. Rev. C 86 (2012)

Solve quantum motion in collective space

$$|\Psi(t)\rangle = \int_{\mathbf{q}} g(\mathbf{q}, t) |\xi(\mathbf{q})\rangle d\mathbf{q}$$



$$i\hbar \frac{\partial g(\mathbf{q}, t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q}) g(\mathbf{q}, t).$$



Difficulties

Some of this difficulties can be solved using Time-dependent EDF

- Dimensionality: number of collective DOFs. Proper mass require doubling the dimension.

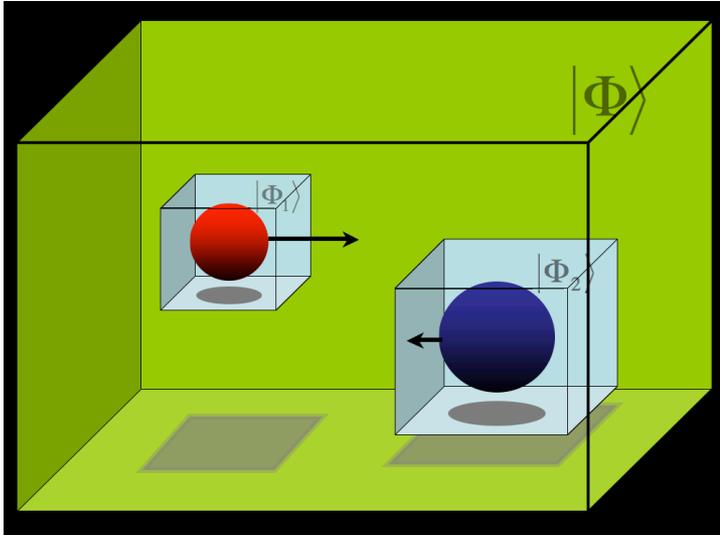
- Energy landscape has discontinuities.

- Full GCM is not well defined within the EDF approach

Lacroix et al, Phys. Rev. C79 (2009); Robledo J. Phys. G 37 (2010),...

- Motion can be non-adiabatic: onset of dissipation, fluctuations, non-Markovian effects.

## Nuclear reaction with superfluid nuclei on a mesh



TDHF is a standard tool  $|\Phi_i\rangle$ : Slater

$$i\hbar \frac{d\rho}{dt} = [h(\rho), \rho] \quad \rightarrow \text{Single-particle evolution}$$

Simenel, Lacroix, Avez, arXiv:0806.2714v2

Introduction of pairing: TDHFB

$$i\hbar \frac{d\mathcal{R}}{dt} = [\mathcal{H}(\mathcal{R}), \mathcal{R}] \quad \mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho \end{pmatrix}$$

$\rightarrow$  Quasi-particle evolution

(Active Groups: France, US, Japan...)

**TDHFB = 1000 \* (TDHF)**

$\rightarrow$  Full TDHFB (Skyrme-spherical symmetry)

Avez, Simenel, Chomaz, PRC 78 (2008).

Full TDHFB (Skyrme-symmetry unrestricted)  
(Gogny-axial symmetry)

Stetcu, Bulgac, Magierski, and Roche, PRC 84 (2011)

Y. Hashimoto, PRC 88 (2013).

$\rightarrow$  Symmetry unrestricted TDBCS limit of TDHFB (also called Canonical basis TDHFB)

Neglect  $\Delta_{ij} \rightarrow |\Phi(t)\rangle = \prod_{k>0} \left( u_k(t) + v_k(t) a_k^\dagger(t) a_{\bar{k}}^\dagger(t) \right) |-\rangle.$

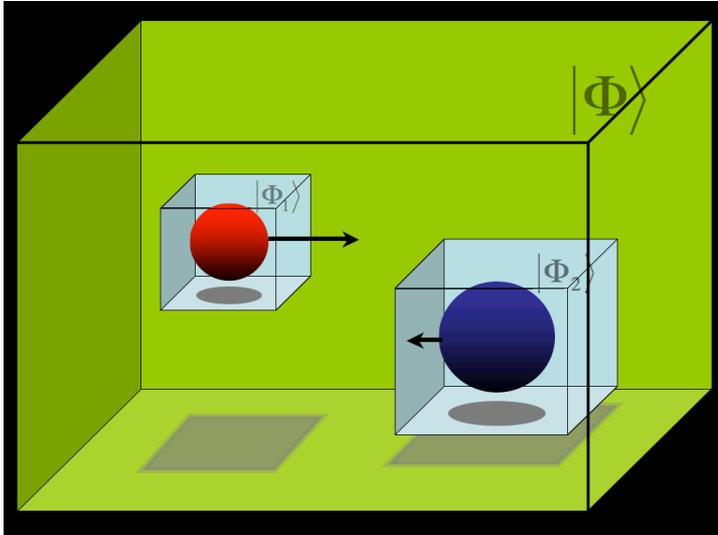
**TDBCS = 2-3 \* (TDHF)**

Ebata, Nakatsukasa et al, PRC82 (2010)

Scamps, Lacroix, PRC88 (2013).

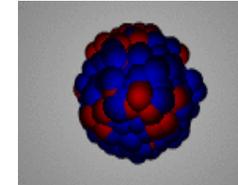
$\rightarrow$  Very good predictive power

### Nuclear reaction with superfluid nuclei on a mesh



Applied to a number of physical process

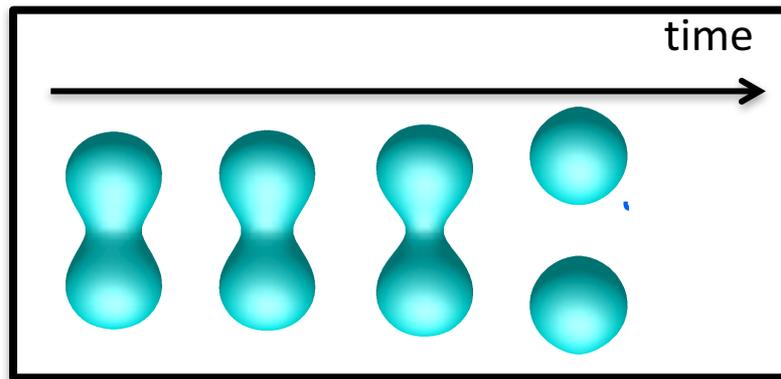
Vibrations



Fusion/Transfert

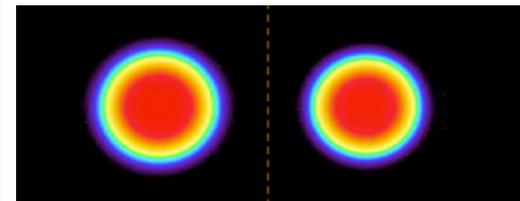
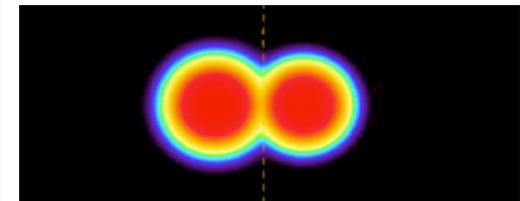
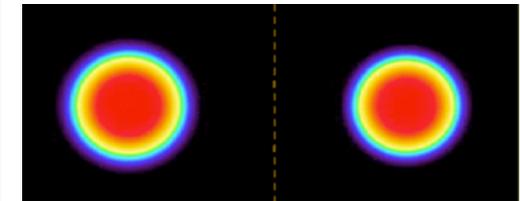
Scamps, Tanimura, Regnier, Lacroix (2012-2017)

Fission



$^{48}\text{Ca}$

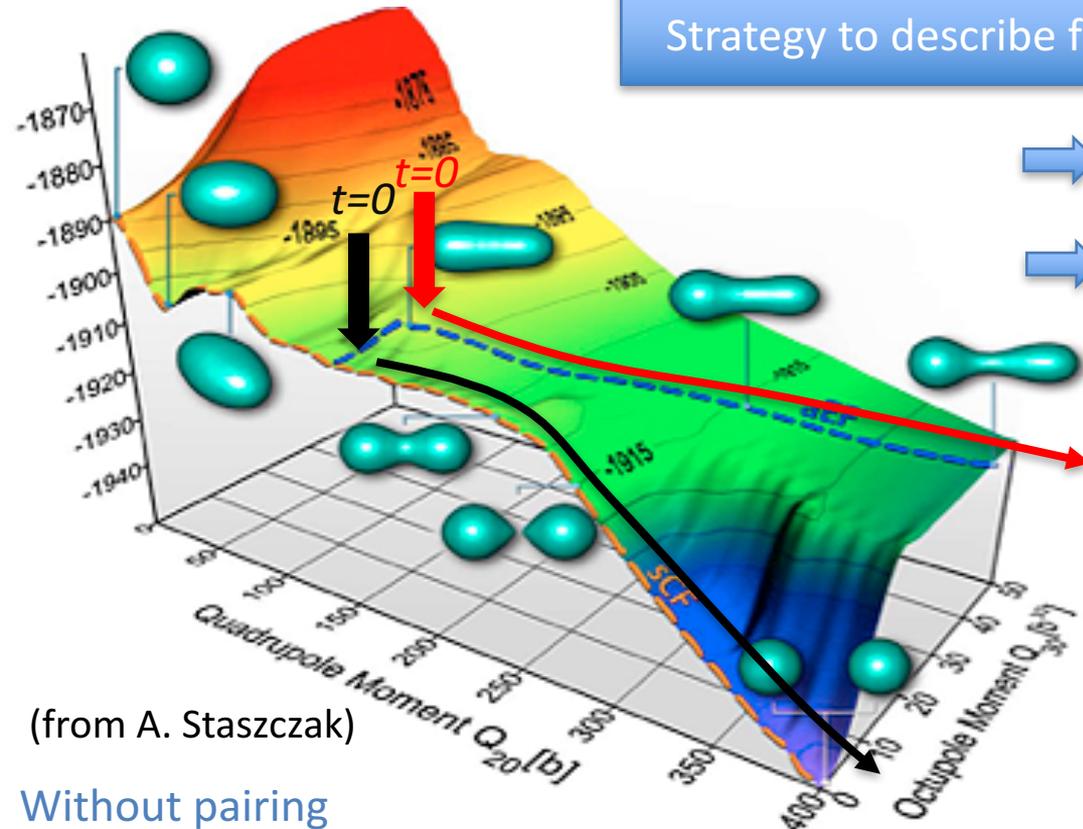
$^{40}\text{Ca}$



time

# Description of fission in a time-dependent mean-field framework

Strategy to describe fission in mean-field



Choose an initial condition

Follow the system in time until something happens (fission)

Advantages

- fully microscopic time-dependent
- non-adiabatic theory
- symmetry unrestricted  
(however with no spontaneous symmetry breaking)

Drawback

- almost classical in collective space  
(fluctuations are underestimated,  
no quantum tunneling, interferences ...)

(from A. Staszczak)

Without pairing

Simenel, Umar, PRC C89 (2014).

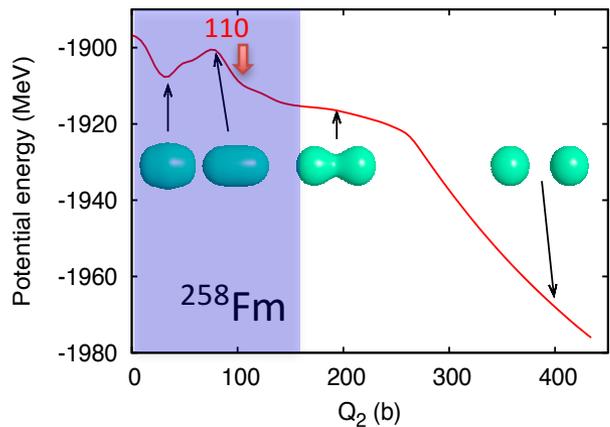
Goddard, Stevenson, Rios, PRC 92 (2015), 93 (2016)

With pairing

Scamps Simenel, Lacroix, PRC92 (2015)

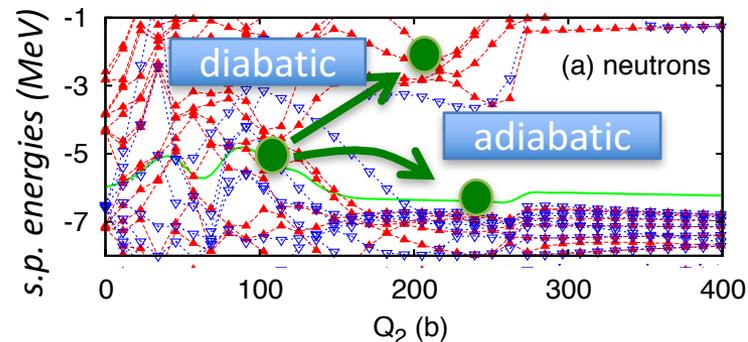
Tanimura, Lacroix, Scamps, PRC 92 (2015)

Bulgac, Magierski, Roche, and Stetcu, PRL 116, 122504 (2016)



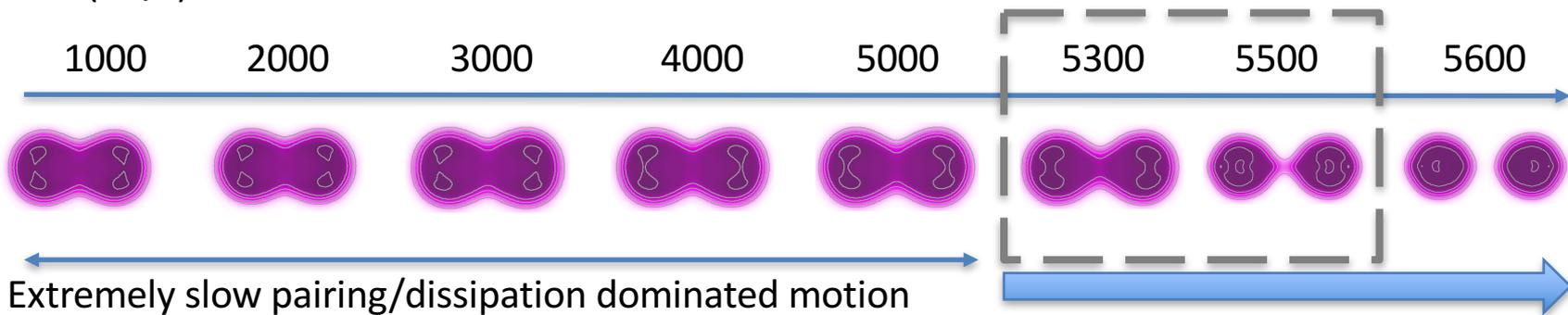
Without pairing the system do not fission:  
Mean-field without pairing is too diabatic!

## Time-dependent mean-field with pairing Accounting for non-adiabaticity



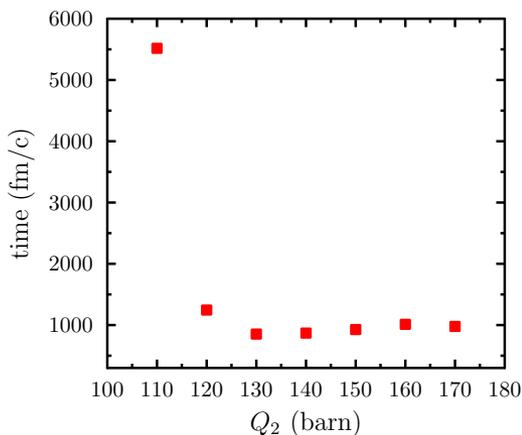
TDHFB or TDHF+BCS solve this problem

Time (fm/c)



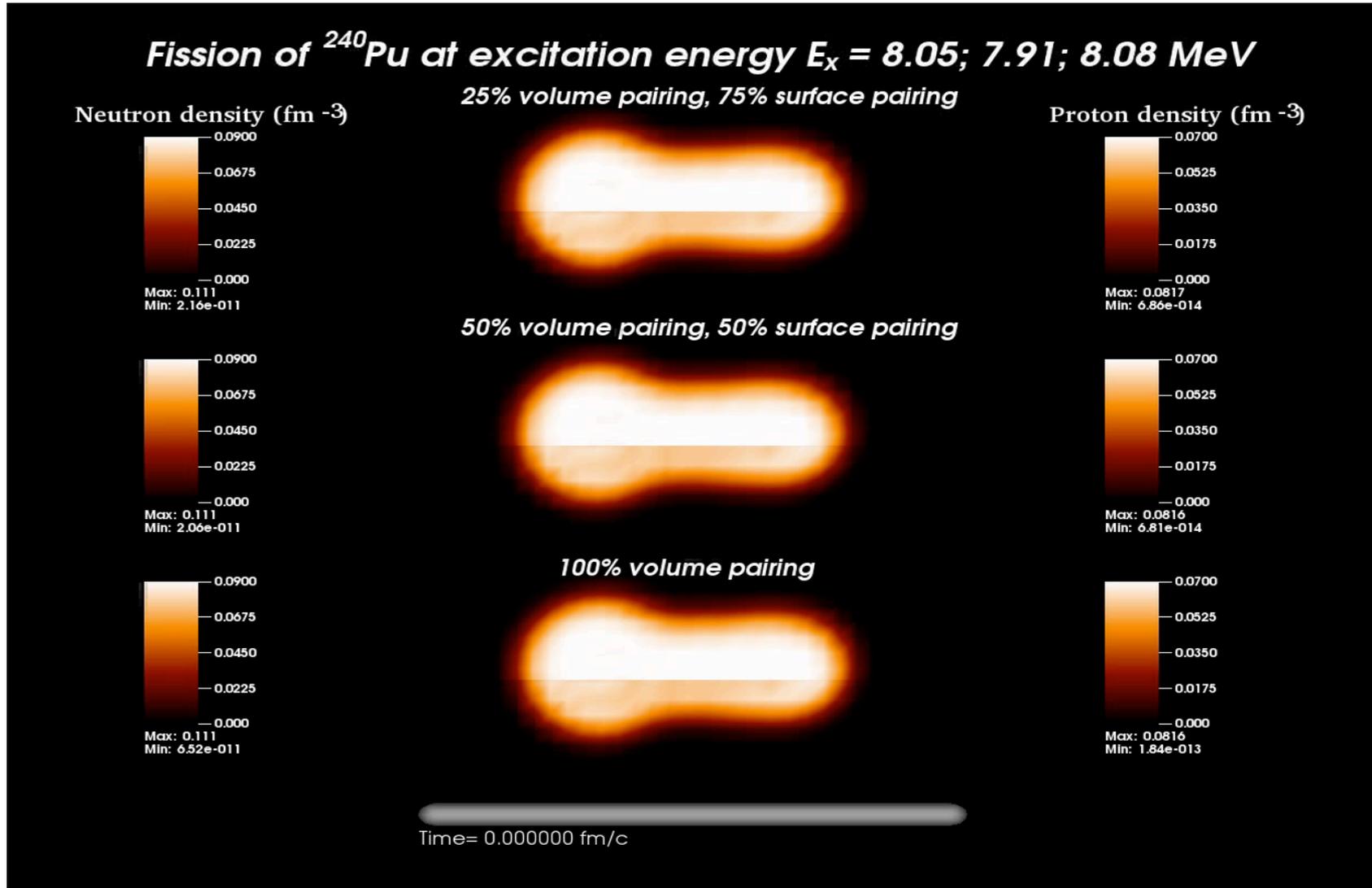
Fission time with  
TDHF+BCS

Scamps, Simenel, DL PRC 92 (2015)  
Tanimura, DL, Ayik, PRL 118 (2017)

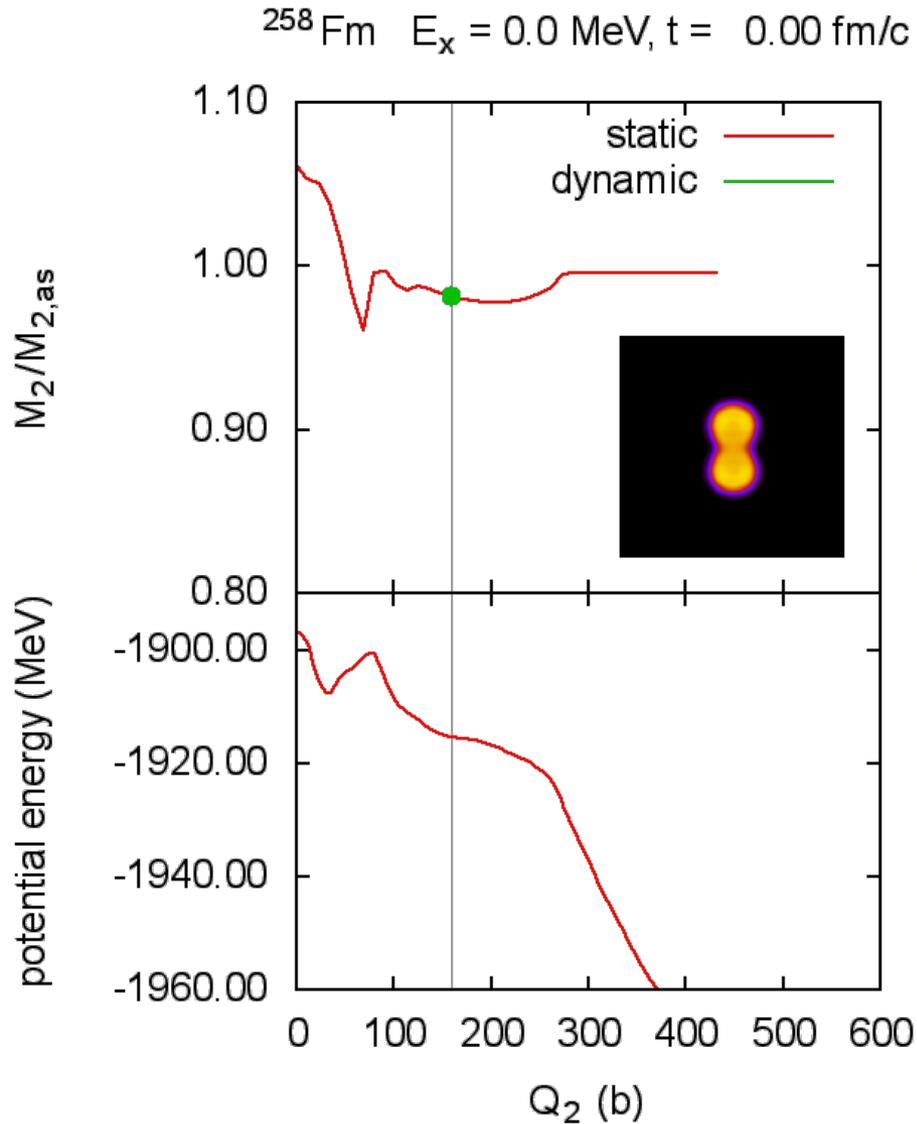


Confirms the finding of:

Bulgac, Magierski, Roche, and Stetcu  
Phys. Rev. Lett. 116, 122504 (2016)



Tanimura, DL, Scamps, PRC 92 (2015)



Microscopic dynamic

$$\frac{dq_\alpha}{dt} = -\frac{i}{2\hbar m} \text{Tr}([Q_\alpha, p^2]\rho(t)) \equiv \frac{p_\alpha}{M_\alpha},$$

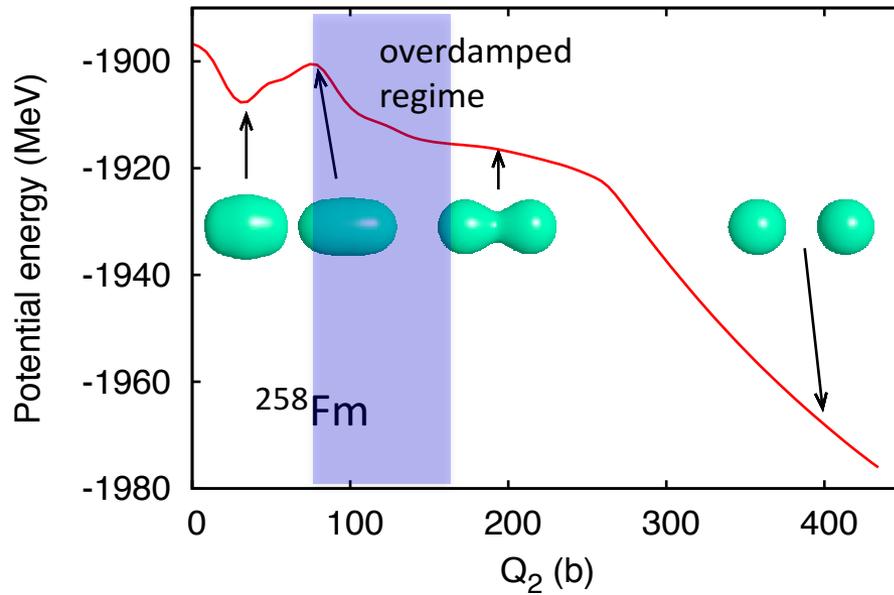
$$\hat{P}_\alpha \equiv -i \frac{M_\alpha}{2\hbar m} \sum_{ij} \langle i | [\hat{Q}_\alpha, \hat{p}^2] | j \rangle \hat{a}_i^\dagger \hat{a}_j.$$

$$\langle [\hat{Q}_\alpha, \hat{P}_\alpha] \rangle = i\hbar, \quad \Rightarrow \quad \frac{1}{M_\alpha(t)} = \frac{1}{m} \text{Tr}[\rho(t) \nabla Q_\alpha \cdot \nabla Q_\alpha],$$

 Macroscopic evolution:  
Dissipation, non-adiabatic effects...

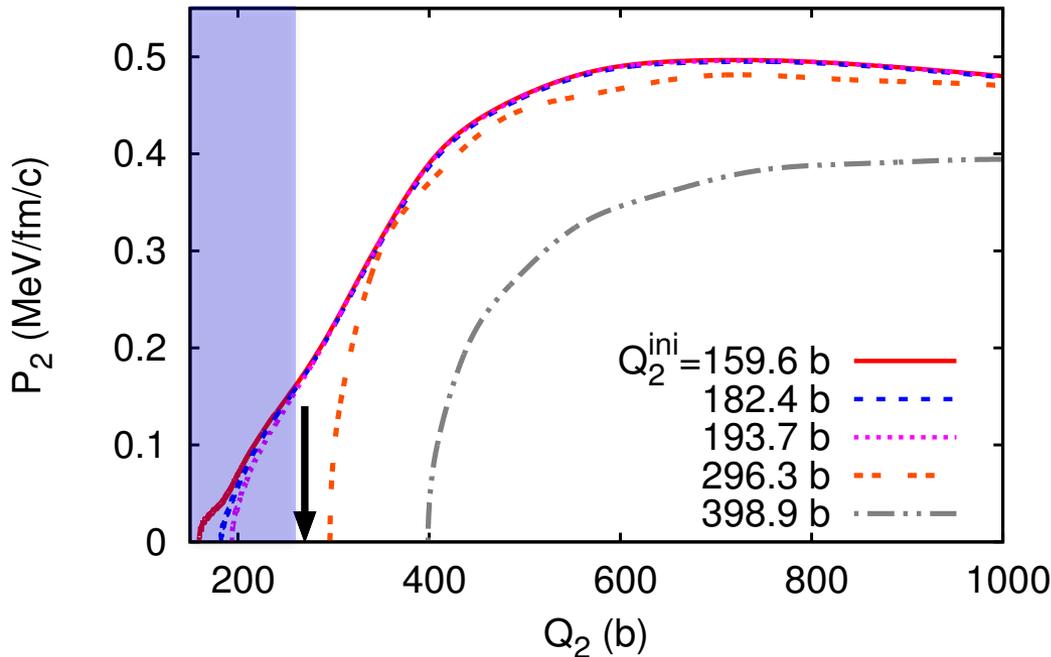
- ➔ The system first follows the adiabatic limit
- ➔ Around scission, dynamic is faster and Becomes non-adiabatic

$$E_{\text{diss}} \simeq 20\text{MeV} \quad \text{TKE} \simeq 250\text{MeV}$$

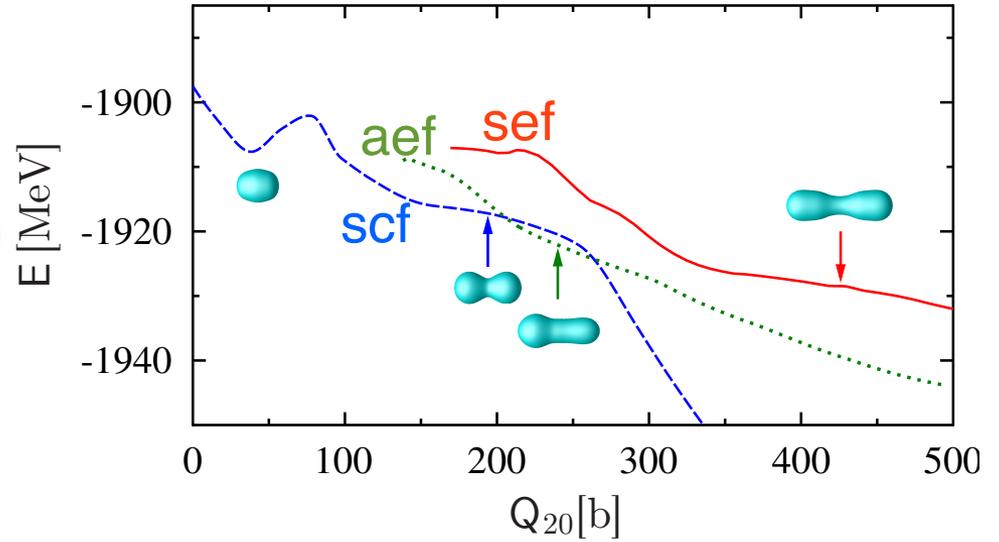
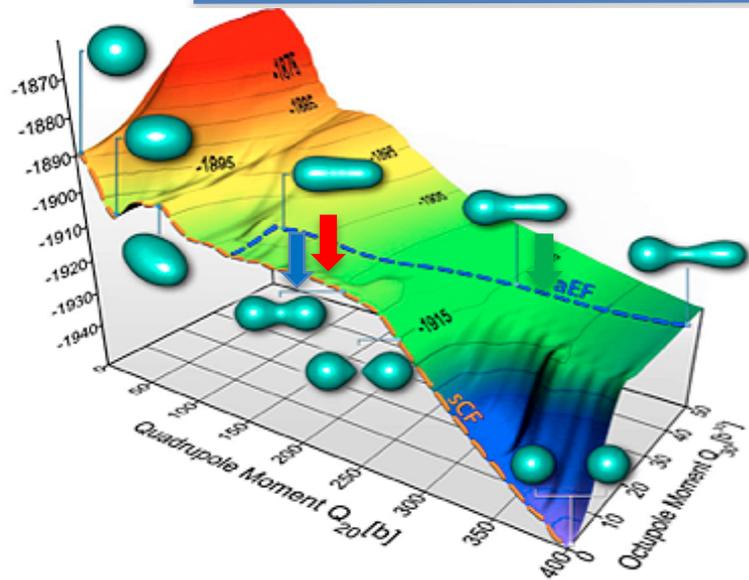


➔ More or less we confirm the overdamped regime before scission (Randrup, Moller model)

## Collective momentum evolution

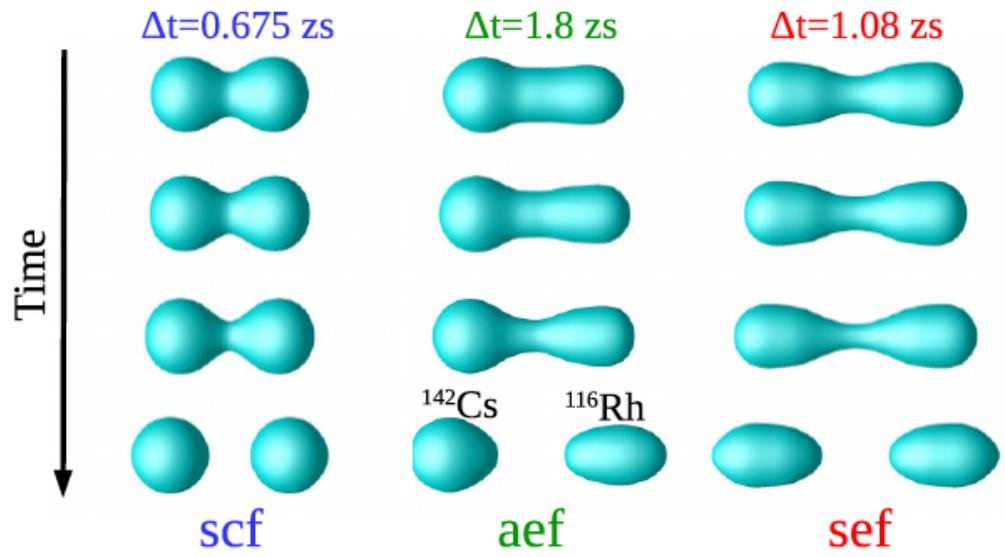


➔ Still open : Precise values of dissipative transport coefficients



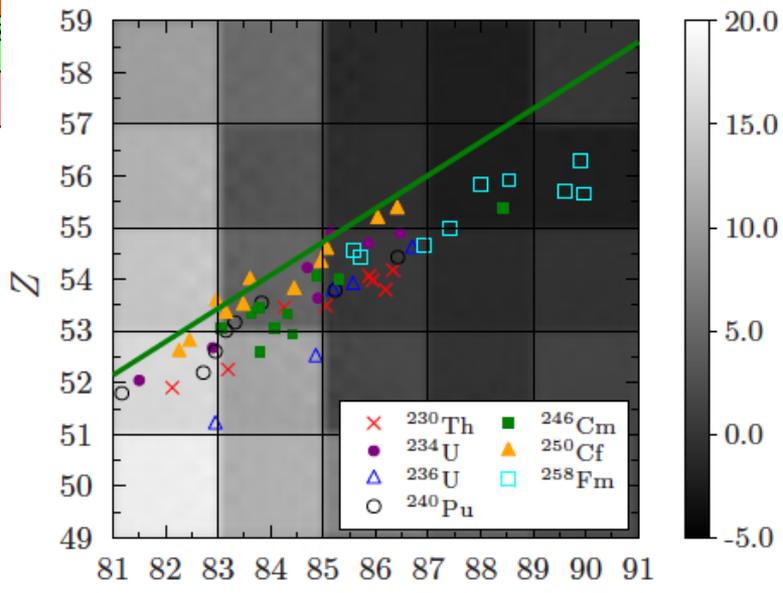
Identification of main fission paths

1 zs =  $10^{-21}$  s



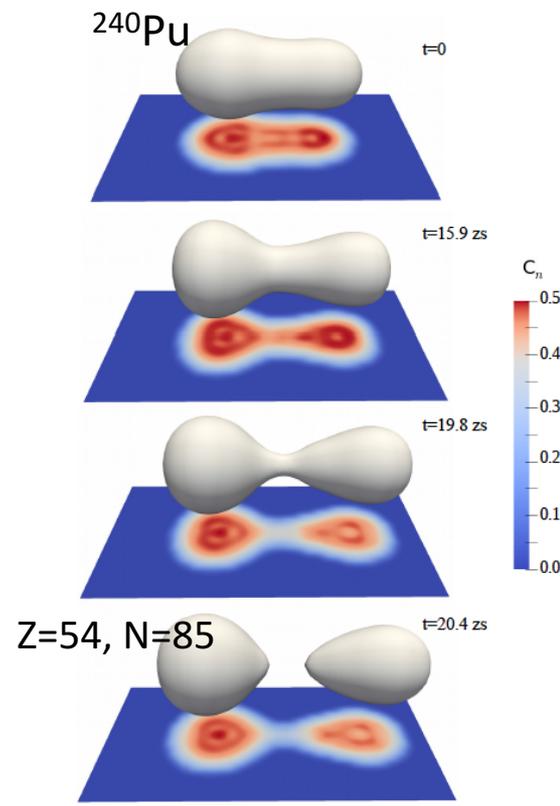
98		Cf237	21.1 S	Cf238	21.1 MS	Cf239	39 S	Cf240	1.06 M	Cf241	3.78 M	Cf242	3.4 M	Cf243	10.7 M	Cf244	19.4 M	Cf245	45.0 M	Cf246	35.7 H	Cf247	3.11 H	Cf248	333.5 D	Cf249	351 Y	Cf250	13.08 Y	Cf251	868 Y
97	Bk235	Bk236	Bk237	Bk238	Bk239	Bk240	Bk241	Bk242	Bk243	Bk244	Bk245	Bk246	Bk247	Bk248	Bk249	Bk250															
96	Cm234	Cm235	Cm236	Cm237	Cm238	Cm239	Cm240	Cm241	Cm242	Cm243	Cm244	Cm245	Cm246	Cm247	Cm248	Cm249															
95	Am233	Am234	Am235	Am236	Am237	Am238	Am239	Am240	Am241	Am242	Am243	Am244	Am245	Am246	Am247	Am248															
94	Pu232	Pu233	Pu234	Pu235	Pu236	Pu237	Pu238	Pu239	Pu240	Pu241	Pu242	Pu243	Pu244	Pu245	Pu246	Pu247															
93	Np231	Np232	Np233	Np234	Np235	Np236	Np237	Np238	Np239	Np240	Np241	Np242	Np243	Np244																	
92	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242																		
91	Pa229	Pa230	Pa231	Pa232	Pa233	Pa234	Pa235	Pa236	Pa237	Pa238	Pa239	Pa240																			
90	Th228	Th229	Th230	Th231	Th232	Th233	Th234	Th235	Th236	Th237	Th238																				

Recent systematic analysis: N/Z physics  
The Z=54 attractor

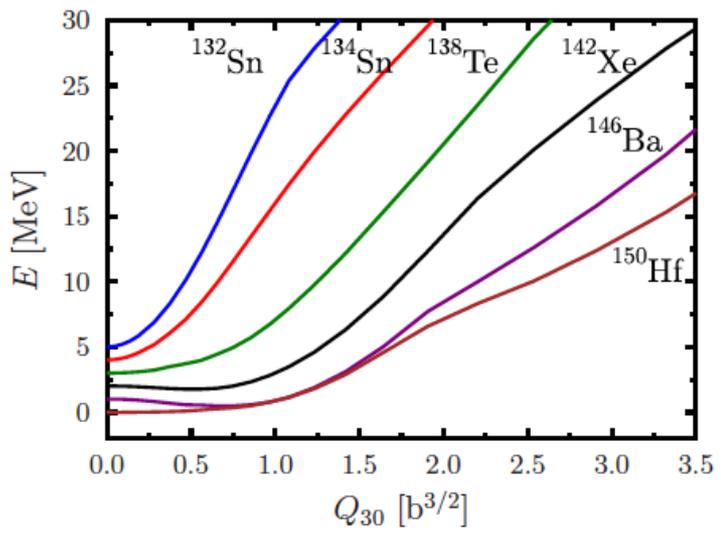


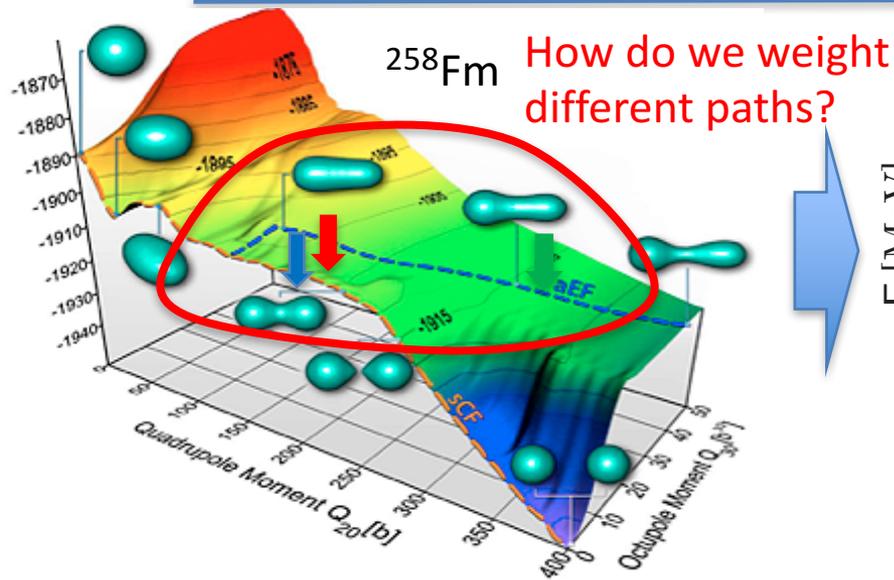
Scamps, Simenel, arxiv (2018)

<http://www.nuclear.nsd.c.cn/nuclear/chart17.asp>

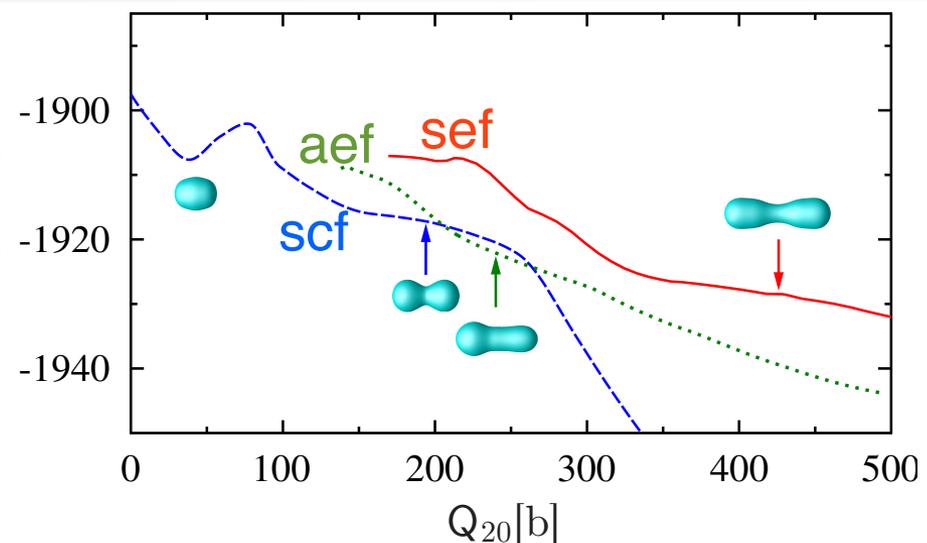


→ The preferential fission towards fragments with Z=52-56 might stems from the octupole softness around Barium.

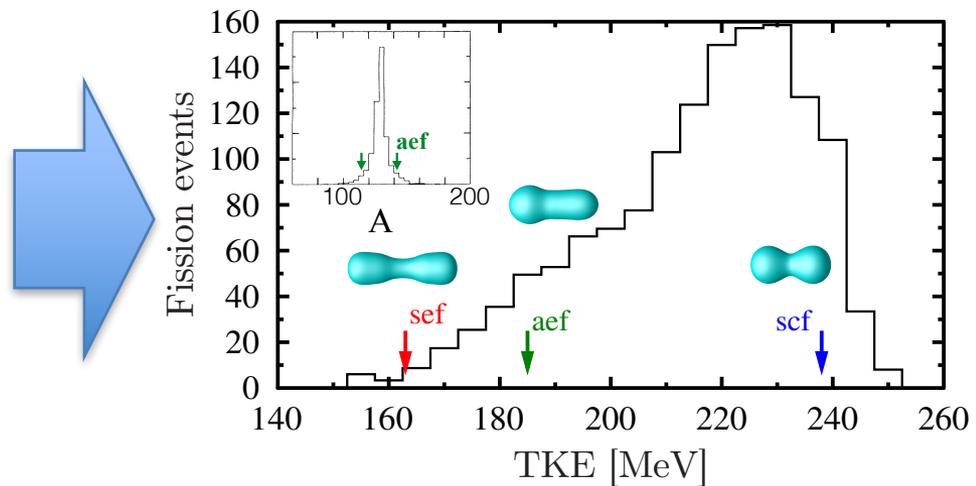




E [MeV]



Total Kinetic Energy



Some conclusions

- ➔ TKE seems compatible with experiments
- ➔ Dynamic seems almost adiabatic up to scission point and then is Well describe by TDHF-BCS

Remaining problem

- ➔ Fluctuations are underestimated
- ➔ Weight of each paths?

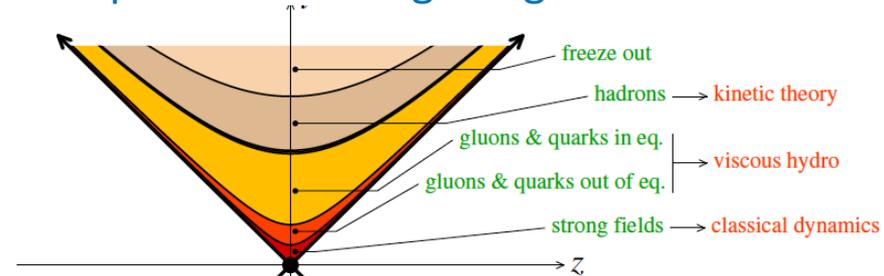
Our objective: use the *stochastic mean-field* approach to describe fission

Lacroix, Ayik, EPJA (Review) 50 (2014)

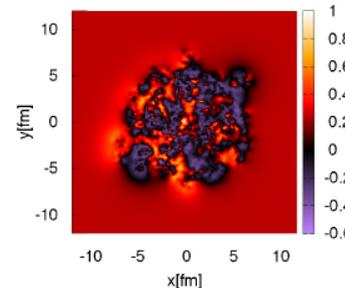
Quantum fluctuations can be treated approximately by sampling initial zero-point motion followed by classical trajectories (here classical=mean-field)

Related approaches:

-description of little big-bang at RHIC or LHC

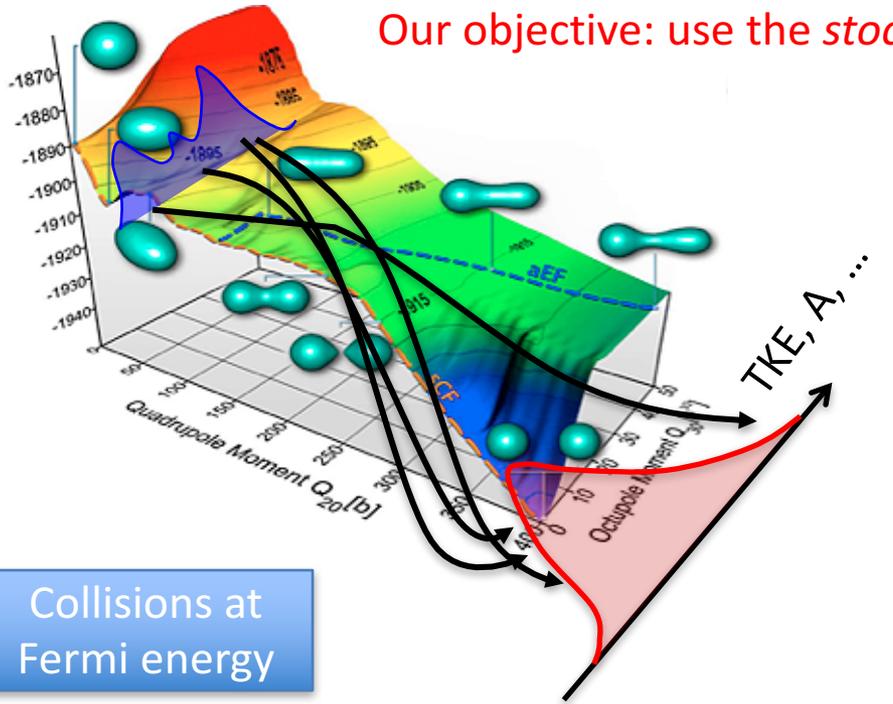


Gelis, Schenke, arxiv:1604:00335



Truncated Wigner theory  
For Bose-Einstein condensates

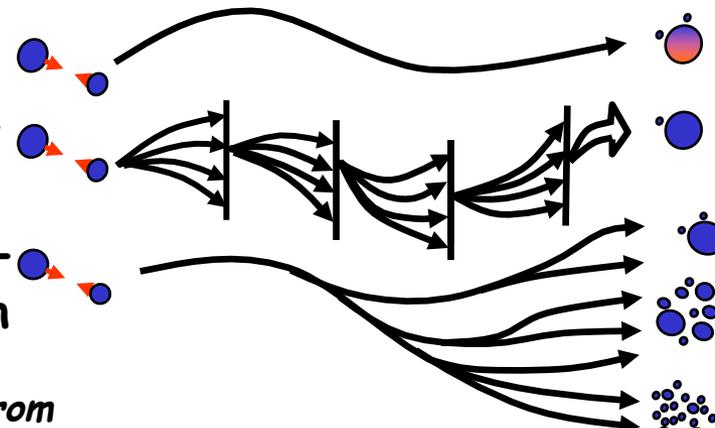
Sinatra, Lobo, and Castin, J. Phys. B 35 (2002)



Vlasov

BUU, BNV

Boltzmann-Langevin



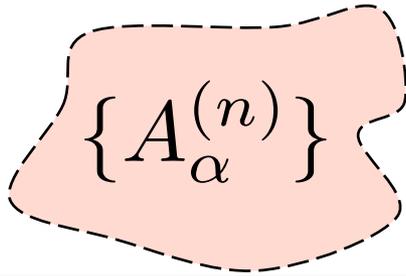
Adapted from  
J. Randrup et al, NPA538 (92).

Mean-Field theory

$$\frac{d\langle A_\alpha \rangle}{dt} = \mathcal{F}(\{\langle A_\beta \rangle\}) \quad \text{at all time} \quad \sigma_Q^2 = \langle A^2 \rangle - \langle A \rangle^2$$

Stochastic Mean-Field

$$\frac{dA_\alpha^{(n)}}{dt} = \mathcal{F}(\{A_\beta^{(n)}\})$$



$$\text{at all time} \quad \Sigma_C^2 = \overline{A^{(n)} A^{(n)}} - \overline{A^{(n)}}^2$$

$$\text{Constraint:} \quad \Sigma_C^2(t=0) = \sigma_Q^2(t=0)$$

SMF in density matrix space: simple initial state

$$\rho(\mathbf{r}, \mathbf{r}', t_0) = \sum_i \Phi_i^*(\mathbf{r}, t_0) n_i \Phi_j(\mathbf{r}', t_0)$$

$$\rho^\lambda(\mathbf{r}, \mathbf{r}', t_0) = \sum_{ij} \Phi_i^*(\mathbf{r}, t_0) \rho_{ij}^\lambda \Phi_j(\mathbf{r}', t_0)$$

$$\overline{\rho_{ij}^\lambda} = \delta_{ij} n_i$$

$$\overline{\delta \rho_{ij}^\lambda \delta \rho_{j'i'}^\lambda} = \frac{1}{2} \delta_{jj'} \delta_{ii'} [n_i(1 - n_j) + n_j(1 - n_i)].$$

S. Ayik, PLB 658 (2008)



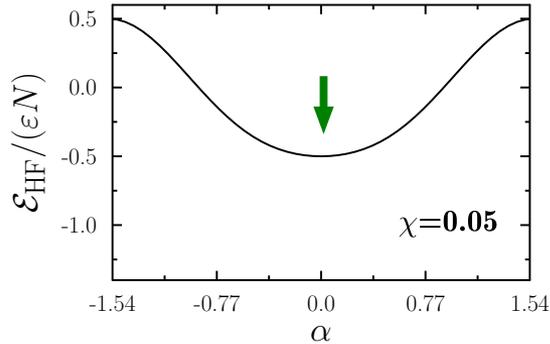
It gives a natural link with the theory of open quantum systems (quantum Langevin approach, non-Markovian, ...)

$$m \frac{dv(t)}{dt} = F - \gamma v(t) + \eta(t)$$



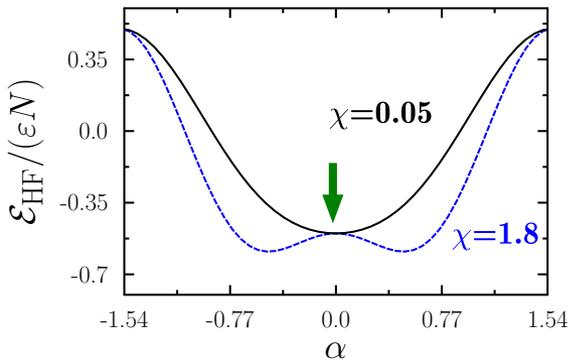
The noise comes from the complexity of the bath that is treated through random initial conditions

Harmonic collective space

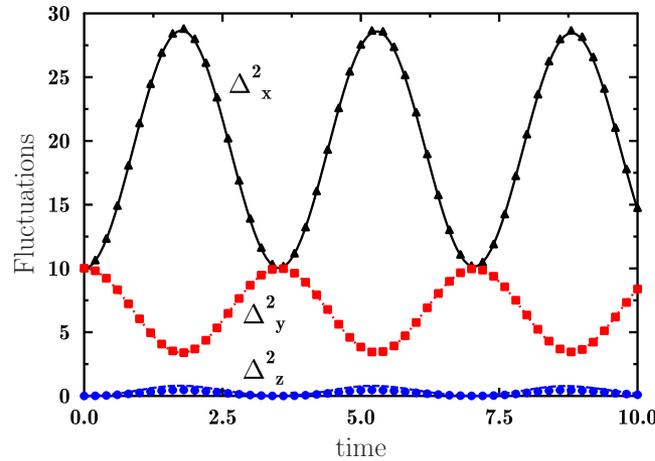
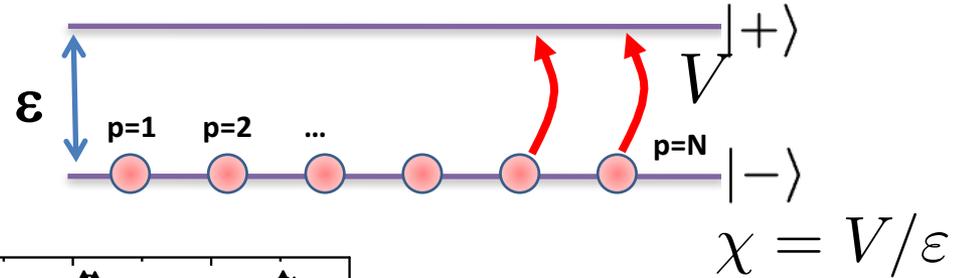


DL, Ayik, Yilmaz, PRC (2012)  
DL, Tanimura, Ayik, EPJA (2016)

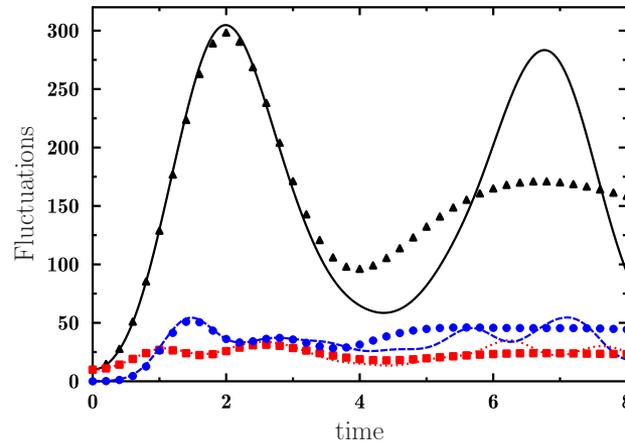
Anharmonic unstable collective space



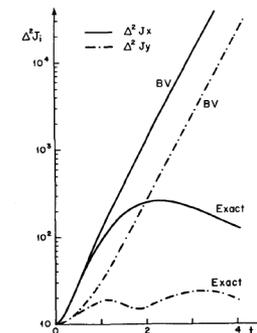
Two-Level Lipkin Model



Effect beyond mean-field (RPA like) almost exactly treated!



Short time is properly treated. Decay time also...



BV result

$$\chi = 1.5$$

Bonche, Flocard, NPA437 (1985)

Progress

➔ Extension to superfluid systems: TDHFB with fluctuations

Lacroix, Gambacurta, Ayik, Yilmaz, PRC C 87, 061302(R) (2013)

➔ Mapping initial fluctuations with complex initial correlations

Yilmaz, Lacroix, Curecal, PRC C 90, 054617 (2014).

➔ Application to optical lattice: better than non-equilibrium 2-body green functions

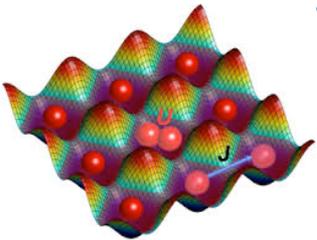
Lacroix, Hermanns, Hinz, Bonitz, PRB90 (2014)

➔ Equivalent to simplified *un-truncated* BBGKY hierarchy

Lacroix, Tanimura, Ayik, EPJA52 (2016)

DL, Ayik, Yilmaz, PRC (2012)

DL, Ayik, EPJA [Review] (2016)



SMF in density matrix space

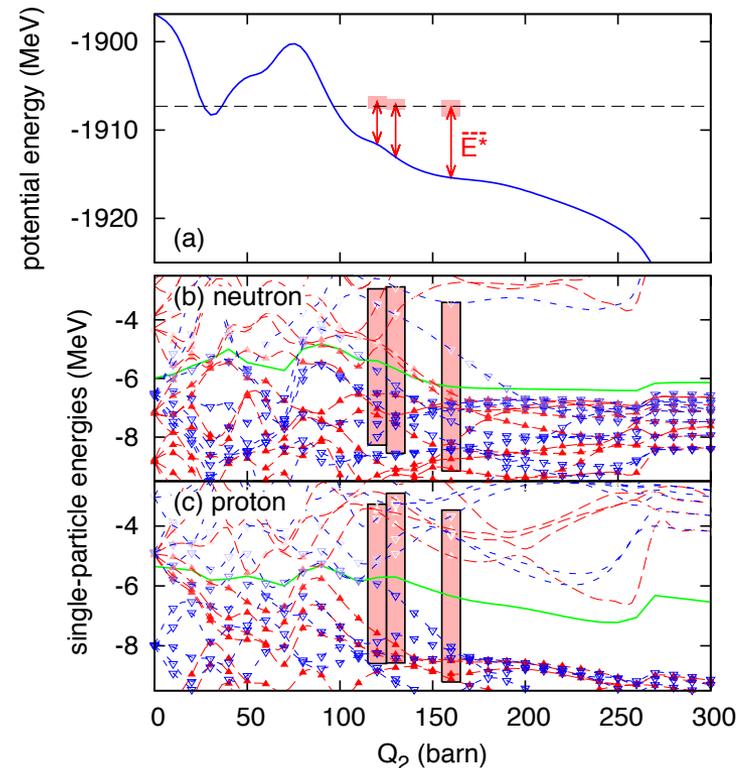
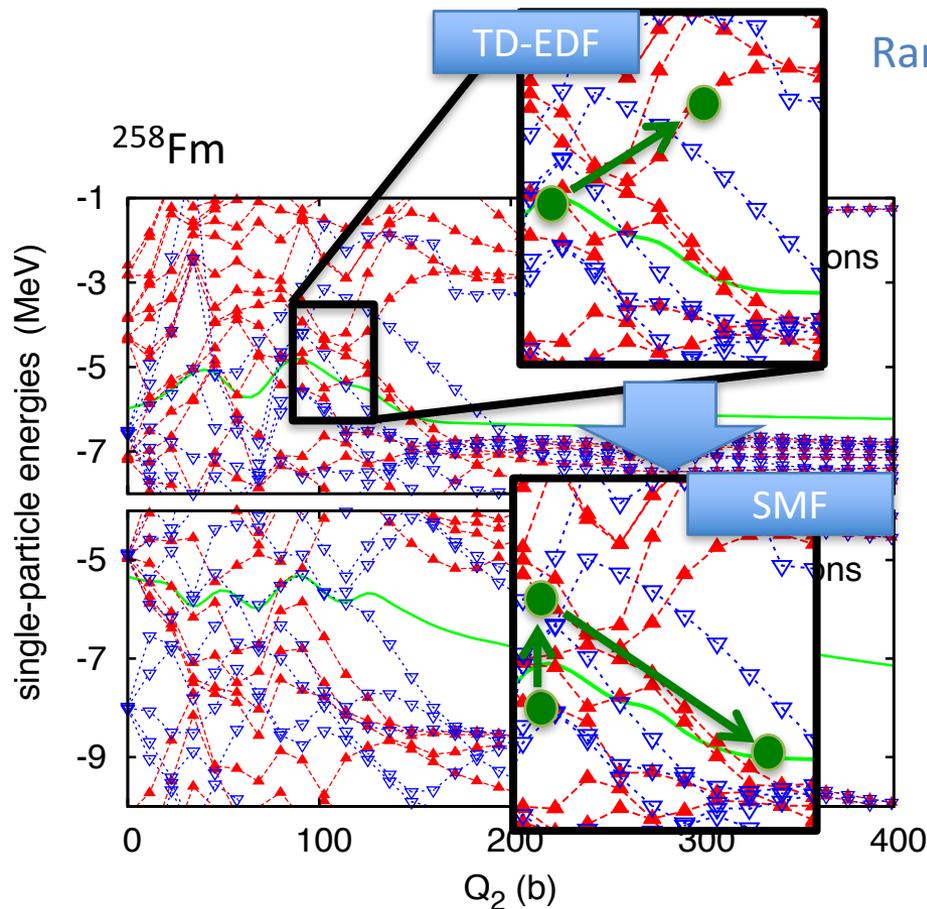
$$\rho(\mathbf{r}, \mathbf{r}', t_0) = \sum_i \Phi_i^*(\mathbf{r}, t_0) n_i \Phi_j(\mathbf{r}', t_0)$$

$$\rho^\lambda(\mathbf{r}, \mathbf{r}', t_0) = \sum_{ij} \Phi_i^*(\mathbf{r}, t_0) \rho_{ij}^\lambda \Phi_j(\mathbf{r}', t_0)$$

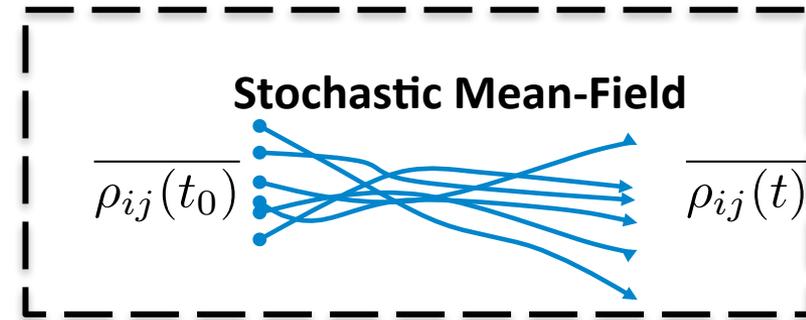
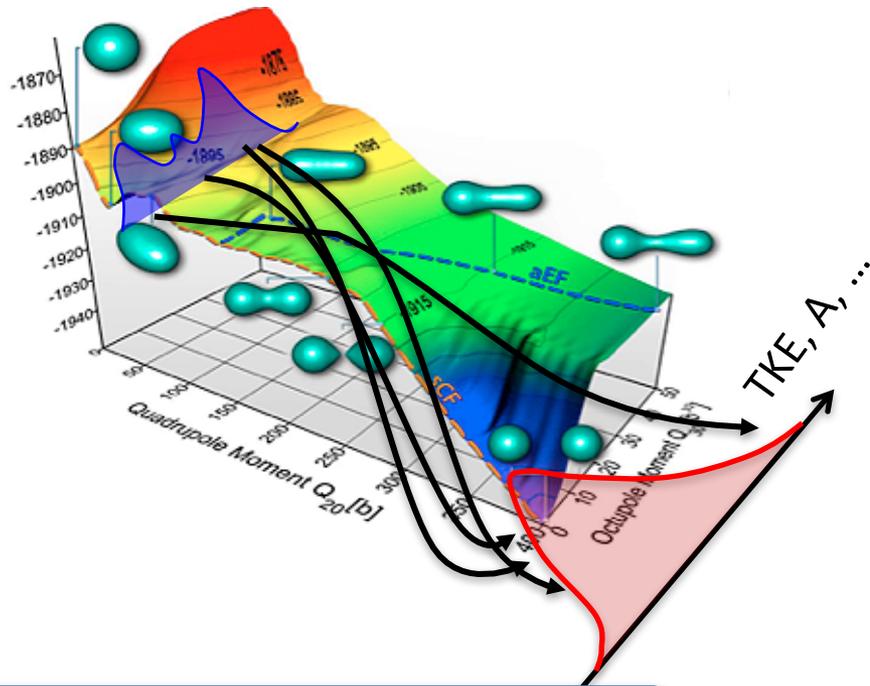
$$\overline{\rho_{ij}^\lambda} = \delta_{ij} n_i$$

$$\overline{\delta \rho_{ij}^\lambda \delta \rho_{j'i'}^\lambda} = \frac{1}{2} \delta_{jj'} \delta_{ii'} [n_i(1 - n_j) + n_j(1 - n_i)].$$

Range of fluctuation fixed by energy conservation



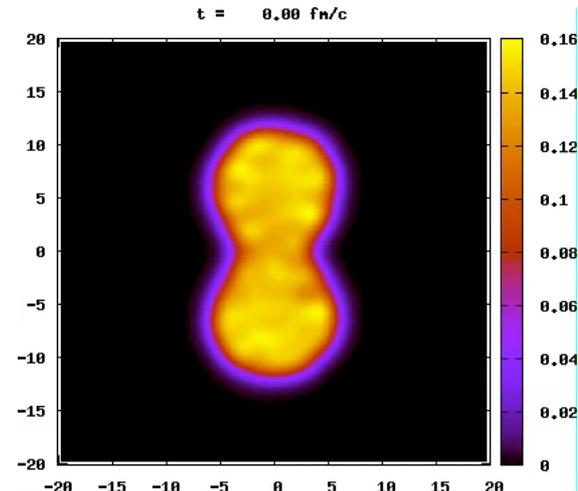
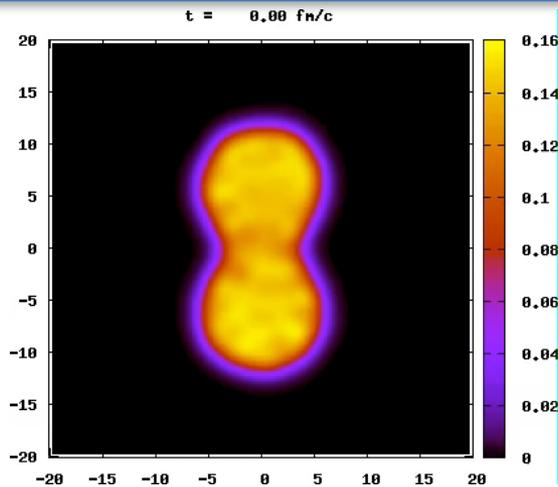
# How to conceal microscopic deterministic approach and randomness ?



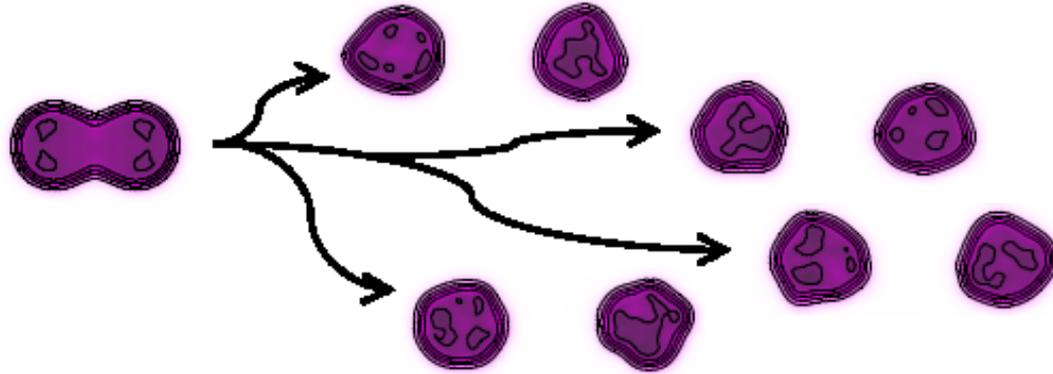
Numerical effort:

- Generates a sample of microscopic trajectories (typically 300 to 1000)
- Each trajectory is 8-10 days CPU time

Some trajectories illustration



# Phase-space average method: experiment versus theory

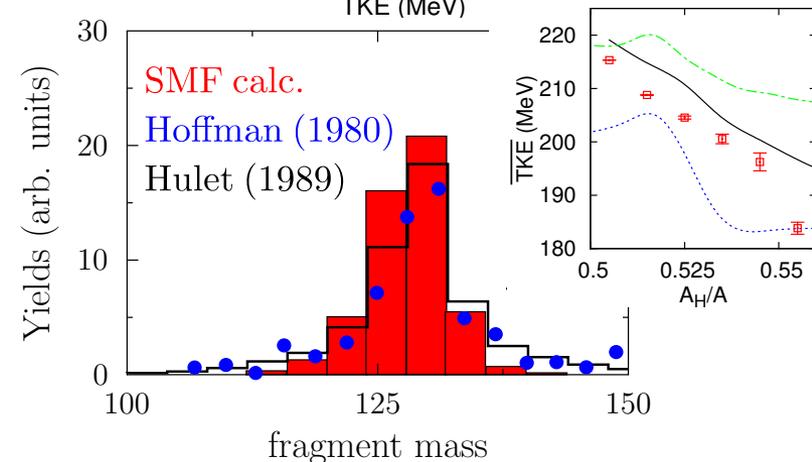
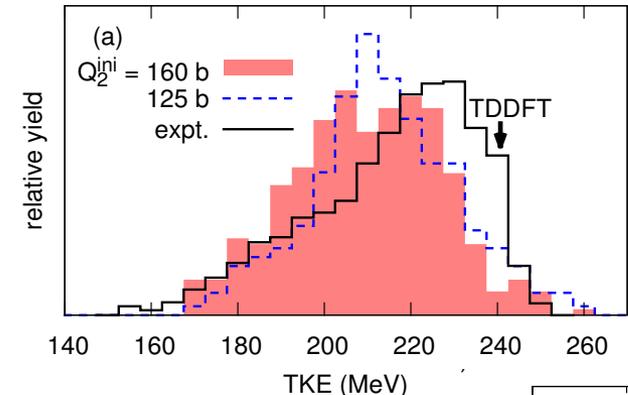
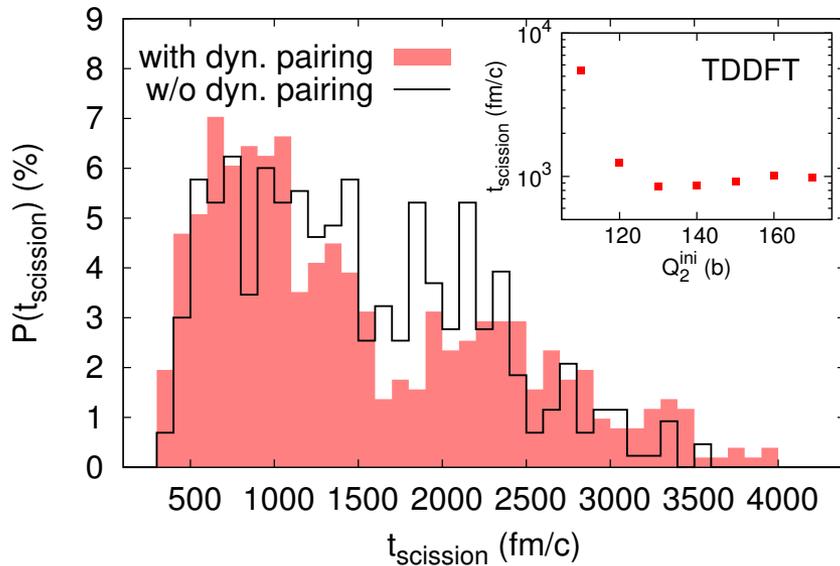


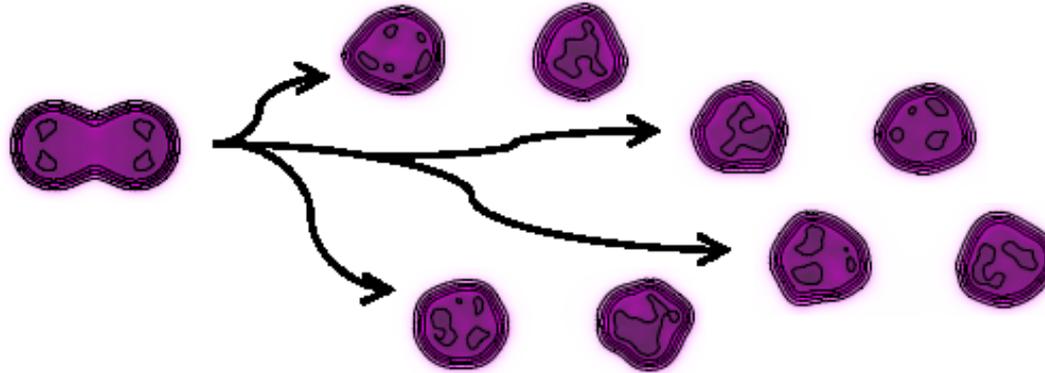
Tanimura, Lacroix, Ayik, PRL (2017)

Theory vs experiment

From deterministic to statistical approach

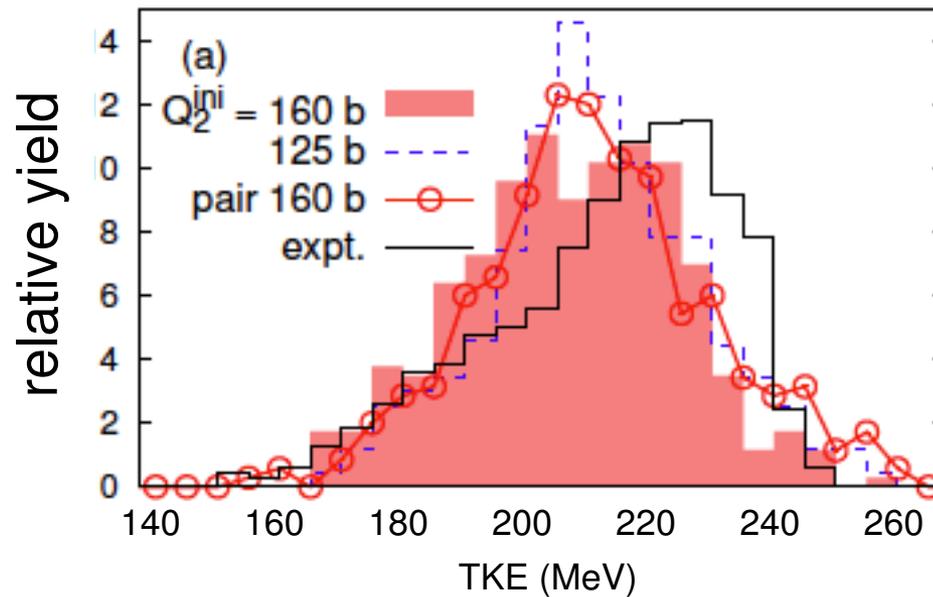
Time to reach scission point



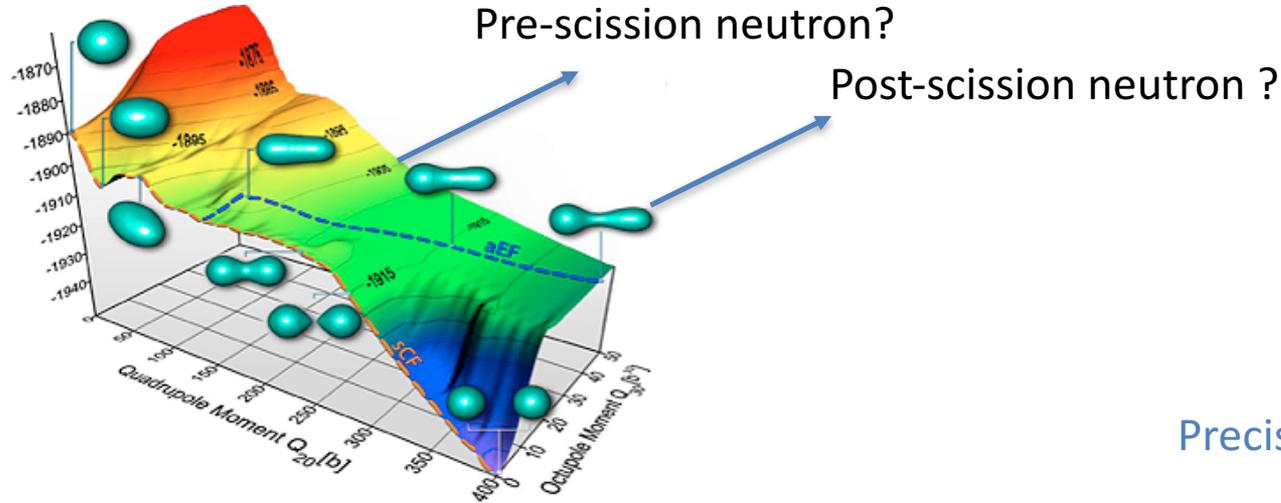


Tanimura, Lacroix, Ayik, PRL (2017)

## Quantum fluctuation versus dynamical pairing

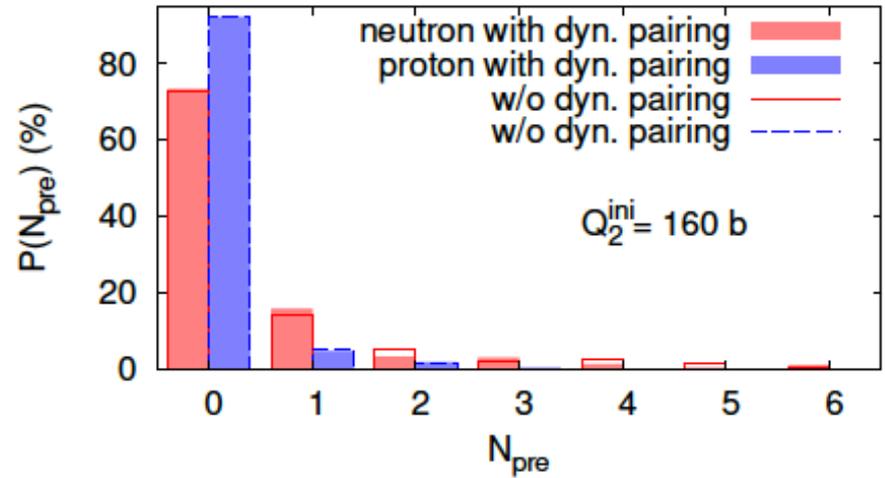
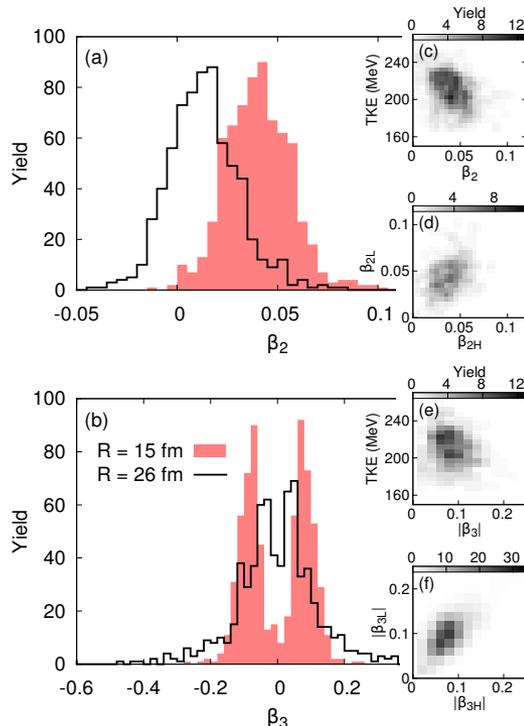


# How to conceal microscopic deterministic approach and randomness ?



Precision neutron emission

## Internal deformation of fission fragments



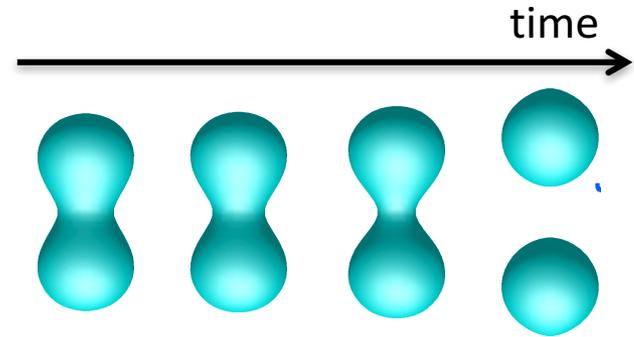
- ➔ TDDFT codes including pairing are now developed
- ➔ This opens new applications perspectives

Applications to fission

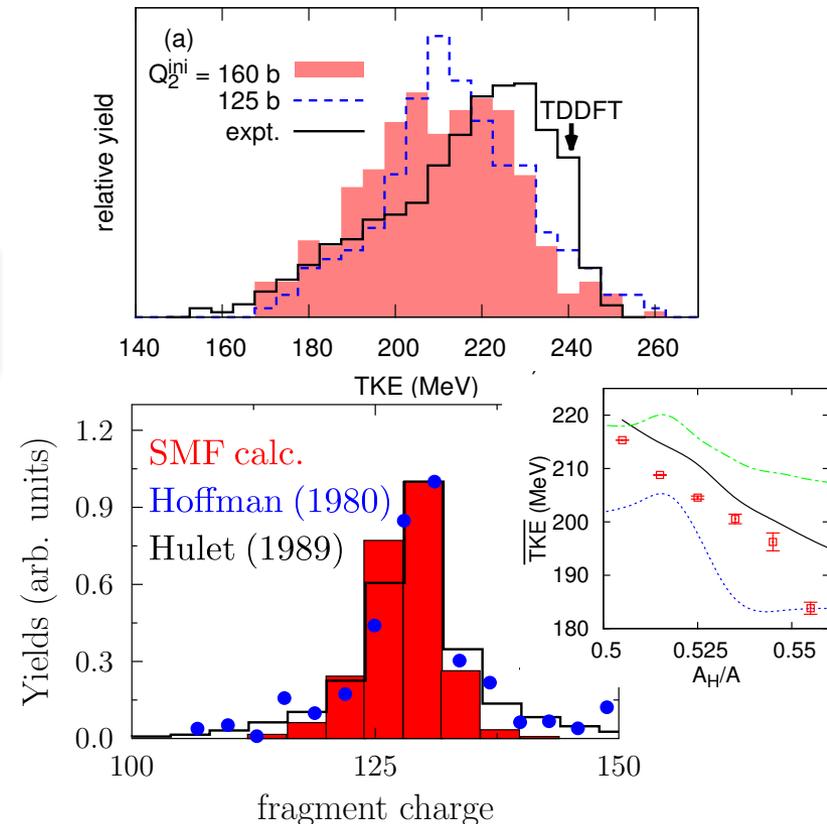
- ➔ Fission of superfluid nuclei
- ➔ Collective mass and dissipation
- ➔ Dynamical time-scale to scission

Beyond mean-field with quantum fluctuations

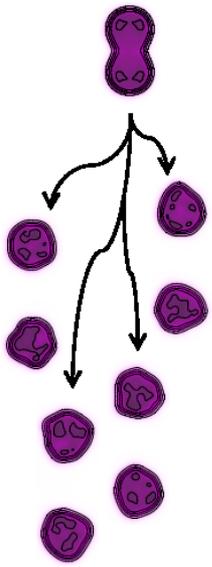
- ➔ First application with sampling of initial phase-space in TD-EDF
- ➔ TKE and mass distribution of  $^{258}\text{Fm}$
- ➔ Towards a systematic study of spontaneous and induced fission



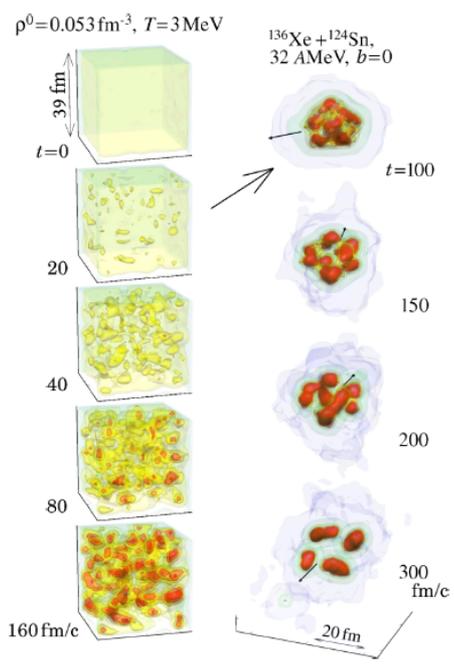
Theory vs experiment



Unifying low and Fermi energy theories

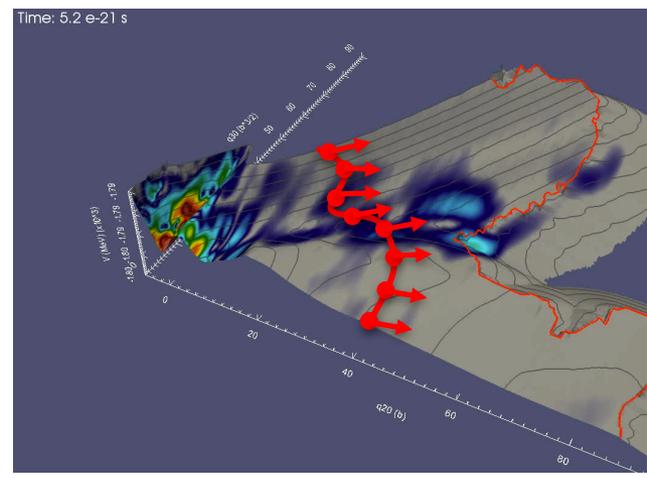
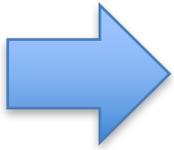
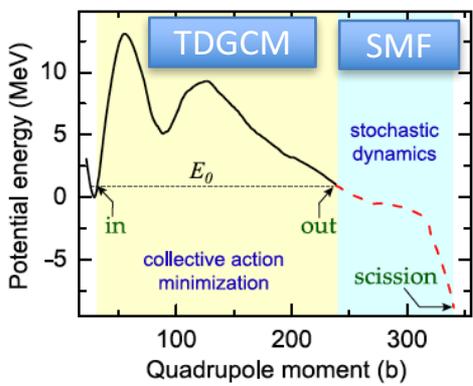


Tanimura et al, PRL118, (2017)



Napolitani, Colonna, PRC 96, (2017)

Nuclear Fission from the early stage



Regnier, Schunck, DL (2018)