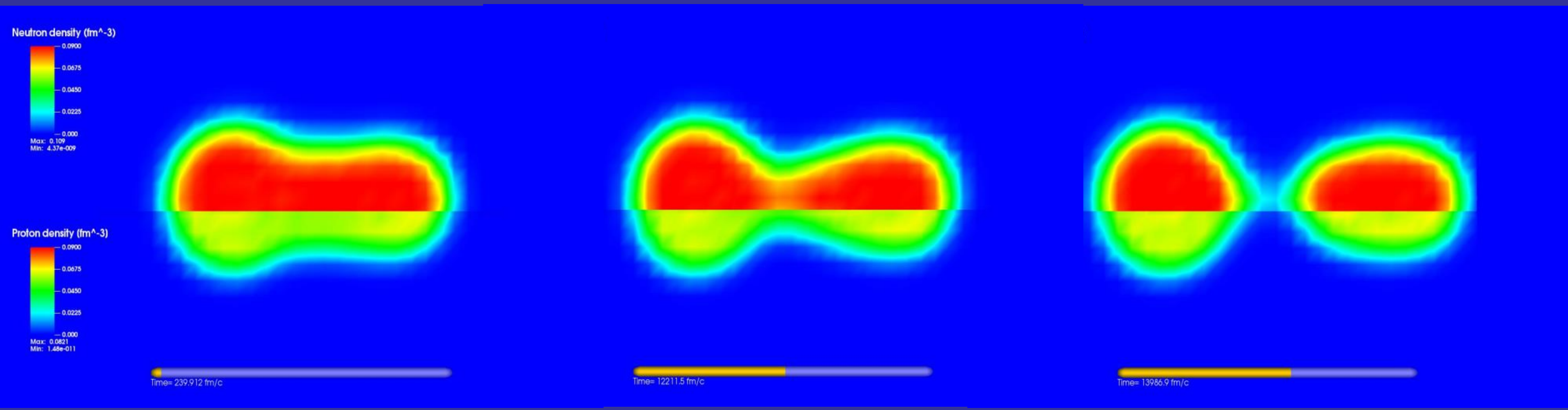
# *Selected problems of nuclear dynamics at low energies*





***Piotr Magierski***

***(Warsaw University of Technology)***

Collaborators:

Aurel Bulgac (Univ. of Washington)

Janina Grineviciute (WUT)

Kenneth J. Roche (PNNL)

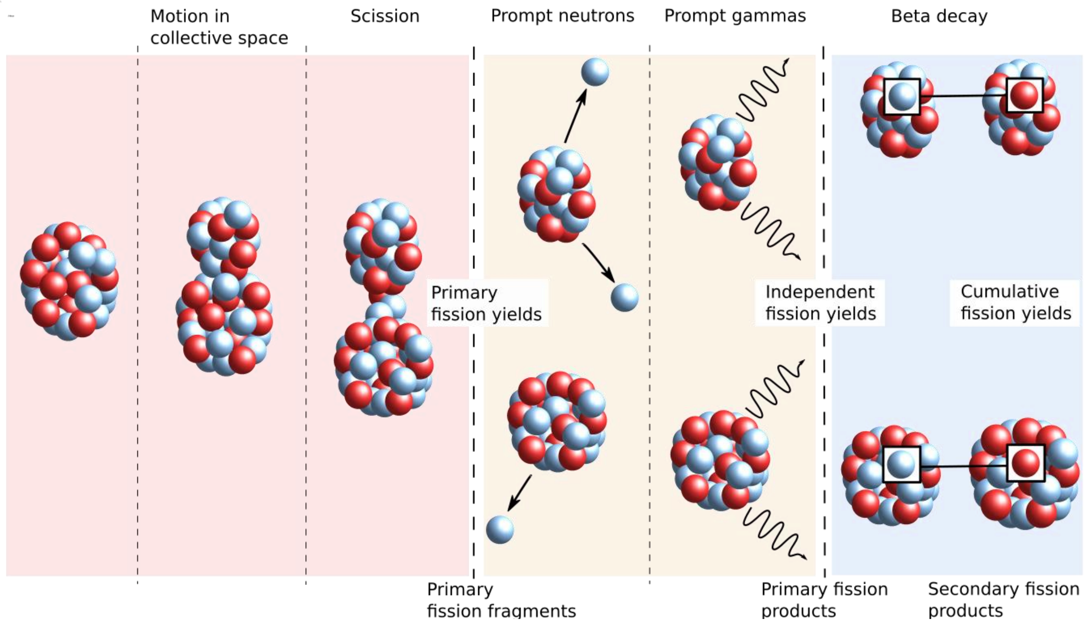
Shi Jin (Univ. of Washington)

Nicolas Schunck (LLNL)

Kazuyuki Sekizawa (Niigata Univ.)

Ionel Stetcu (LANL)

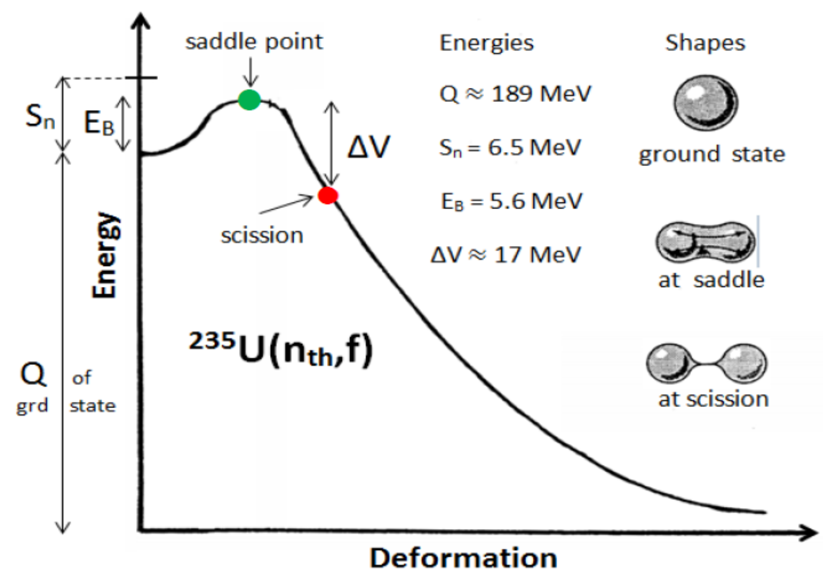
Gabriel Wlazłowski (WUT)




From LLNL-PRES-758023

**Nuclear dynamics of interest**

## Potential energy versus deformation

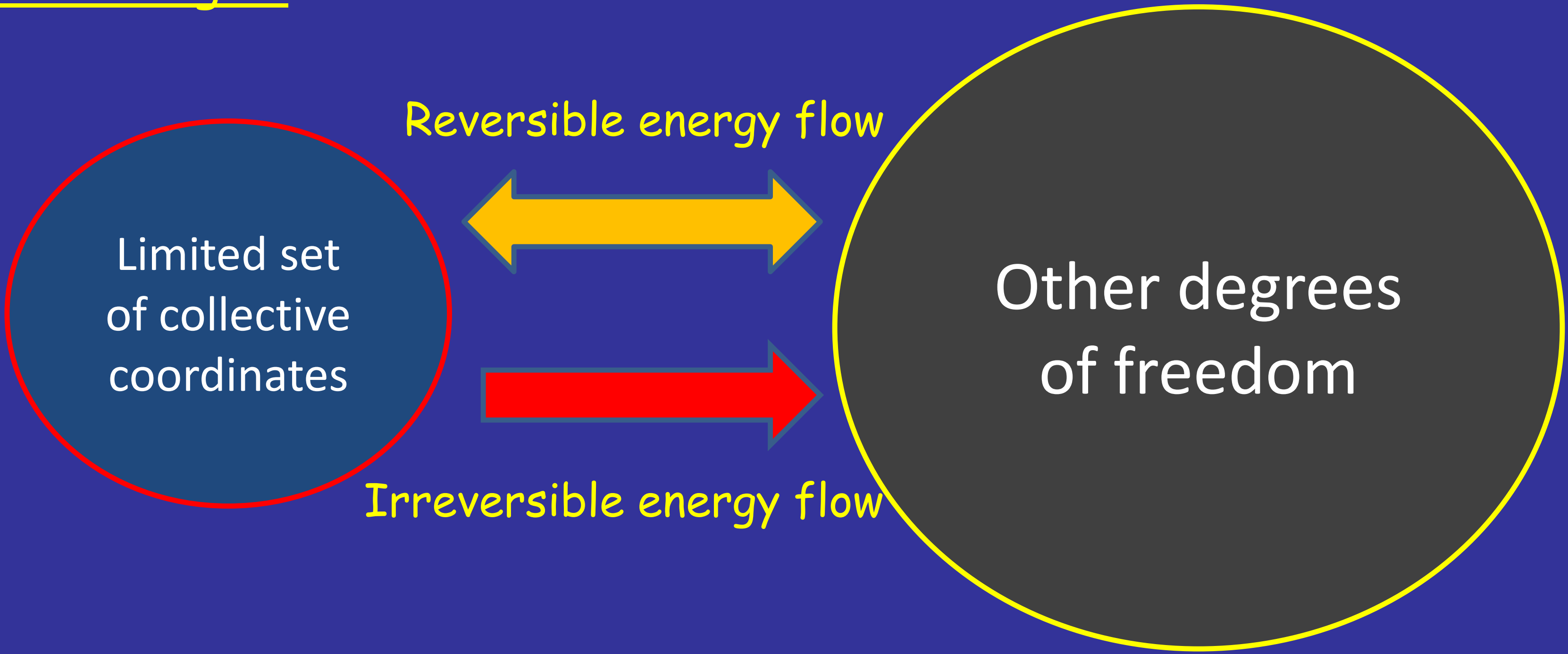



From F. Gonnenwein FIESTA2014

**Estimation of characteristic time scales for low energy fission ( <10MeV ):**

| | | |
|---|---|---|
| **Ground state to saddle** | **-** | **1 000 000 zs** |
| **Saddle to scission** | **-** | **10-100 zs** |
| **Acceleration of fission fragments to 90% of their final velocity** | **-** | **10 zs** |
| **Neutron evaporation** | **-** | **1 000 zs** |

# Typical framework for the theoretical description of nuclear dynamics at low energies

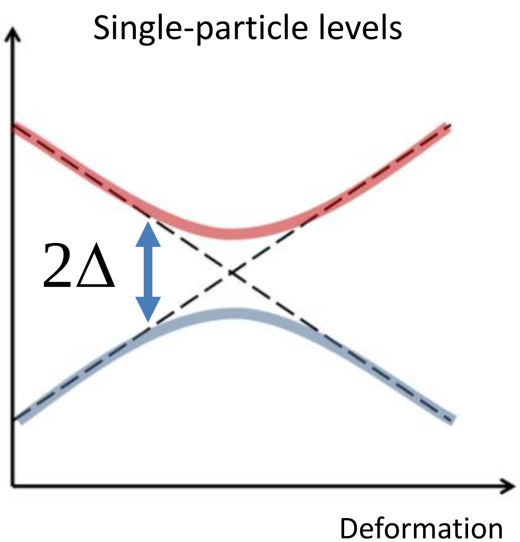



Reversible energy flow is determined by: mass parameters, potential energy surface.

Irreversible energy flow is determined by friction coefficients and leads to collective energy dissipation.

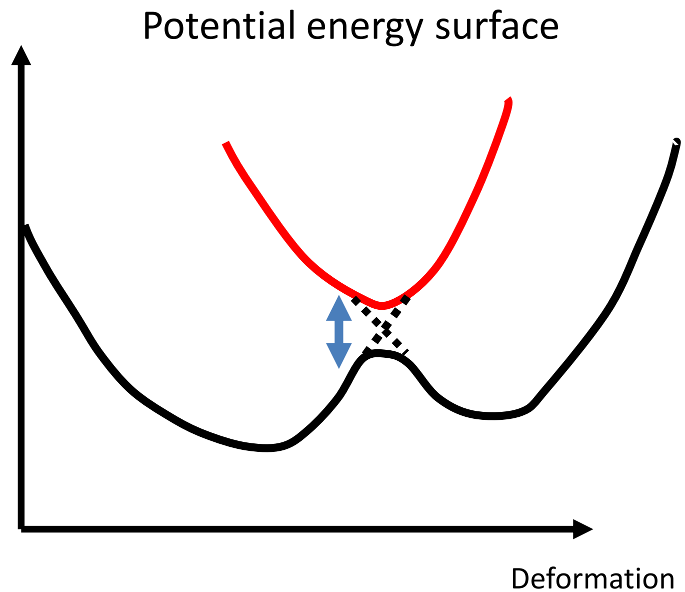
Consequently, questions associated with nuclear dynamics are directly related to the treatment of various components of this framework:
- Determination of the set of collective variables and their eq. of motion
- Treatment of other degrees of freedom
- Assumptions concerning energy flows

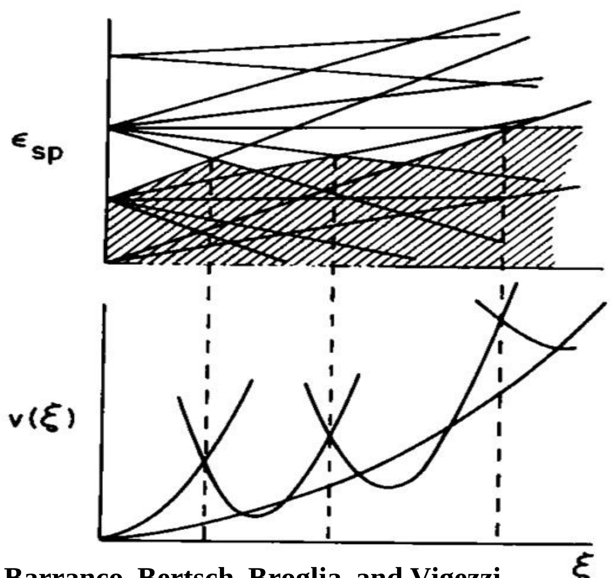
# Physics of nuclear superfluid dynamics




Quasiparticle energy:

$$\boxed{E_{qp} = \sqrt{(\varepsilon - \mu)^2 + |\Delta|^2}}$$




**From Barranco, Bertsch, Broglia, and Vigezzi**
**Nucl. Phys. A512, 253 (1990)**

As a consequence of pairing correlations large amplitude nuclear motion becomes more adiabatic.

While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored
Hill and Wheeler, PRC, 89, 1102 (1953)
Bertsch, PLB, 95, 157 (1980)

# Induced fission – theoretical approaches

Potential energy surface (PES) + Langevin dynamics

Dissipative classical motion within the space spanned by chosen collective coordinates (not more than 5).

**Features:**

- Easy to use scheme, especially if for PES a micro-macro model is used.
- Allows for global systematic calculations.
- **Mass/charge distribution** is obtained.
- **Total kinetic energies** can be extracted once the scission point is defined.
- Both spontaneous and induced fission can be studied.

$$\dot{q}_i = \sum_j M_{ij}^{-1}(\vec{q})\, p_j$$

$$\dot{p}_i = -\frac{\partial V}{\partial q_i} - \frac{1}{2}\sum_{j,k}\frac{\partial M^{-1}{}_{jk}}{\partial q_i} p_j p_k \overbrace{- \sum_j \gamma_{ij} M^{-1}{}_{jk}(\vec{q})\, p_k}^{\text{friction}} + \overbrace{\sum g_{ij}(\vec{q})\,\xi_j(t)}^{\text{stochastic force}}$$

$$\sum_k g_{ik} g_{jk} = \gamma_{ij} T$$ Fluctuation-dissipation theorem (classical)

P. Frobrich, I.I. Gontchar, Phys. Rep. 292 (1998) 131

The main problem with this approach lies in the fact that it contains various components which are included inconsistently. Once we face a problem (comparing results to exp. data) we do not know which component of the approach need to be corrected, and what is more important, how to do it in a consistent way.

# Time dependent generator coordinate method (TDGCM)

Fully quantum motion on the PES instead of classical Langevin-like equation.

However there is no irreversible energy flow – i.e. the motion is fully adiabatic. The system remains cold during motion: no energy transfer from collective degrees of freedom to other degrees of freedom.

$$\left|\Psi(t)\right\rangle = \int f(\vec{q},t)\left|\Phi(\vec{q})\right\rangle d^N q$$ - Ansatz for the wave function

$$\left\langle \Phi(\vec{q}) \,|\, \Phi(\vec{q}\,')\right\rangle \sim exp(-\sum_k |\sigma_k(\vec{q}) - \sigma_k(\vec{q}\,')|^2/2)$$ - GOA approx.

Instead of Langevin equation the evolution on the PES is governed by:

$$i\hbar\frac{\partial}{\partial t} g(\vec{q},t) = H_{coll}(\vec{q})\, g(\vec{q},t)$$

$$H_{coll}(\vec{q}) = -\frac{\hbar^2}{\gamma^{1/2}(\vec{q})}\sum_{i,j}\frac{\partial}{\partial q_i}\gamma^{1/2}(\vec{q})B_{ij}(\vec{q})\frac{\partial}{\partial q_j} + V(\vec{q})$$

$\gamma$ - Metric tensor

$B(\vec{q})$ - Mass tensor

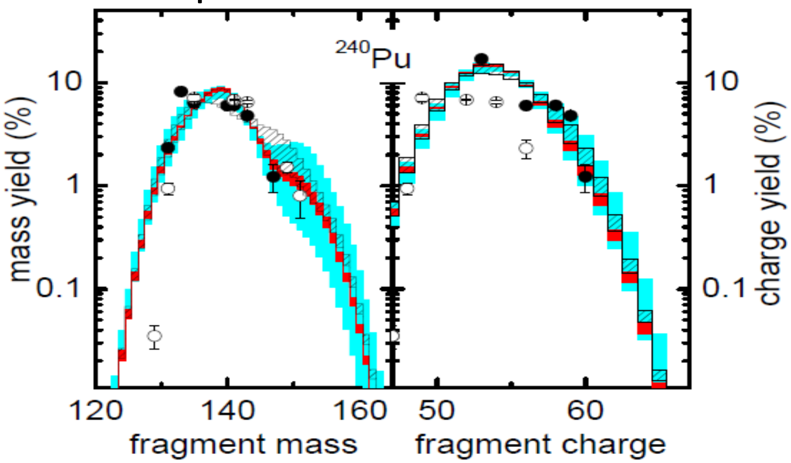
$g(\vec{q},t)$ - Probability amplitude for the system to be at point **q**

see eg.: D. Regnier et al. CPC 200, 350 (2016)

TDGCM is best suited to account for mass/charge distribution of fragments: the scission line has to be determined and the probabiliy flux through the scission line is calculated determining yields.

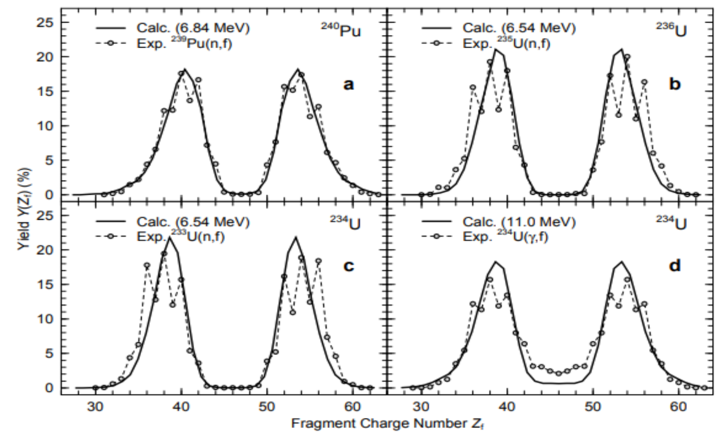
# Mass/charge distribution in PES + Langevin approach

Spontaneous fission




J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC **93**, 011304(2016),

Induced fission

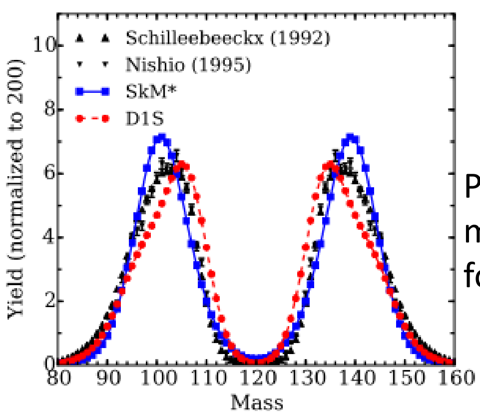



J. Randrup and P. Möller, PRL **106**, 132503 (2011)

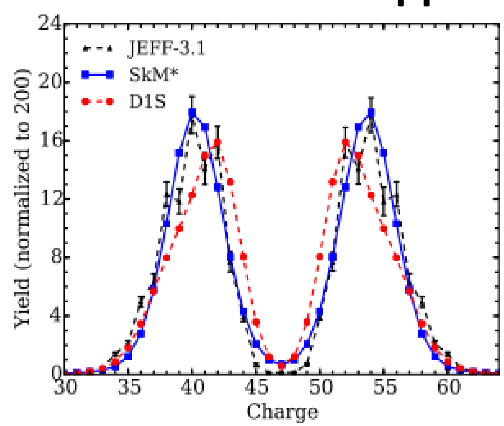
Strongly damped nuclear dynamics

P. Nadtochy and G. Adeev, PRC **72**, 054608 (2005); P. N. Nadtochy, A. Kelić, and K.-H. Schmidt, PRC **75**, 064614 (2007); J. Randrup and P. Möller, PRL **106**, 132503 (2011); J. Randrup, P. Möller, and A. J. Sierk, PRC **84**, 034613 (2011); P. Möller, J. Randrup, and A. J. Sierk, PRC **85**, 024306 (2012); J. Randrup and P. Möller, PRC **88**, 064606 (2013); J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC **93**, 011304 (2016), J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC **96**, 061361 (2017).

# Mass/charge distribution in TDGCM approach




Pre-neutron mass yields for: 239Pu(n,f)




Charge yields for: 239Pu(n,f)

J.-F. Berger, M. Girod, D. Gogny, CPC **63**, 365 (1991); H. Goutte, J.-F. Berger, P. Casoli, D. Gogny, PRC **71** 024316 (2005); D. Regnier, N. Dubray, N. Schunck, and M. Verrière, PRC **93**, 054611 (2016); D. Regnier, M. Verriere, N. Dubray, and N. Schunck, CPC **200**, 350 (2016)

Mass and charge distributions are not sensitive to the character of nuclear motion  prior to the scision point.

They depend predominantly on the structure of the collective energy surface

# Time dependent selfconsistent mean-field (time dependent density functional theory)

$$V(\vec{r},t) \Rightarrow \Psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N,t) \Rightarrow \rho(\vec{r},t)$$

**Runge-Gross mapping(1984):**

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle, \quad \left|\psi_0\right\rangle = \left|\psi(t_0)\right\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\rho(\vec{r}) \leftrightarrow e^{i\alpha(t)}\Psi[\rho](\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$$

TDDFT variational principle also exists but it is more tricky:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1} \left\langle\psi[\rho]\right|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\left|\psi[\rho]\right\rangle dt$$


E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

# Kohn-Sham procedure

**Suppose we are given the density of an interacting system.**
**There exists a unique noninteracting system with the same density.**

**Interacting system**

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = (\hat{T}+\hat{V}(t)+\hat{W})|\psi(t)\rangle$$

**Noninteracting system**

$$i\hbar\frac{\partial}{\partial t}|\varphi(t)\rangle = (\hat{T}+\hat{V}_{KS}(t))|\varphi(t)\rangle$$

$$\rho(\vec{r},t) = \langle\psi(t)|\hat{\rho}(\vec{r})|\psi(t)\rangle = \langle\varphi(t)|\hat{\rho}(\vec{r})|\varphi(t)\rangle$$

**Hence the DFT approach is essentially exact.**

A new local extension of DFT to superfluid systems (SLDA) and time-dependent phenomena (TDSLDA) has been developed.

Reviews: A. Bulgac, *Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids*, Ann. Rev. Nucl. Part. Sci. 63, 97 (2013);
P. Magierski, *Nuclear Reactions and Superfluid Time Dependent Density Functional Theory*, *Frontiers in Nuclear and Particle Physics* vol. 2, 57 (2019)

# Pairing correlations in time-dependent DFT

$$S = \int_{t_0}^{t_1} \left( \left\langle 0(t) \left| i\frac{d}{dt} \right| 0(t) \right\rangle - E[\rho(t), \chi(t)] \right) dt$$

Stationarity requirement produces the set of equations:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r},t) & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -h^*(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix},$$

$$B(t) = \begin{pmatrix} U(t) & V^*(t) \\ V(t) & U^*(t) \end{pmatrix} = \exp[iG(t)] \qquad G(t) = \begin{pmatrix} h(t) & \Delta(t) \\ \Delta^\dagger(t) & -h^*(t) \end{pmatrix}$$

Orthogonality and completeness has to be fulfilled: $\boxed{B^\dagger(t)B(t) = B(t)B^\dagger(t) = I,}$

In order to fulfill the completenes relation of Bogoliubov transform all states need to be evolved!
Otherwise Pauli principle is violated, i.e. the evolved densities do not describe a fermionic system (spurious bosonic effects are introduced).

**Consequence:** the computational cost increases considerably.

## Advantages of TDDFT for nuclear reactions

- The same framework describes various limits: eg. linear and highly nonlinear regimes, adiabatic and nonadiabatic (dynamics far from equilibrium).
- Interaction with basically any external probe (weak or strong) easy to implement.
- TDDFT does not require introduction of hard-to-define collective degrees of freedom and there are no ambiguities arising from defining potential energy surfaces and inertias.
- One-body dissipation, the window and wall dissipation mechanisms are automatically incorporated into the theoretical framework.
- All shapes are allowed and the nucleus chooses dynamically the path in the shape space, the forces acting on nucleons are determined by the nucleon distributions and velocities, and the nuclear system naturally and smoothly evolves into separated fission fragments.
- There is no need to introduce such unnatural quantum mechanical concepts as "rupture" and there is no worry about how to define the scission configuration.

Sometimes simplified assumptions are made eg. replacing TDHFB by TDBCS :

$\Delta(\vec{r},t) \rightarrow \Delta(\rho(\vec{r},t))$ - severe limitation in pairing degrees of freedom.

e.g. G.Scamps. D. Lacroix, G.F. Bertsch, K. Washiyama, PRC85, 034328 (2012).

More precisely:
BCS as compared to HFB approach neglects <u>the quasiparticle scattering</u> and consequently all effects originated from this effect are missed.

**The main advantage of TDSLDA over TDHF (+BCS) is related to the fact that in TDSLDA the pairing correlations are described as a true <u>complex field which has its own modes of excitations</u>, which include spatial variations of both amplitude and phase. Therefore in TDSLDA description the evolution of nucleon Cooper pairs is treated consistently with other one-body degrees of freedom.**

# *Open problems of TDDFT*

1) There are easy and difficult observables in DFT.
   In general: easy observables are one-body observables. They are easily extracted and reliable.

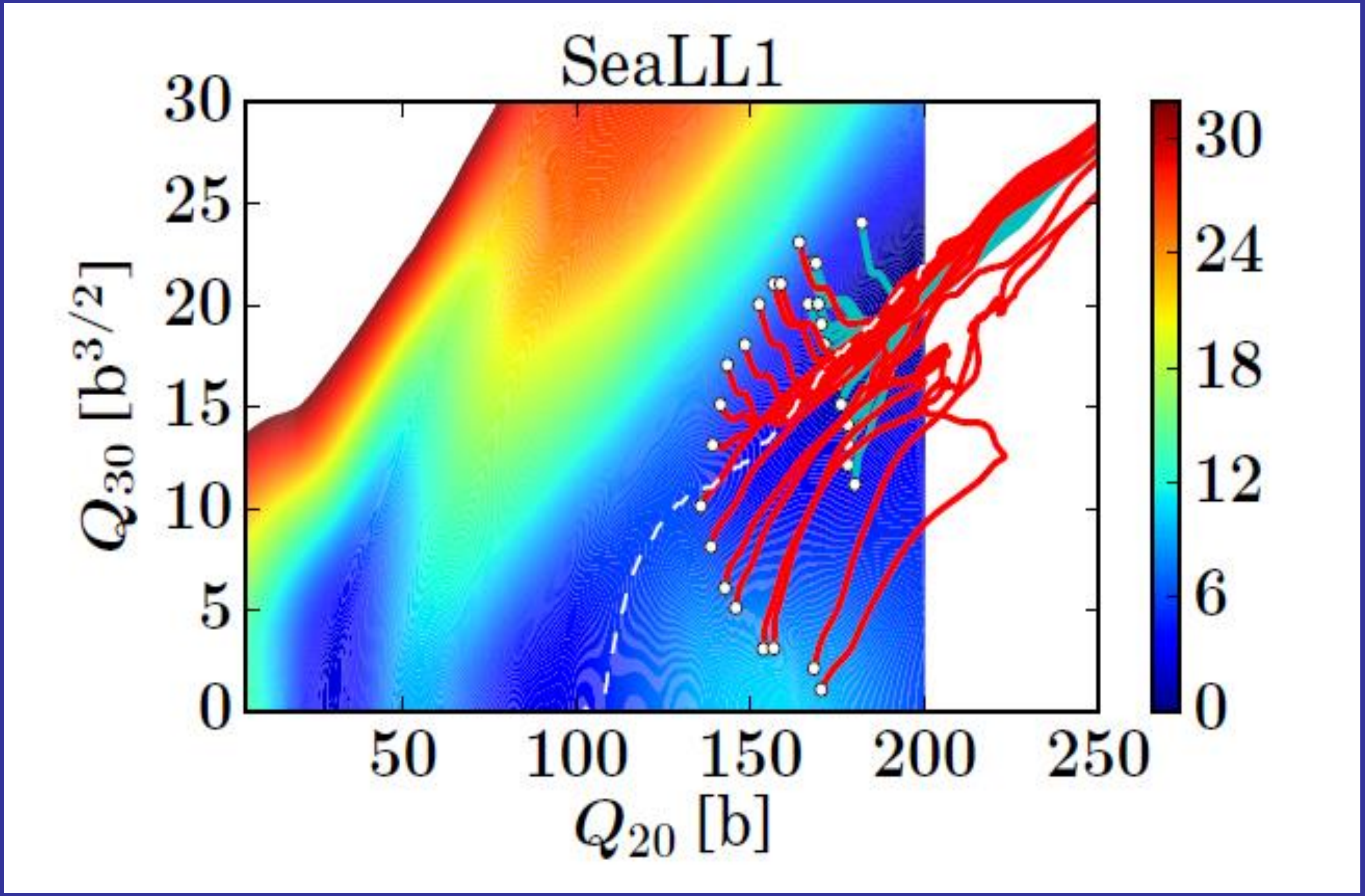
2) But there are also important observables which are difficult to extract.
   For example:
   - S matrix
   - momentum distributions
   - transitional densities (defined in linear response regime)
   - various conditional probabilities
   - mass distributions

   Stochastic extensions of TDDFT are under investigation:

   D. Lacroix, A. Ayik, Ph. Chomaz, Prog.Part.Nucl.Phys.52(2004)497
   S.Ayik, Phys.Lett. B658 (2008) 174
   A. Bulgac, S.Jin, I. Stetcu, arxiv:1806.00694

3 ) Dissipation: transition between one-body dissipation regime and two-body dissipation regime.

# TDSLDA trajectories on the collective potential surface originating from various initial configurations

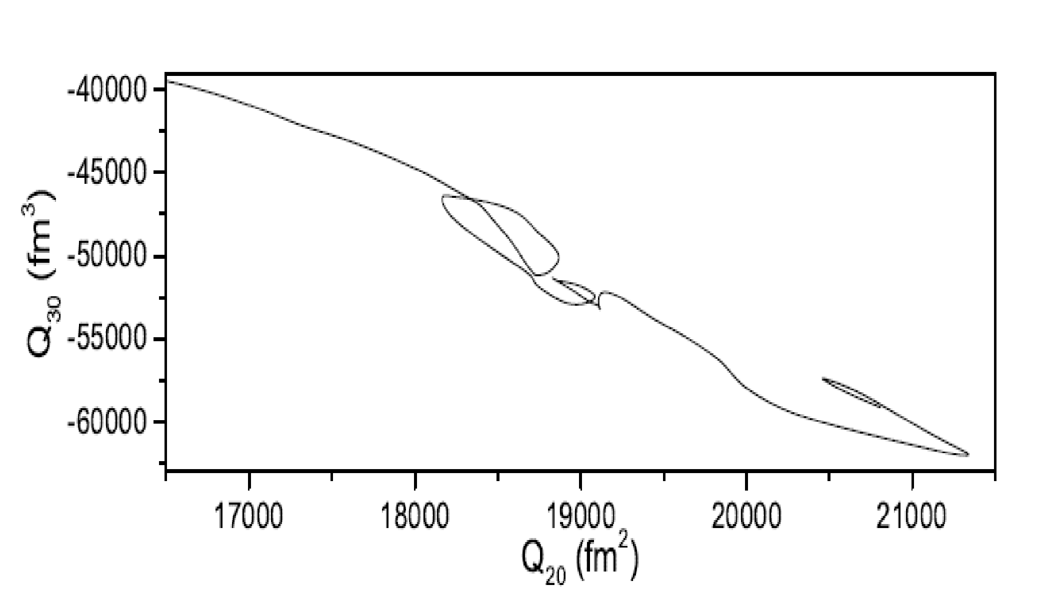



A. Bulgac, et al., arXive: 1806.00694

**The final scission configuration is relatively independent on the initial condition (providing it starts at or beyond the saddle point).**
**One needs a kind of stochastic extension to account for fluctuations.**

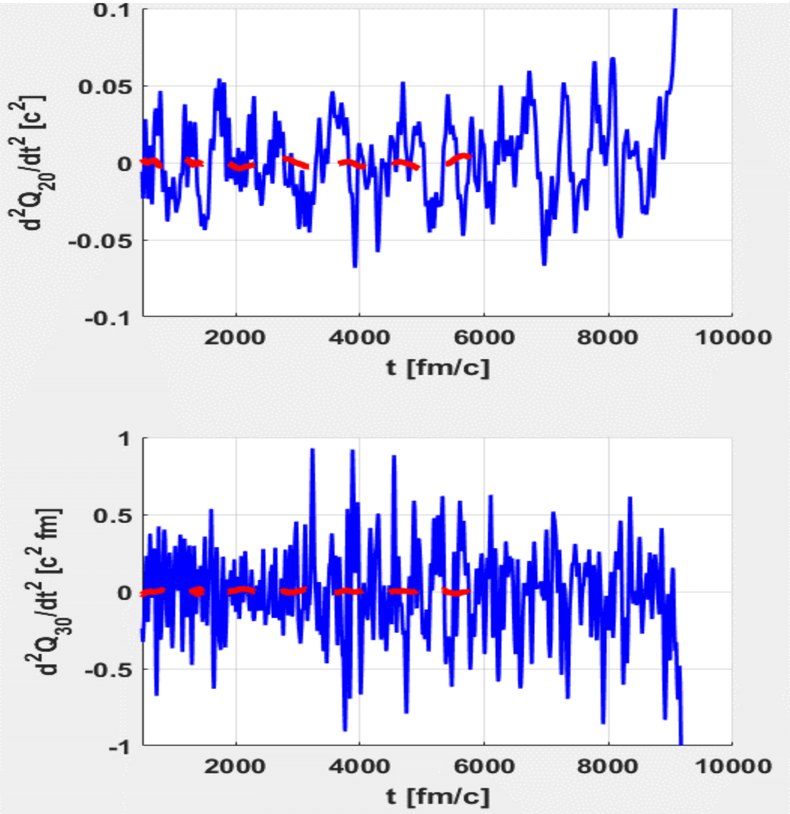
# Nature of fission dynamics of $^{240}Pu$ in TDDFT

A typical trajectory of fissioning $^{240}Pu$ in the collective space at excitation excitation energy of *E=8-9 MeV*:




J. Grinevicute, etal. (in preparation).

**Accelerations in quadrupole and octupole moments along the fission path**



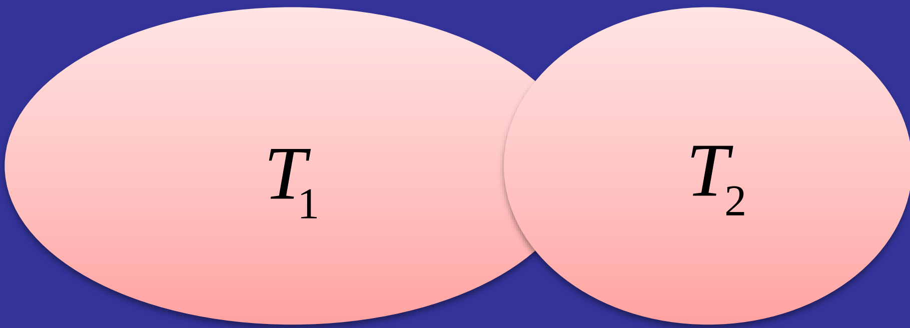

Note that despite the fact that nucleus is already beyond the saddle point the collective motion on the time scale of 1000 fm/c and larger is characterized by the constant velocity (*see red dashed line for an average acceleration*) till the very last moment before splitting. Within the time scale, of the order of 300 fm/c and shorter, the collective motion is a subject to random-like kicks indicating strong coupling to internal degrees of freedom.

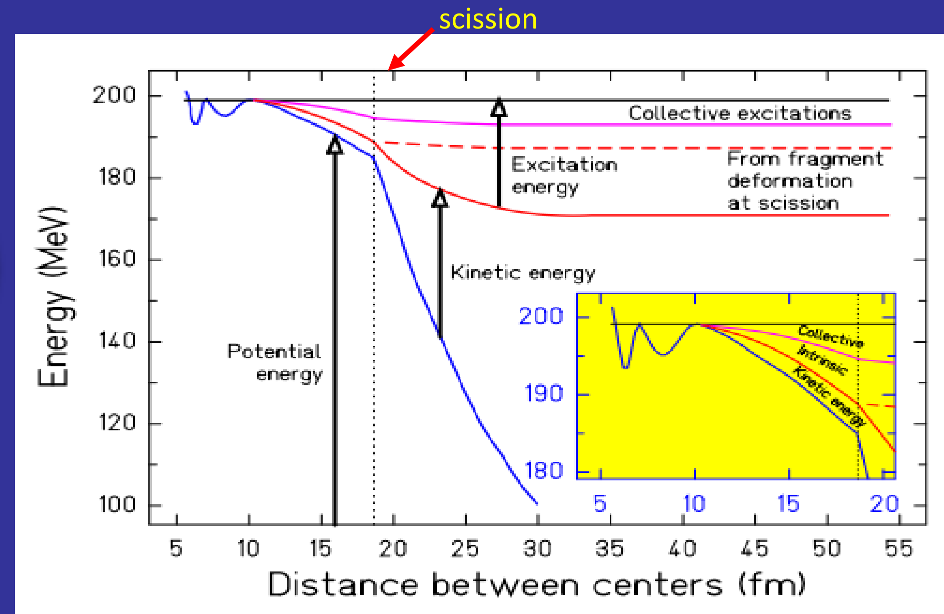
## Nuclear induced fission dynamics:

It is important to realize that these results indicate that the motion is not adiabatic, although it is slow.

Although the average collective velocity is constant till the very last moment before scission, the system heats up as the energy flows irreversibly from collective to intrinsic degrees of freedom.

# Remarks on the fragment kinetic and excitation energy sharing within the TDDFT




Schmidt&Jurado:Phys.Rev.C83:061601,2011

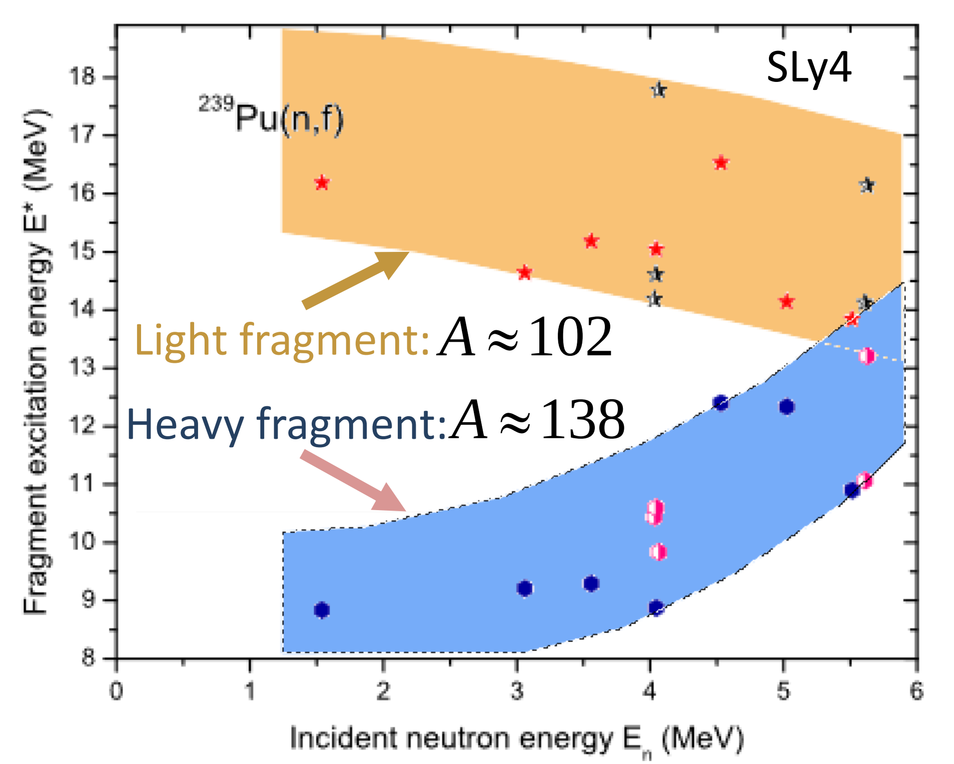
In the to-date approaches it is usually assumed that the excitation energy has 3 components (Schmidt&Jurado:Phys.Rev.C83:061601,2011 Phys.Rev.C83:014607,2011):

- deformation energy
- collective energy (energy stored in collective modes)
- intrinsic energy (specified by the temperature)

It is also assumed that the intrinsic part of the energy is sorted according <u>to the total entropy maximization</u> of two nascent fragments (i.e. according to temperatures, level densities) and the <u>fission dynamics does not matter.</u>

In TDDFT such a decomposition can be performed as well.
The intrinsic energy in TDDFT will be partitioned <u>dynamically</u> (no sufficient time for equilibration).

# Induced fission of 240Pu




| $E^*$ (MeV) | $E_n$ (MeV) | $TKE_{TDSLDA}$ (MeV) | $TKE_{syst}$ (MeV) | $err$ (%) | $Z_L$ | $N_L$ |
|---|---|---|---|---|---|---|
| 8.08 | 1.542 | 173 | 177.26 | 1.95 | 40.825 | 62.246 |
| 9.60 | 3.063 | 174 | 176.73 | 1.13 | 40.500 | 61.536 |
| 10.10 | 3.560 | 179 | 176.56 | 1.43 | 41.625 | 62.783 |
| 10.57 | 4.032 | 173 | 176.39 | 1.55 | 40.092 | 61.256 |
| 10.58 | 4.043 | 173 | 176.39 | 1.70 | 40.146 | 61.388 |
| 10.58 | 4.047 | 175 | 176.39 | 0.72 | 40.313 | 61.475 |
| 10.60 | 4.065 | 174 | 176.38 | 0.92 | 40.904 | 62.611 |
| 11.07 | 4.534 | 176 | 176.22 | 0.14 | 41.495 | 63.134 |
| 11.56 | 5.024 | 175 | 176.05 | 0.51 | 40.565 | 61.894 |
| 12.05 | 5.515 | 176 | 175.88 | 0.49 | 40.412 | 61.809 |
| 12.15 | 5.610 | 176 | 175.84 | 0.29 | 40.355 | 61.695 |
| 12.16 | 5.626 | 176 | 175.84 | 0.15 | 41.386 | 62.764 |

The lighter fragment is more excited (and strongly deformed) than the heavier one.

Excitation energies are not shared proportionally to mass numbers of the fragments!

$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

**Calculated TKEs slightly reproduce experimental data with accuracy < 2%**

J. Grineviciute, et al. (in preparation)

see also:

A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

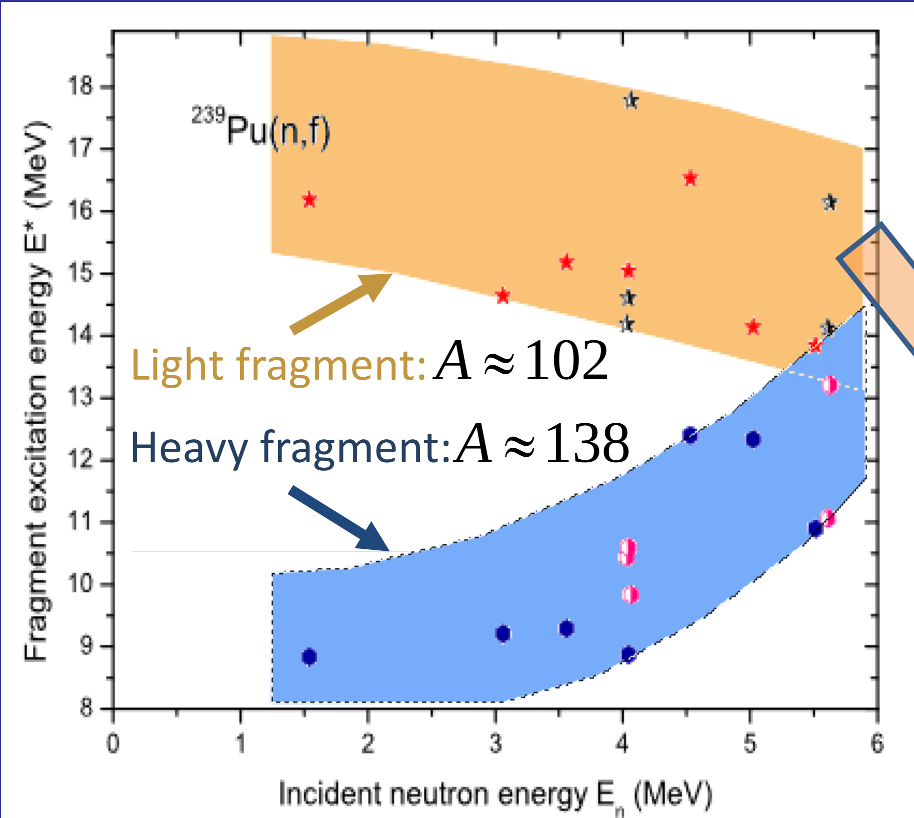
# Decomposition of the excitation energy into collective and noncollective part

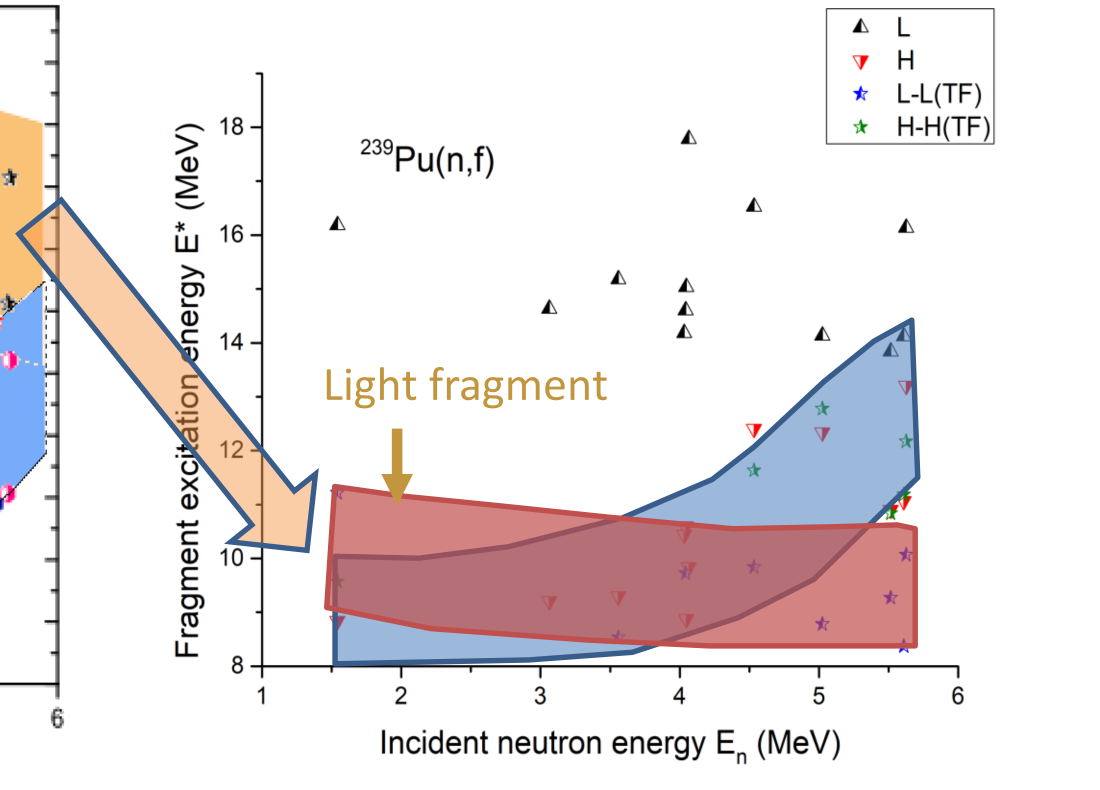
Intrinsic excitation energy of the fragments:

$$E^{\mathrm{int}}_{exc.} = E^{tot}_{exc.} - \bar{E}_{Thomas-Fermi}$$

$$\bar{E}_{Thomas-Fermi} = \frac{1}{\Delta T}\int_{T_{scission}}^{T_{scission}+\Delta T} E_{Thomas-Fermi}(t)dt$$

Total excitation energy of the fragments




J. Grineviciute, et al. (in preparation)

Energy stored in collective modes: < 2MeV

The intrinsic energy is not shared proportionally to fragment masses at low excitation energy!

# Usefulness of various fission observables

**Mass/charge distribution** – does not provide us insight into nuclear dynamics e.g. it is relatively well reproduced both by PES+Langevin and TDGCM theories, despite of the fact that completely different character of nuclear motion is assumed.

**Odd-even mass effect** – so far it is difficult to compare it to any theory without making uncontrollable asumptions. All theories that were presented are unable to incorporate consistently odd-particle system in the dynamics.

**Total kinetic energy distributions** - this quantity is determined practically at the scission point. So similarly to mass/charge distributions it is not very sensitive to nuclear dynamics prior to the scission point.

**Scission neutrons** - extremely useful quantity as it can be easily extracted in TDDFT, without further assumptions. Measurement of scission neutrons can provide stringent test for the applicability of TDDFT theory to describe neutron emission in real-time.

**Excitation energy sharing** - depending on dynamics and density of states at scission.
**Very severe test for TDDFT: theoretical predictions already exist.**

**Primary gamma emission** - may give some information on ang. momentum distribution of fragments, but as far as I know, not directly comparable to theories presented here.