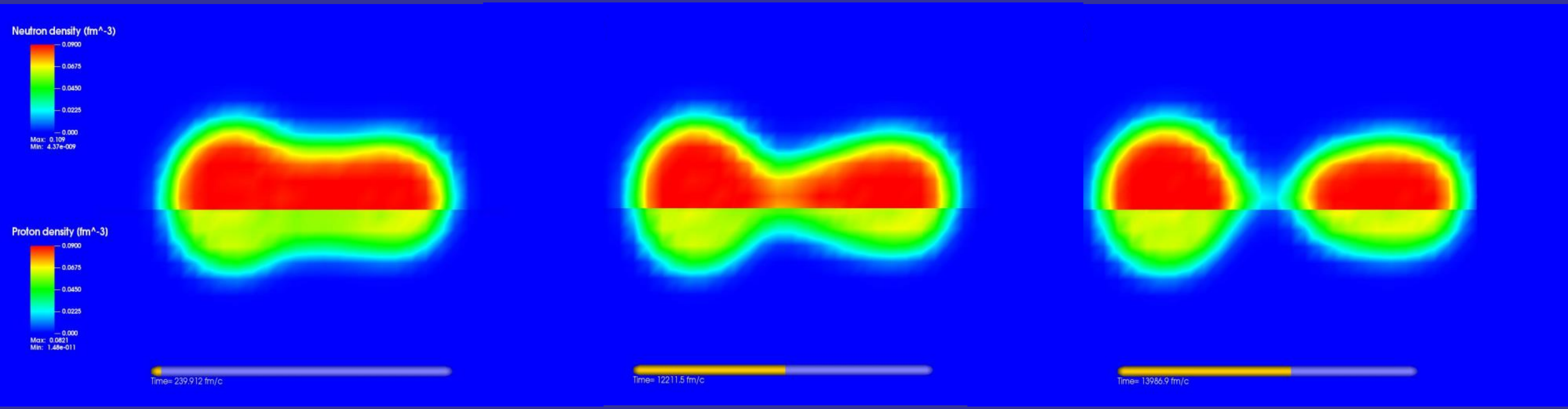
Towards exascale simulations of nuclear dynamics at low energies



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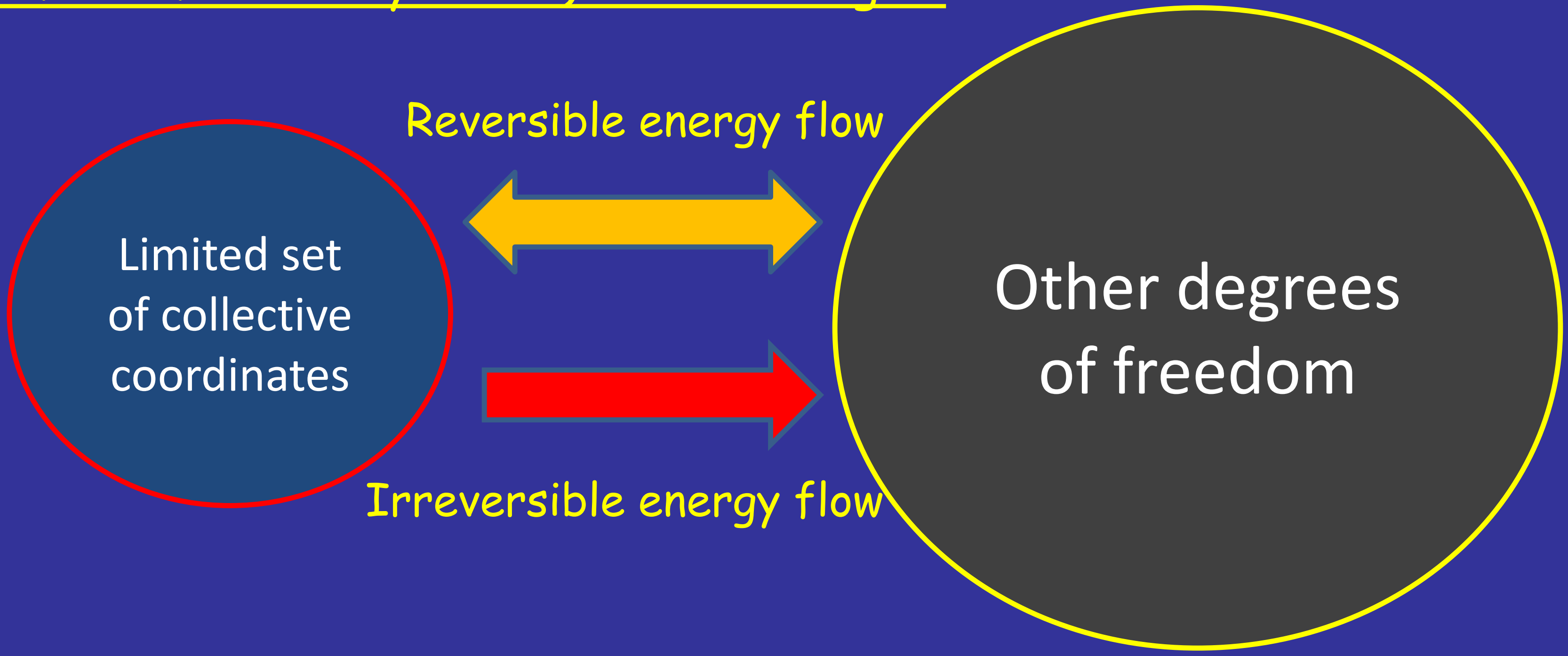
Typical framework for the theoretical description of nuclear dynamics (of medium or heavy nuclei) at low energies



Reversible energy flow

Limited set of collective coordinates

Other degrees of freedom

Irreversible energy flow

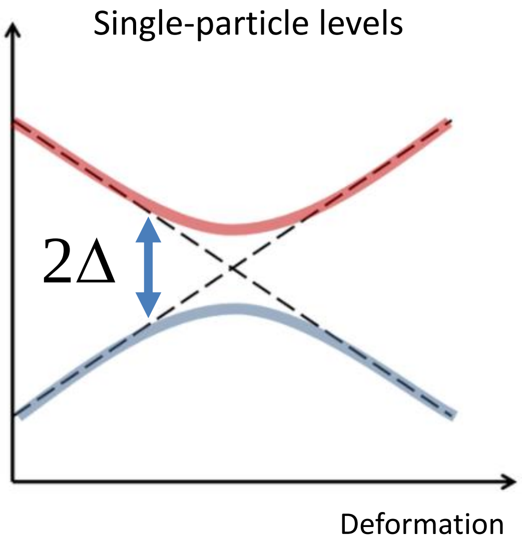
Reversible energy flow is determined by: mass parameters, potential energy surface.

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:

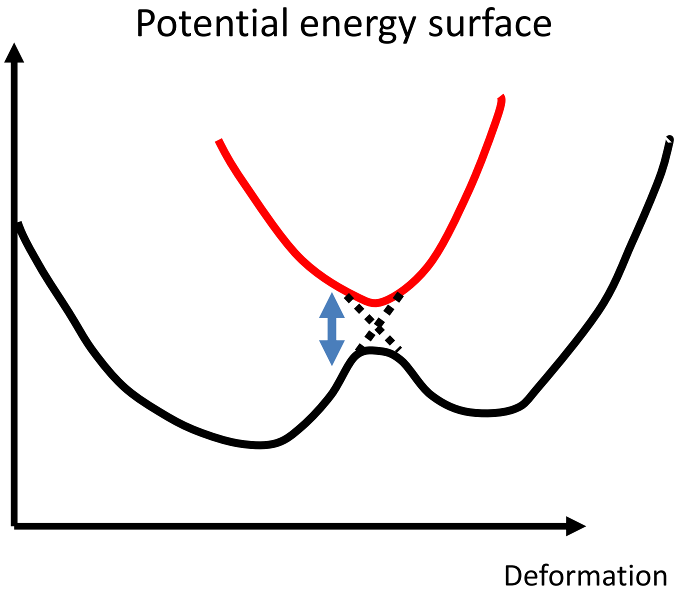
- Determination of the set of collective variables and their eq. of motion
- Treatment of other degrees of freedom
- Assumptions concerning energy flows

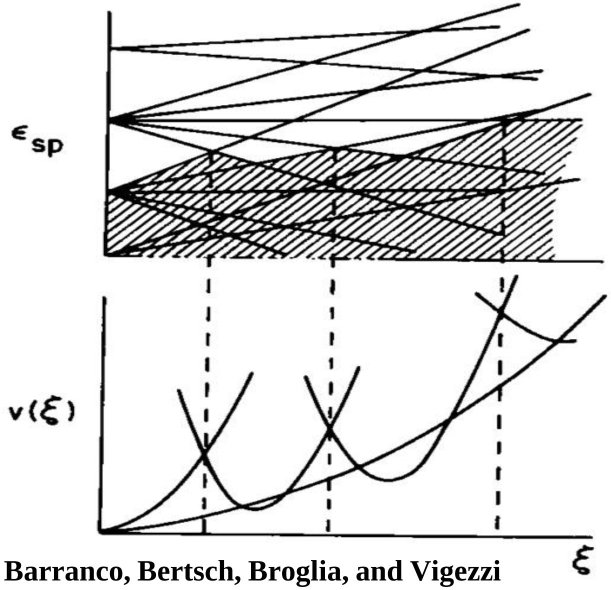
Physics of nuclear superfluid dynamics



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.

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.

Time dependent generator coordinate method (TDGCM)

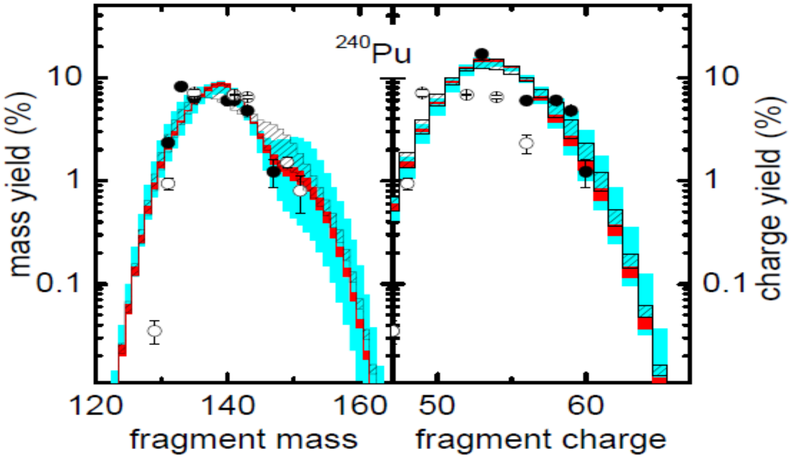
Fully quantum motion on the PES instead of classical Langevin-like equation.

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.

- Mostly used for calculating **mass/charge distribution**.

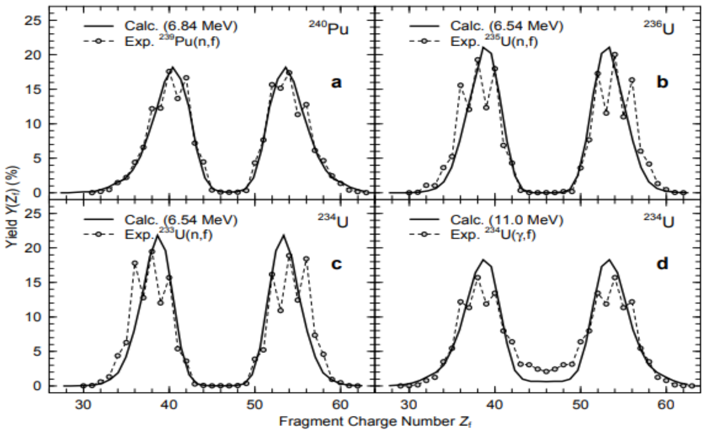
Mass/charge distribution in PES + Langevin approach

Spontaneous fission



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

Induced fission

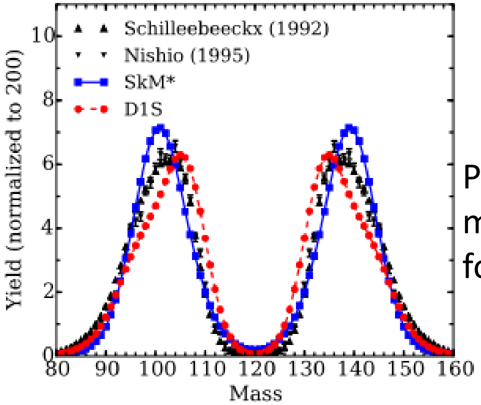


J. Randrup and P. Möller, PRL **106**, 132503 (2011)

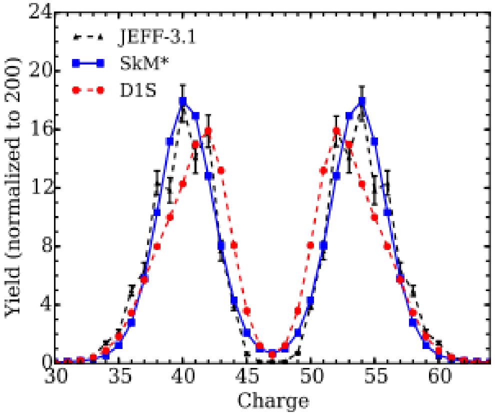
Strongly damped nuclear dynamics

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).

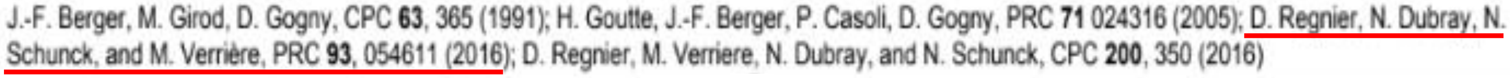
Mass/charge distribution in TDGCM approach



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)

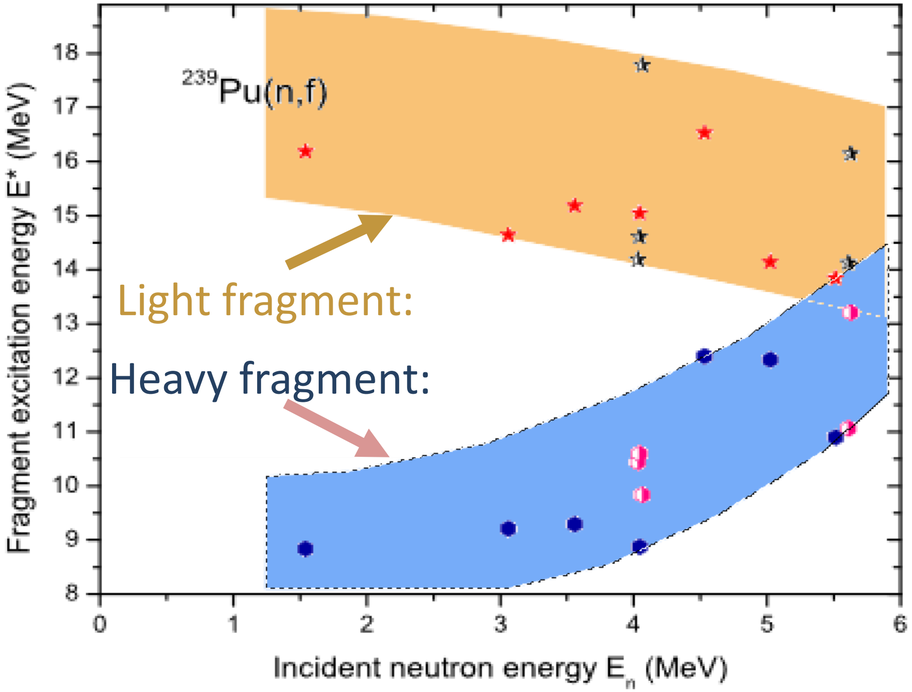
Time dependent Density Functional Theory

Time evolution of all nucleonic degrees of freedom (can be treated as time evolving mean field including pairing field).

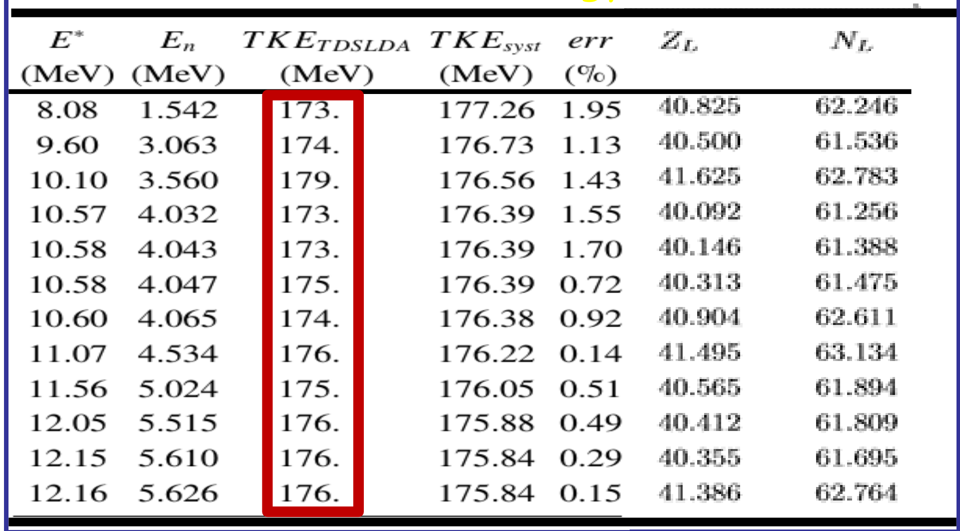
Features:

- No need to introduce collective degrees of freedom, inertias or to define scission point.
- One-body dissipation, the window and wall dissipation mechanisms are automatically incorporated into the theoretical framework.
- Requires supercomputers.
- Average description within unified framework: provides TKE, TXE, energy sharing between fragments.
- no information about mass/charge/TKE distributions

Excitation energy of the fragments vs neutron incident energy



Total kinetic energy of the fragments vs neutron incident energy



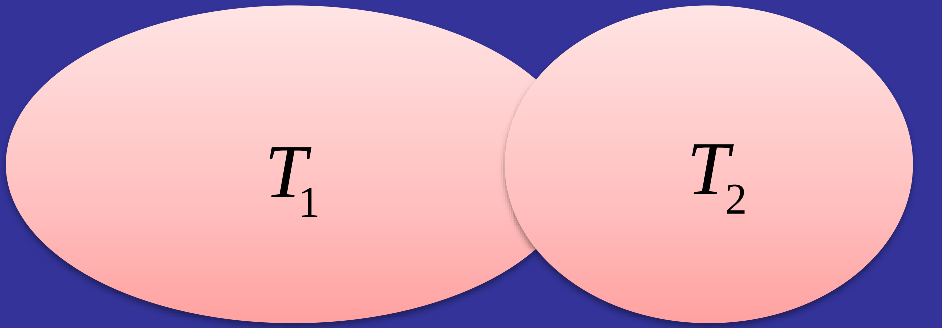
E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173.	177.26	1.95	40.825	62.246
9.60	3.063	174.	176.73	1.13	40.500	61.536
10.10	3.560	179.	176.56	1.43	41.625	62.783
10.57	4.032	173.	176.39	1.55	40.092	61.256
10.58	4.043	173.	176.39	1.70	40.146	61.388
10.58	4.047	175.	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

J. Grineviciute, et al. (in preparation)

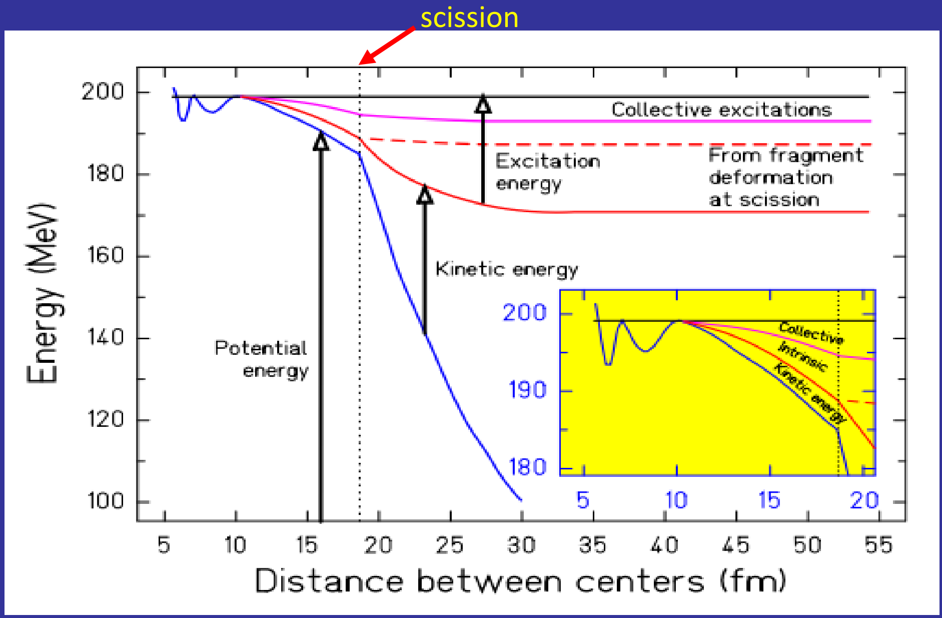
A. Bulgac, et al., arXive: 1806.00694

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

Excitation energy sharing between fragments



Excitation energy is produced and shared between nascending fragments during saddle-to-scission evolution.



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

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 to the total entropy maximization of two nascent fragments (i.e. according to temperatures, level densities) and the fission dynamics does not matter.

TDDFT naturally provides excitation energy sharing.
The intrinsic energy in TDDFT is partitioned dynamically (no sufficient time for equilibration).

Is it the correct description?

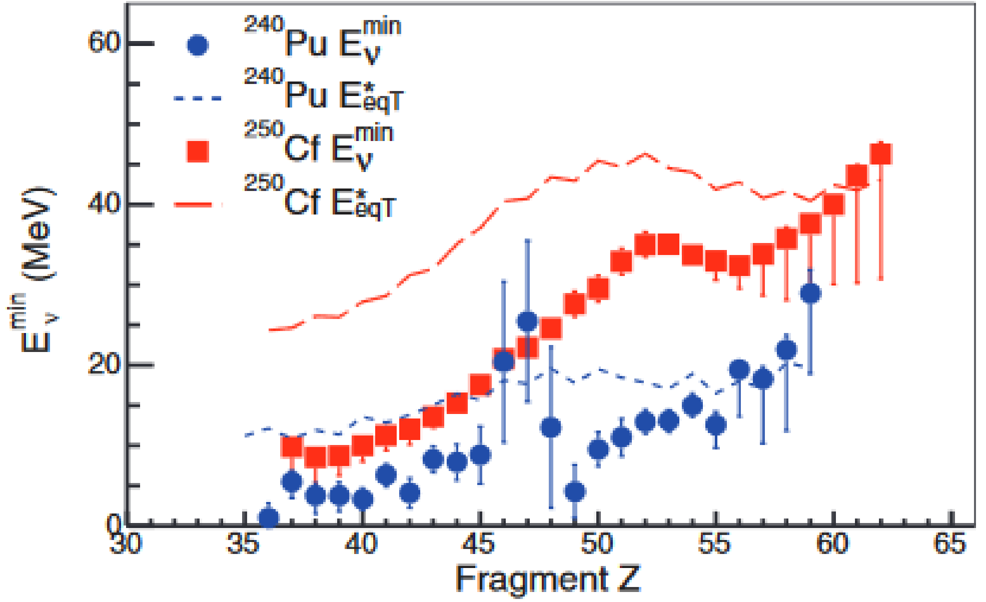
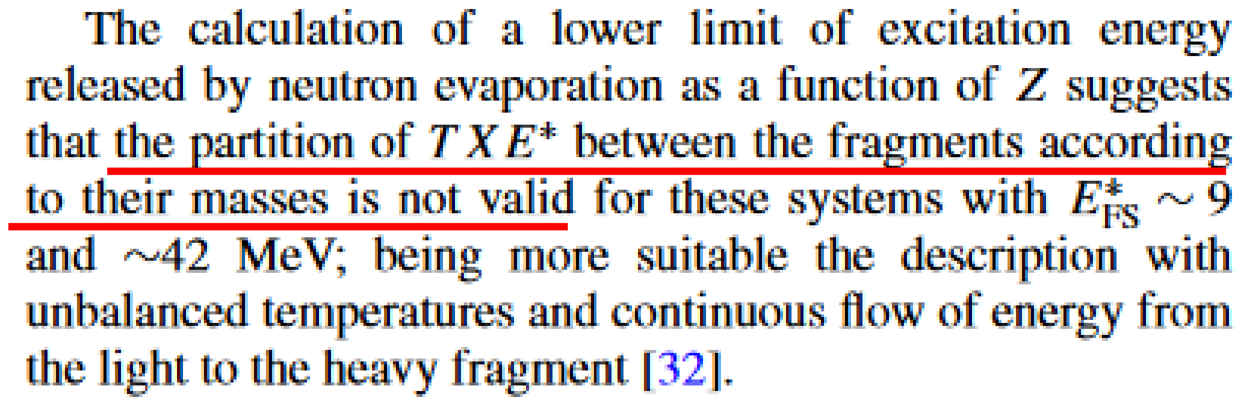


FIG. 7. (Color online) Minimum energy released in neutron evaporation and excitation energy shared according with the mass ratio of the fragments for ^{240}Pu (blue dots and dashed line) and ^{250}Cf (red squares and long-dashed line).

M. Caamaño et al. Phys. Rev. C92 034606 (2015)


The calculation of a lower limit of excitation energy released by neutron evaporation as a function of Z suggests that the partition of TXE^* between the fragments according to their masses is not valid for these systems with $E^*_{FS} \sim 9$ and ~42 MeV; being more suitable the description with unbalanced temperatures and continuous flow of energy from the light to the heavy fragment [32].

Experimental observables vs theory

Mass/charge distribution – important, but do not give us deep 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 – very interesting, but 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 - useful quantity, but as far as we know TKE 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 in principle 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 - extremely important quantity, depending on dynamics and density of states at scission. Very severe test for TDDFT: theoretical predictions already exist.

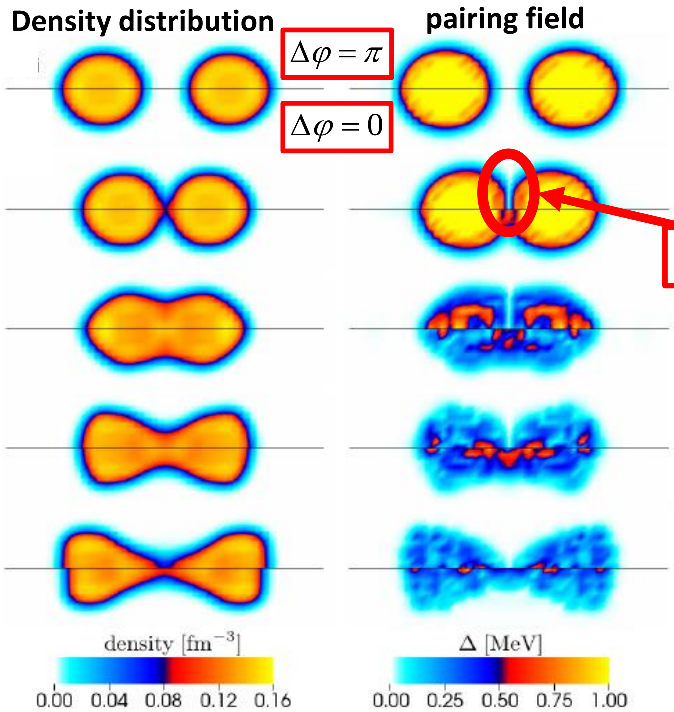
Primary gamma emission - may give some information on ang. momentum distribution of fragments, but as far as I know, not directly comparable to theories presented here.

Manifestation of pairing as a field in nuclear collisions

$$\Delta(\vec{r},t) = \left|\Delta(\vec{r},t)\right| e^{i\phi(\vec{r},t)}$$

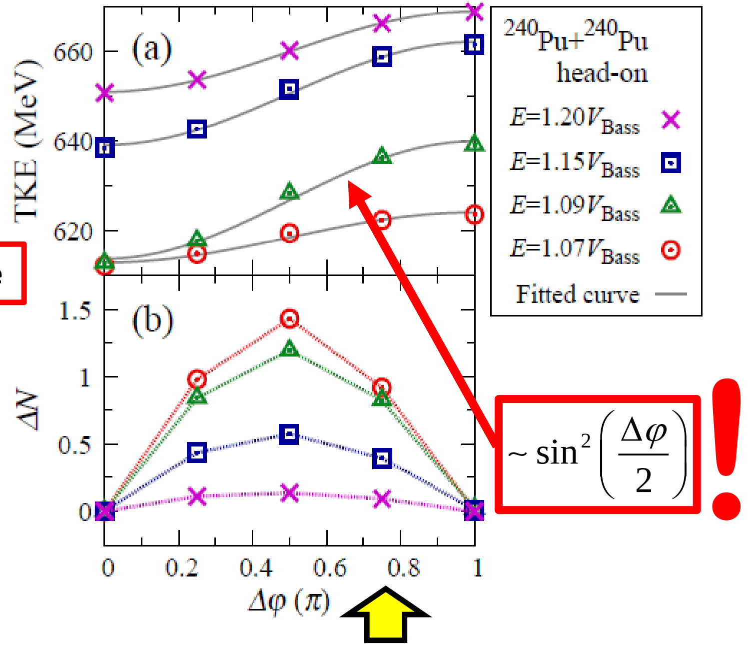
Both magnitude and phase may have a nontrivial spatial and time dependence.

Collision and reseparation of two heavy nuclei for two values of gauge angle difference (TDDFT simulation)



Solitonic structure

Total kinetic energy of the fragments (TKE)



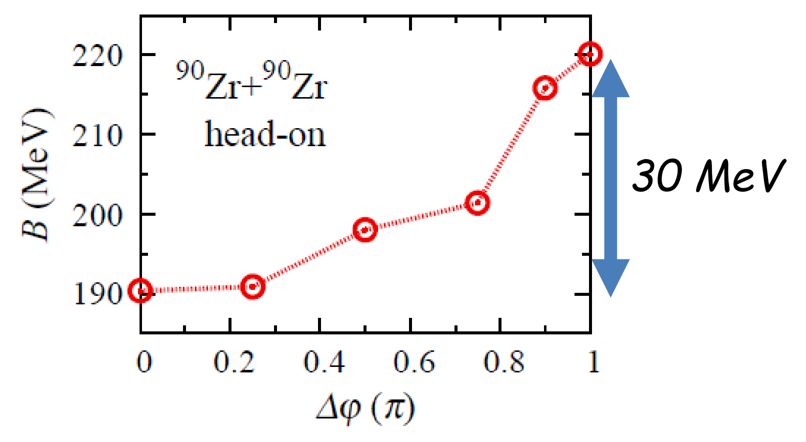
$$\sim \sin^2\left(\frac{\Delta\varphi}{2}\right)$$

!

Average particle transfer between fragments.

Creation of the solitonic structure of the pairing field between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently enhances the kinetic energy of outgoing fragments.
Surprisingly, the gauge angle dependence from the Ginzburg-Landau approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

Effective barrier height for fusion as a function of the phase difference



What is an average extra energy needed for the capture?

$$\boxed{E_{extra}=\frac{1}{\pi}\int_0^{\pi}\left(B(\Delta\varphi)-V_{Bass}\right)d(\Delta\varphi)\approx 10MeV}$$

The effect is found (within TDDFT) to be of the order of 30MeV for medium nuclei and occur for energies up to 20-30% of the barrier height.

P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

It raises an interesting question:

to what extent systems of hundreds of particles can be described using the concept of pairing field?

G. Scamps, Phys. Rev. C 97, 044611 (2018): barrier fluctuations extracted from experimental data indicate that the effect exists although is weaker than predicted by TDDFT