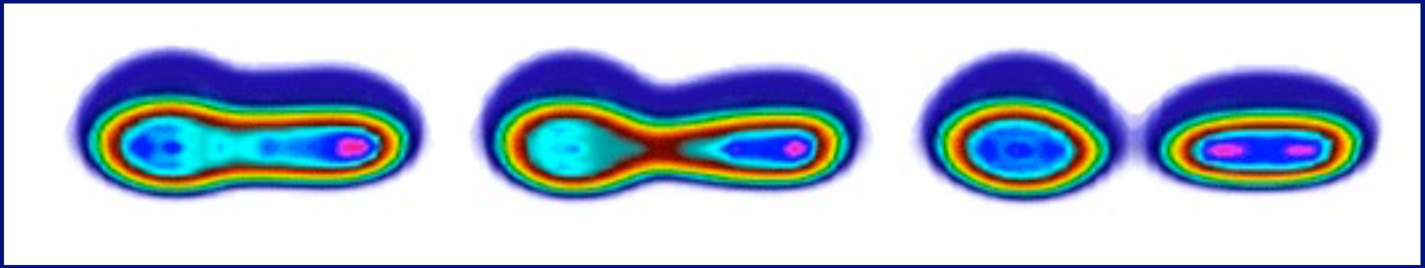
Fission Dynamics



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Most of the modeling of fission since 1939 is still performed mostly phenomenologically, *which is distinct from microscopic approaches!*

"Microscopic" approaches (TDGCM, ATDHF) assume the decoupling of collective and intrinsic motion (adiabaticity), making thus the introduction of a collective Hamiltonian legitimate.

Schunck and Robledo, Microscopic theory of nuclear fission, Rep. Prog. Phys. 79, 116301 (2016)
Krappe and Pomorski, Theory of Nuclear Fission, Springer, 2012.

What <u>microscopic</u> conclusions have been firmly established so far?

- **Fission is controlled by the competition between Coulomb and surface energies.** ***Meitner and Frisch (1939)***

- **The formation of a compound nucleus and a very slow evolution of the nuclear shape towards the outer barrier.** ***Bohr and Wheeler* (1939)**

- **The crucial role of shell effects at large deformations and of the pairing correlations while the nuclear shape evolves.** ***Strutinski, 1967, Bertsch, 1980***

- **The decay of the fission fragments can be described in a statistical approach.** ***Weisskopf (1937), Hauser and Feshbach (1952)***

The Main Theoretical Tool: DFT

(formulated in 1964 by Kohn and Hohenberg and further extended ever since)

TDSLDA- An extension to Superfluids and Time-Dependent Phenomena of DFT and is based on Verification and Validation for a variety of strongly interacting fermions systems (cold atoms, neutron star crust, nuclei).

- **Since DFT/SLDA is not an approximation, but in principle an exact theoretical framework (unlike HF, HFB, etc.), one has to convincingly prove that its specific realization is equivalent to the Schrödinger equation!**
- ***(The fine print: There is a continuous debate on whether DFT exist for self-bound systems, but this will not be discussed today. If you feel more confortable for the sake of the discussion replace DFT with EDF.)***
- **<u>The DFT and the Schrödinger descriptions of observables should be identical.</u>**
- **One expects that DFT also describes correctly Nature!**
- **And, of course, that the numerical implementation faithfully reproduces the theory.**

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} \mathrm{u}_{n\uparrow}(\vec{r},t) \\ \mathrm{u}_{n\downarrow}(\vec{r},t) \\ \mathrm{v}_{n\uparrow}(\vec{r},t) \\ \mathrm{v}_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{\mathrm{h}}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{\mathrm{h}}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{\mathrm{h}}_{\downarrow\uparrow}(\vec{r},t) & \hat{\mathrm{h}}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{\mathrm{h}}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{\mathrm{h}}^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -\hat{\mathrm{h}}^*_{\downarrow\uparrow}(\vec{r},t) & -\hat{\mathrm{h}}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} \mathrm{u}_{n\uparrow}(\vec{r},t) \\ \mathrm{u}_{n\downarrow}(\vec{r},t) \\ \mathrm{v}_{n\uparrow}(\vec{r},t) \\ \mathrm{v}_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

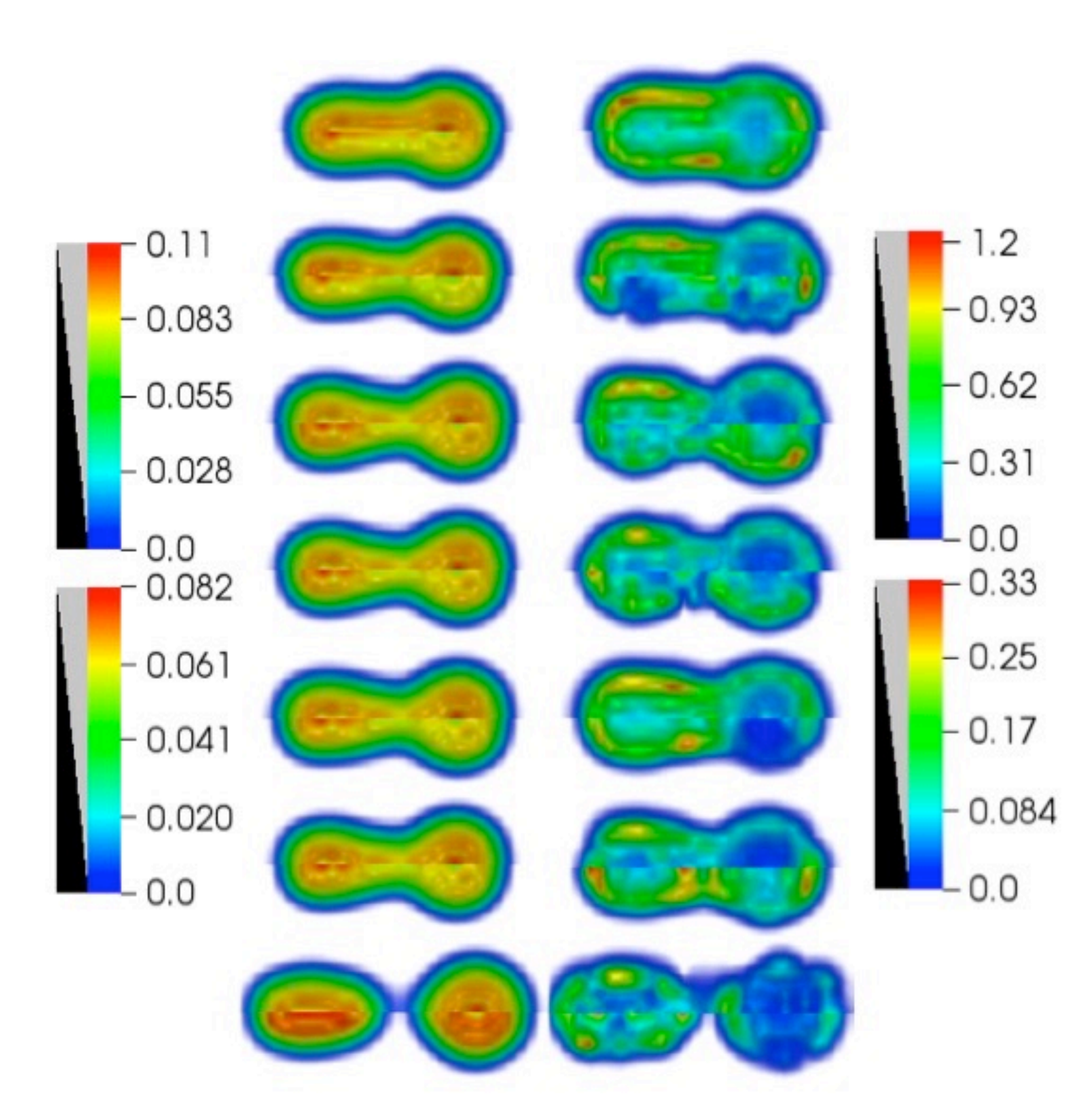
The Main Computational Tool

Titan, Cray XK7, ranked at peak ≈ 27 Petaflops (Peta – 10^{15})

On Titan there are <u>18,688 GPUs</u> which provide <u>24.48 Petaflops !!!</u>
and <u>299,008 CPUs</u> which provide <u>only 2.94 Petaflops</u>.

A single GPU on Titan (#7 on Top 500) performs the same amount of FLOPs as approximately 134 CPUs. In our codes we observed a ≈150x speed-up with GPUs vs CPUs

Induced fission of ^{240}Pu



Neutron/proton densities (left and top/bottom)
Neutron/proton pairing gaps (right and top/bottom)

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

TABLE I. The simulation number, the pairing parameter η, the excitation energy (E^*) of $^{240}_{94}\mathrm{Pu}_{146}$ and of the fission fragments [$E^*_{H,L} = E_{H,L}(t_{SS}) - E_{gs}(N_{H,L}, Z_{H,L})$], the equivalent neutron incident energy (E_n), the scaled initial mass moments $q_{20}(0)$ and $q_{30}(0)$, the "saddle-to-scission" time t_{SS}, TKE evaluated as in Ref. [71], TKE, atomic (A_L^{syst}), neutron (N_L^{syst}), and proton (Z_L^{syst}) extracted from data [72] using Wahl's charge systematics [73] and the corresponding numbers obtained in simulations, and the number of postscission neutrons for the heavy and light fragments ($\nu_{H,L}$), estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8,74,75]. Units are in MeV, fm^2, fm^3, fm/c as appropriate.

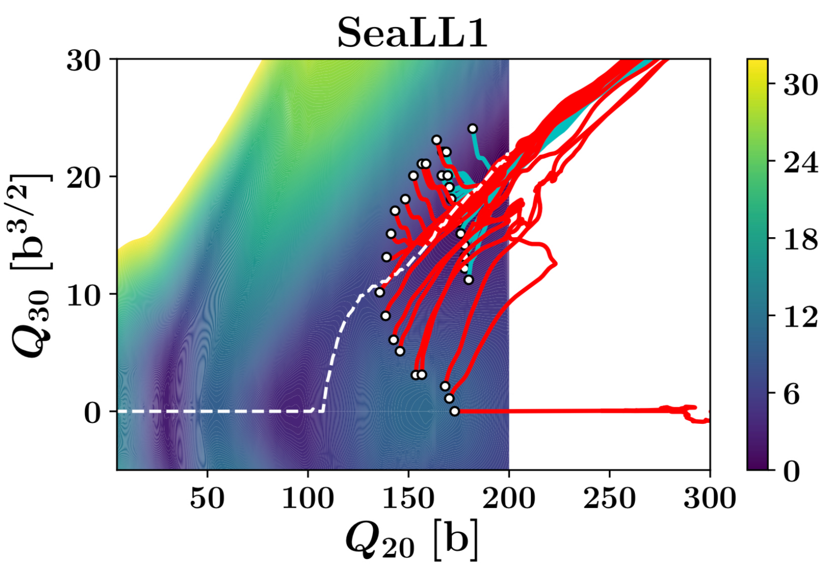
S no.	η	E^*	E_n	q_{zz}	q_{zzz}	t_{SS}	TKE$^{\text{syst}}$	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L	E_H^*	E_L^*	ν_H	ν_L
$S1$	0.75	8.05	1.52	1.78	−0.742	14 419	177.27	182	100.55	104.0	61.10	62.8	39.45	41.2	5.26	17.78	0	1.9
$S2$	0.5	7.91	1.38	1.78	−0.737	4360	177.32	183	100.56	106.3	60.78	64.0	39.78	42.3	9.94	11.57	1	1
$S3$	0	8.08	1.55	1.78	−0.737	14 010	177.26	180	100.55	105.5	60.69	63.6	39.81	41.9	3.35	29.73	0	2.9
$S4$	0	6.17	−0.36	2.05	−0.956	12 751	177.92	181		103.9		62.6		41.3	7.85	9.59	1	1

NEDF	E^*_{ini}	TKE	N_{H}	Z_{H}	N_{L}	Z_{L}	E^*_{H}	E^*_{L}	TXE	TKE+TXE	$\tau_{s\to s}$ (fm/c)
SeaLL1-1asy	7.9(1.7)	177.8(3.1)	83.4(0.4)	53.2(0.4)	62.9(0.5)	41.1(0.4)	17.1(3.0)	20.3(2.0)	37.4(3.1)	215.2(2.5)	2317(781)
SeaLL1-2asy	2.6(1.8)	178.0(2.3)	82.9(0.4)	52.9(0.2)	63.3(0.5)	41.5(0.3)	19.5(3.8)	14.0(1.9)	33.5(5.1)	211.5(3.3)	1460(176)
SeaLL1-sy	9.2	147.1	77.5	48.9	68.8	45.4	45.2	29.0	74.2	221.3	10103
SkM*-asy	8.2(3.0)	174.5(2.5)	84.1(0.9)	53.0(0.5)	61.8(0.9)	40.9(0.5)	16.6(3.1)	14.9(2.3)	31.5(3.8)	206.0(2.4)	1214(448)
SkM*-sy	9.6	149.0	73.4	47.2	72.6	46.7	29.4	28.5	57.9	206.9	3673

Table I. The NEDF, the initial excitation energy E^*_{ini}, TKE, neutron, proton number number and excitation energies N_{H}, N_{L}, Z_{H}, Z_{L} of the heavy and light fragments, total excitation energy of fragments TXE, and the sum of TKE and TXE, and the average saddle-to-scission times and their corresponding variances in parentheses. All energies are in MeV and S***sy, S***asy stand for symmetric and antisymmetric channels.

Agreement with observations is pretty good and without any fitting parameters, as long as the basic nuclear properties (saturation, surface tension, symmetry energy, Coulomb, spin-orbit, pairing) are well described !

^{240}Pu potential energy surface $E(Q_{20},Q_{30})$ together with fission trajectories in case of SeaLL1



E_{init}=-1813.9±1.1 MeV

N_H = 82.9±0.4, Z_H = 52.9±0.2, T_H = 1.15±0.08 MeV, Q_{20} = 2.58 ± 0.61b

N_L = 63.3±0.5, Z_L = 41.5±0.3, T_L = 1.19±0.12 MeV, Q_{20} = 17.09 ± 1.09b

TKE = 178.0±2.3 MeV

TXE = 33.5±5.1 MeV, E^*_H=19.5±3.8 MeV, E^*_L=14.0±1.9 MeV

TKE+TXE = 211.5±3.3 MeV

$$E^* = \frac{A}{10}T^2$$

E_{init}=-1808.0±2.4 MeV

N_H = 83.5±0.4, Z_H = 53.2±0.4, T_H = 1.11±0.08 MeV, Q_{20} = 2.59 ± 0.47b

N_L = 62.8±0.5, Z_L = 41.1±0.4, T_L = 1.39±0.07 MeV, Q_{20} = 15.65 ± 0.91b

TKE = 177.8±2.8 MeV

TXE = 37.1±2.7 MeV, E^*_H=17.0±2.4 MeV, E^*_L=20.1±2.0 MeV

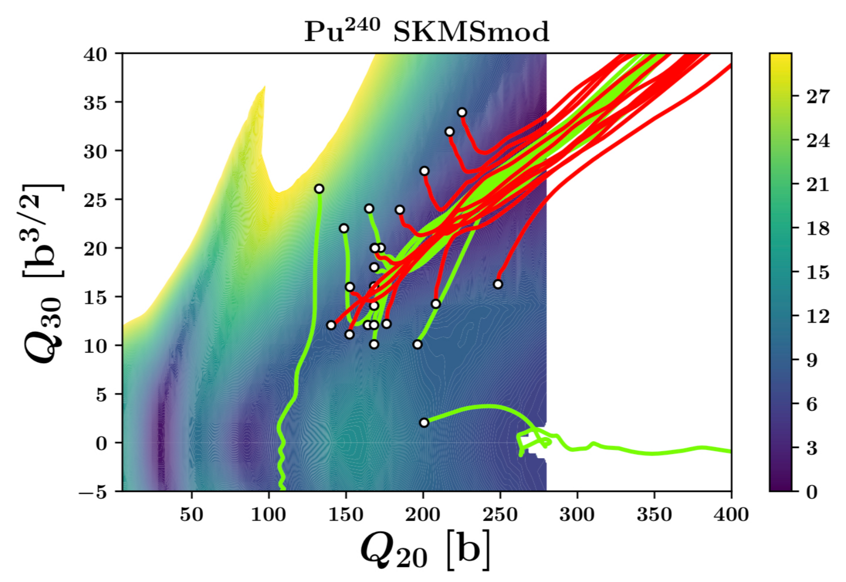
TKE+TXE = 214.9± 2.4MeV

- Irrespective of the initial conditions the final configurations are almost the same!

This behavior is consistent with strong dissipation and overdamped collective motion only.

- The excitation energy/temperature of the fission fragments is determined by the initial energy. The higher the initial excitation energy the higher the temperature of the final light fission fragment. Thus excitation energy sharing in induced and spontaneous fission differ.

^{240}Pu potential energy surface $E(Q_{20},Q_{30})$ together with fission trajectories in case of SkM*



E_{init}=-1780.5±2.2 MeV

N_H = 84.1±0.9, Z_H = 53.0±0.5, T_H = 1.10 ± 0.10 MeV, Q_{20} = 3.5±0.9 b

N_L = 61.8±0.9, Z_L = 40.9±0.5, T_L = 1.20 ± 0.09 MeV, Q_{20} = 11.3±1.3 b

TKE = 174.5±2.5 MeV

TXE = 31.5±3.8 MeV , E^*_H=16.6±3.1 MeV, E^*_L=14.9±2.3 MeV

TKE+TXE = 206.0±2.4MeV

$$E^* = \frac{A}{10} T^2$$

"Symmetric" case

E_{init}=-1780.2 MeV

N_L = 72.6, Z_L = 46.7, E^*_L = 28.5MeV

N_H = 73.4, Z_H = 47.2, E^*_R = 29.4MeV

TKE = 149.0 MeV

TXE = 57.9 MeV

TKE+TXE = 206.9 MeV

Similar qualitative behavior with SeaLL1.

- **Irrespective of the initial conditions the final configurations are almost the same!**

This behavior is consistent with strong dissipation and overdamped collective motion only.

- **The excitation energy/temperature of the fission fragments is determined by the initial energy. The higher the initial excitation energy the higher the temperature of the final light fission fragment. Thus excitation energy sharing in induced and spontaneous fission differ.**

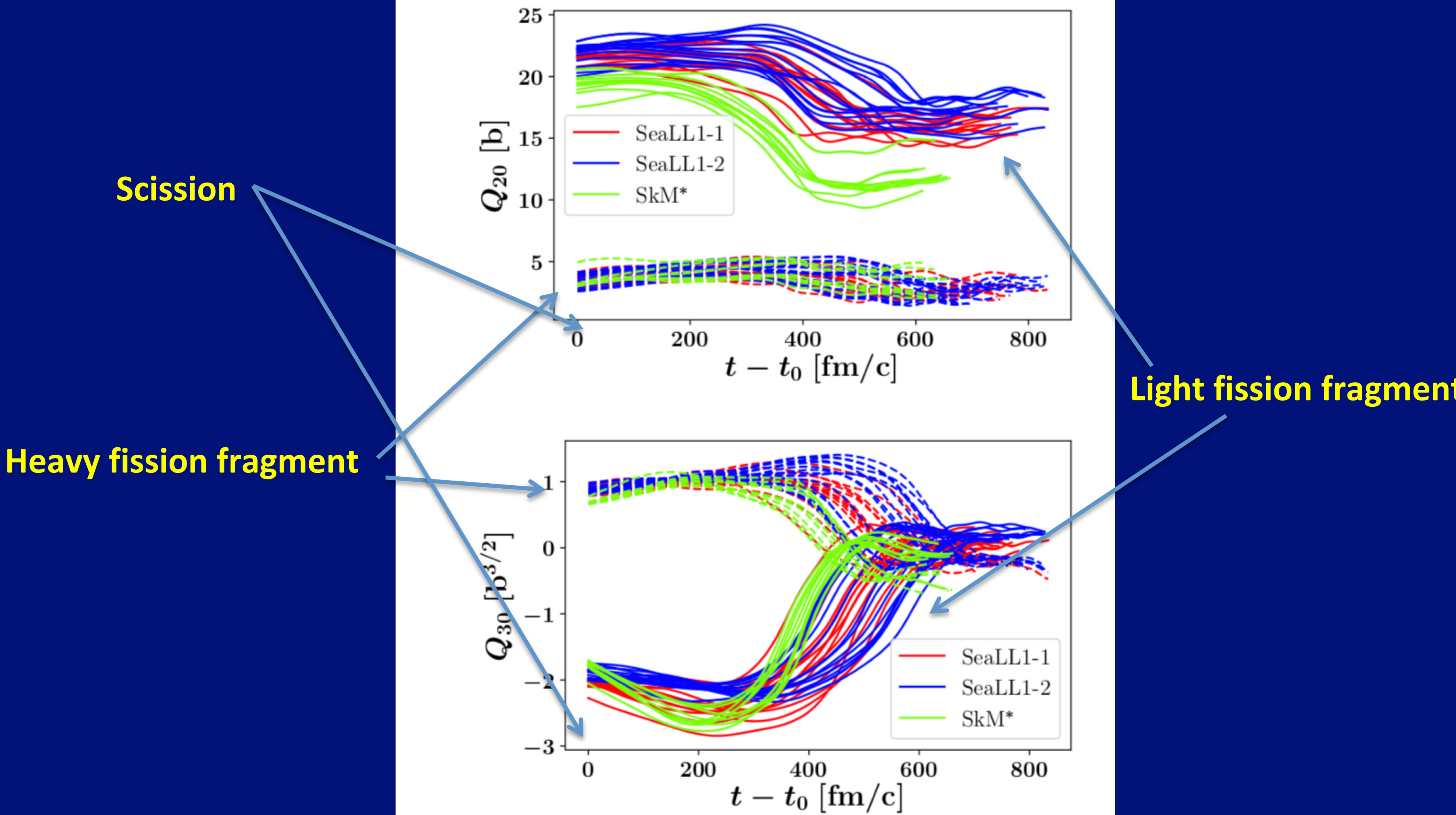


Figure 5. (Color online) The evolution of the quadrupole Q_{20} and octupole Q_{30} moments of the light (solid lines) and heavy (dashed lines) FFs after scission. The color codes are the same as in Fig. 3

The light fission fragment emerges at scission (t_0) very elongated, but it relaxes relatively quickly.

Large Amplitude Collective Motion is strongly dissipative.
It is overdamped!

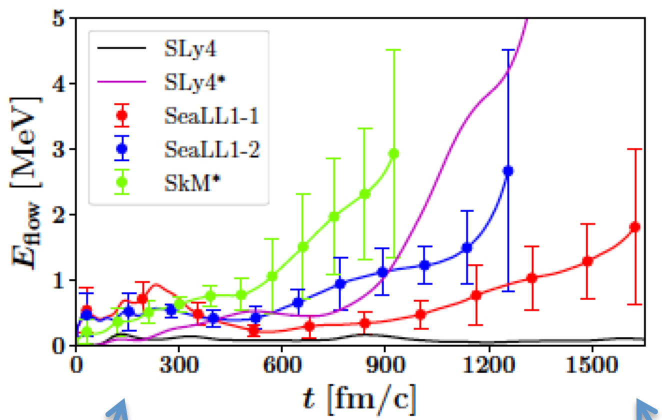
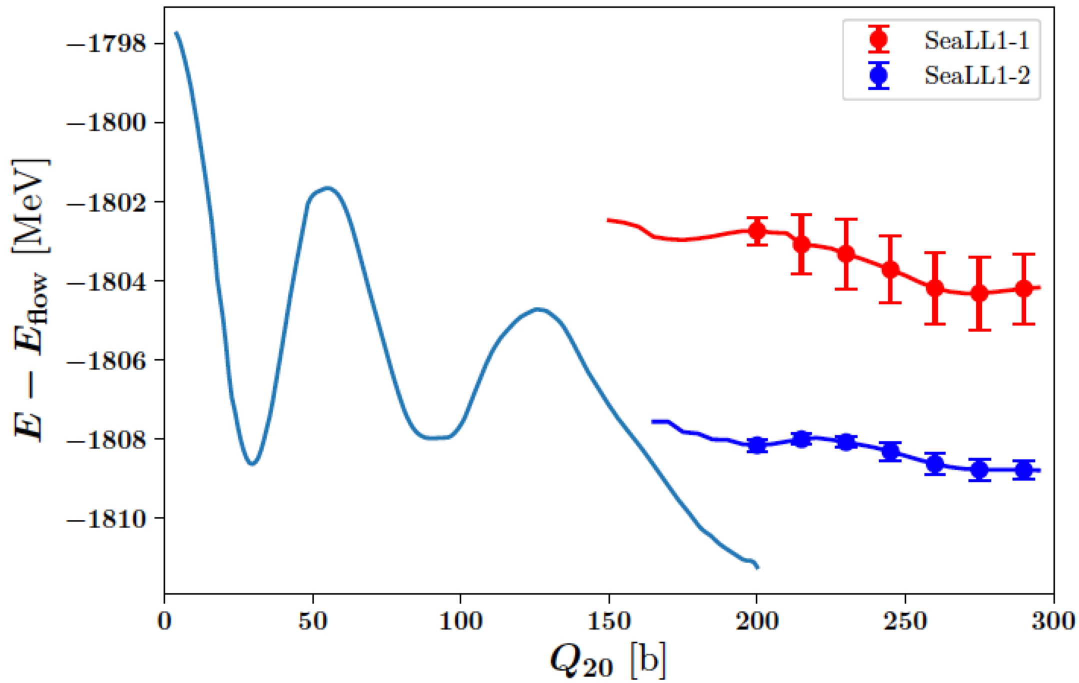


Figure 3. (Color online) The collective flow energy evaluated for NEDFs with realistic pairing SLy4 [41], enhanced pairing SLy4*, and for SkM*, SeaLL1-1 and SeaLL1-2 sets. The error bars illustrate the size of the variations due to different initial conditions.



$$E_{flow} = \int d^3r \frac{\vec{j}^{\,2}(\vec{r},t)}{2mn(\vec{r},t)}$$

$$\vec{j}(\vec{r},t) = \frac{i\hbar}{2}\sum_k \mathrm{v}_k^*(\vec{r},t)\vec{\nabla}\mathrm{v}_k(\vec{r},t) - \mathrm{v}_k(\vec{r},t)\vec{\nabla}\mathrm{v}_k^*(\vec{r},t)$$

$$n(\vec{r},t) = \sum_k \left|\mathrm{v}_k(\vec{r},t)\right|^2$$

$$E_{total} = E_{flow} + E_{\rm int} \approx E_{\rm int}(q,T) \approx const.$$

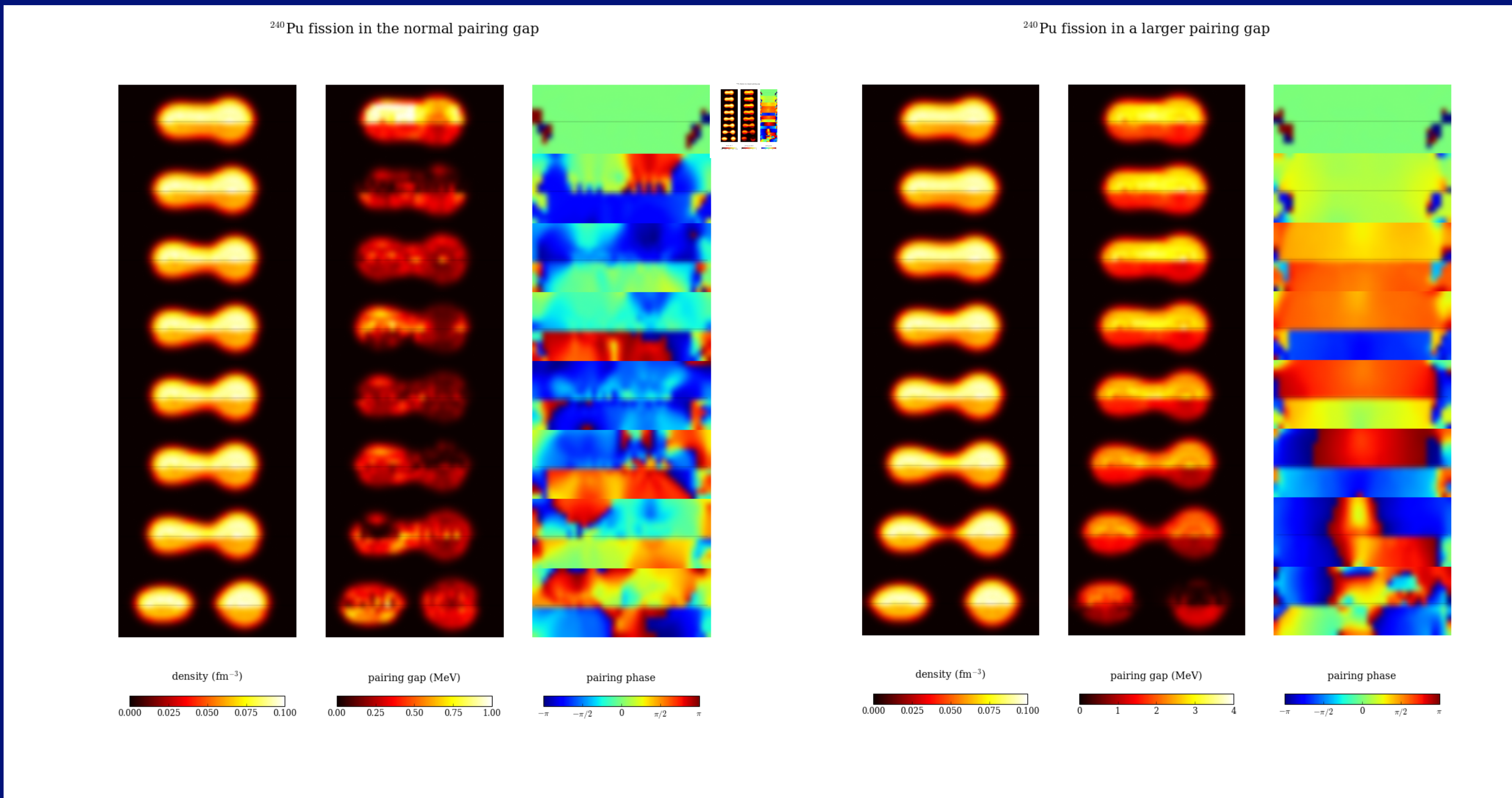
The kinetic energy of the fission fragments at scission is almost negligible, an order of magnitude smaller then expected in all "microscopic" models!

Fission Fragments emerge (relatively) "hot" at scission!

And they will get a bit hotter after their shape relaxes, particularly the light fragments.

How important is pairing?

Without pairing nuclei will either need a long time to fission or typically will fission!!!



Normal pairing strength
Saddle-to-scission 14,000 fm/c

Enhanced pairing strength
Saddle-to-scission 1,400 fm/c !!!

The textbook "microscopic" theories of large amplitude collective motion are based on either ATDHF or TDGCM, and on the derivation of a collective Hamiltonian.

Goeke and Reinhard, Ann. Phys. 124, 249 (1980)

The generator coordinate method with conjugate parameters and the unification of microscopic theories of large amplitude collective motion

$$\left|\psi\right\rangle = \int dq\, f(q)\left|q\right\rangle, \qquad \int dq \left\langle q'\right|H-E\left|q\right\rangle f(q) = 0, \qquad \text{GCM}$$

$$\left|\psi\right\rangle = \int dq\, dp\, f(q,p)\left|qp\right\rangle, \quad \int dq \left\langle q'p'\right|H-E\left|qp\right\rangle f(q,p) = 0 \quad \text{Dynamical GCM}$$

$$\Rightarrow H_C = -\frac{1}{4}\left[\frac{\partial^2}{\partial q^2}\frac{1}{2M(q)} + \frac{\partial}{\partial q}\frac{1}{M(q)}\frac{\partial}{\partial q} + \frac{1}{2M(q)}\frac{\partial^2}{\partial q^2}\right] + V(q)$$

Hill and Wheeler (1953)

Peierls and Yoccoz (1957)

It is remarkable that this Schrödinger equation first contains a collective mass of the form as given by the semiclassical approaches like ATDHF, and second is altogether nearly identical to the one obtained by quantizing the semiclassical theories properly. Second, both sorts of approaches provide identical matrix elements of observables with respect to collective wave functions. A third link concerns properties of the collective basis $|q, p\rangle$: The DGCM requires certain decoupling conditions which are covered by the corresponding equations in ATDHF. Altogether the important result is that both, DGCM and quantized ATDHF, although originating from different starting points, are virtually identical. Since ATDHF is known to be a sophisticated

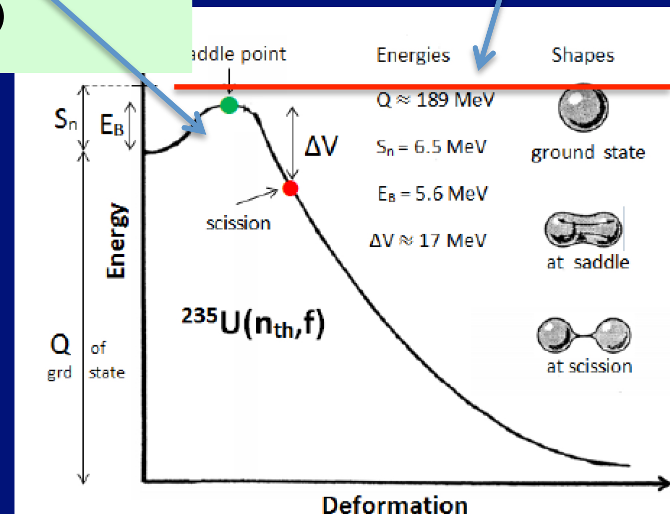
$$|\psi\rangle = \int dq\, f(q)|q\rangle, \qquad \int dq \langle q'|H-E|q\rangle f(q) = 0, \qquad \text{GCM}$$

$$|\psi\rangle = \int dq\, dp\, f(q,p)|qp\rangle, \quad \int dq \langle q'p'|H-E|qp\rangle f(q,p) = 0 \qquad \text{Dynamical GCM}$$

$$\Rightarrow H_C = -\frac{1}{4}\left[\frac{\partial^2}{\partial q^2}\frac{1}{2M(q)} + \frac{\partial}{\partial q}\frac{1}{M(q)}\frac{\partial}{\partial q} + \frac{1}{2M(q)}\frac{\partial^2}{\partial q^2}\right] + V(q)$$

$$\text{Classically (HF or HFB):} \quad E_{tot} = \frac{M(q)\dot{q}^2}{2} + V(q) = \frac{M(q)\dot{q}^2}{2} + E_{\text{int}}(q)$$

$$E_{\text{int}} = V(q,T) \approx const$$



The intrinsic or potential energy is always obtained in a Born-Oppenheimer approximation (with constraints) as in molecular physics. It depends on density alone.

While the nuclear shape evolves the nucleus follows the lowest energy surface (aka the molecular term in atomic physics), and thus the intrinsic entropy is always zero.

(Extending GCM by adding some low lying quasiparticle excitations into the mix does not lead to qualitative Improvements.)

Does the nucleus ever evolve on the lowest potential energy surface? This assumptions was questioned many times but never confirmed.

If that would be the case at scission the collective kinetic energy would be about ≈O(20) MeV.

In fact this kinetic collective energy is about 1-2 MeV.

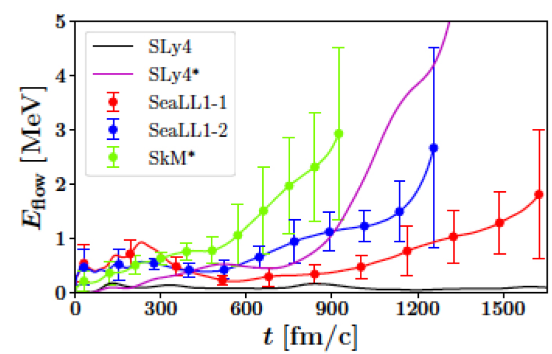


Figure 3. (Color online) The collective flow energy evaluated for NEDFs with realistic pairing SLy4 [41], enhanced pairing SLy4*, and for SkM*, SeaLL1-1 and SeaLL1-2 sets. The error bars illustrate the size of the variations due to different initial conditions.

- **The collective motion it is indeed very slow, much slower than in the case of adiabatic motion, but this fact does not justifies the assumption that collective and intrinsic motions are decoupled, and neither that the assumption that the motion is adiabatic, nor the introduction of a collective Hamiltonian.**

The motion of a nucleus form saddle-to-scission is similar to a train down the slope with its wheels locked and all the gravitational energy turns into heat, hot wheels!

- **Remember, the evolution from the ground state shape, when a neutron is captured, to the outer fission barrier is much much slower.**

But that does not make that part of the nuclear shape evolution adiabatic either.
(an adiabatic transformation should not be conflated with a quasistatic one, both are slow, as we all know from thermodynamics)

- **Nuclei remember and conserve almost exactly their initial intrinsic energy from which they started, while their shape evolves.**
Intrinsic energy (approximately) does not depend on collective velocity.

$$E_{\mathrm{int}} = V(q,T) \approx const$$

But this does not make sense within GCM or ATDHF!
This is at odds with stochastic meanfield as well, where Pauli principle is violated!!!

- The irreversible energy flow from the collective degrees of freedom towards the intrinsic degrees of freedom is simply controlled by the large entropy of the intrinsic system.
  At the scission configuration the level density is about 10^7 MeV^{-1}.

$$S_{tot}(t) = -\mathrm{Tr}_{all}\ \rho_{tot}(t)\ln\rho_{tot}(t) \equiv 0, \quad \rho_{tot}(t) = \left|\Psi(t)\right\rangle\left\langle\Psi(t)\right|,$$
$$S_{\mathrm{int}}(t) = -\mathrm{Tr}_{\mathrm{int}}\ \rho_{\mathrm{int}}(t)\ln\rho_{\mathrm{int}}(t) \quad \geq 0 \Leftarrow \text{Entanglement entropy},$$
$$\rho_{\mathrm{int}}(t) = \mathrm{Tr}_{coll}\ \rho_{tot}(t)$$

Intrinsic entropy is the main driver of the nuclear shape dynamics

Does there exist a GCM/ATDHF-like representation of the total nuclear wave function?

$$\left|\Psi\right\rangle = \int d^n q f(q_1,\ldots,q_n)\left|q_1,\ldots,q_n\right\rangle$$

$$N_s = 24^2 \times 48 = 27{,}648 \text{ sites on spatial lattice in a typical simulation}$$
$$\text{the maximum number of collective coordinates}$$

$$N_{\mathrm{SD}} = \frac{(2N_s)!}{Z!(2N_s - Z)!} \times \frac{(2N_s)!}{N!(2N_s - N)!} \simeq 10^{739} \quad \text{\# of possible Slater det.}$$

<u>The fine print!</u>

Nobody produced yet a theoretical argument which determines how many and what kind of collective degrees of freedom are necessary!

Very likely their number Increases while a nucleus barrels down from near the saddle all the way to scission.

- **Not an exact numerical estimate for N_s, but a reasonable one.**
- **A satisfactory physical framework would require about 10^7 Slater determinants at scission.**

A little gedanken experiment!

The energy flow from the collective degrees of freedom to intrinsic degrees of freedom is <u>irreversible!</u>

The entropy and the temperature of the intrinsic system are increasing while the nucleus evolves towards the scission configuration.

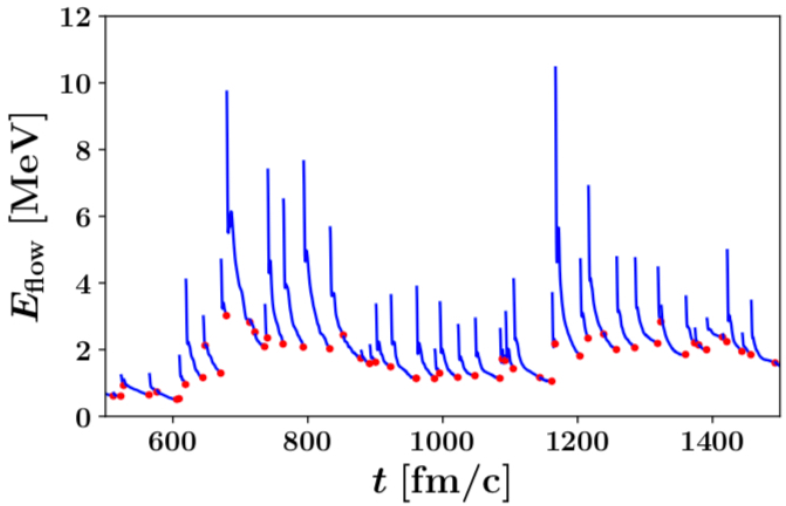


Figure 3. (Color online) At times indicated with red dots we have applied collective quadrupole momentum kicks to both neutrons and protons, see Eq. (15), with random values of η, see Eq. (15).

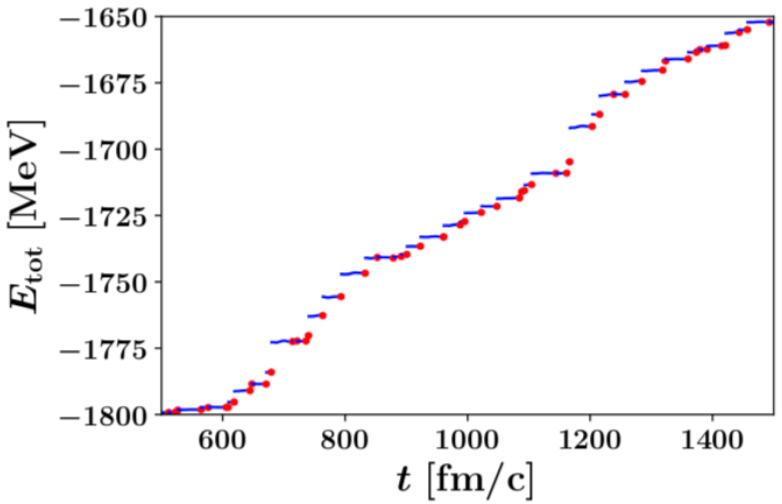


Figure 4. The time evolution of the total energy of the nucleus, in the rest frame of the nucleus, after we have applied collective kicks were to both neutrons and protons with random values of η, see Eq. (15) and Fig. 3.

$$\begin{pmatrix} u_\alpha(\mathbf{r},t) \\ v_\alpha(\mathbf{r},t) \end{pmatrix} \rightarrow \begin{pmatrix} \exp[\ i\eta(2z^2 - x^2 - y^2)]u_\alpha(\mathbf{r},t) \\ \exp[-i\eta(2z^2 - x^2 - y^2)]v_\alpha(\mathbf{r},t) \end{pmatrix}$$

$$E_{tot} = E_{flow} + E_{\text{int}} \approx E_{\text{int}}$$

What have we learned?

Large Amplitude Collective Motion is strongly dissipative, it is overdamped, the role of the collective inertia is negligible!

The introduction of a collective Hamiltonian is illegitimate.

Fluctuations or two-body collisions do not modify this conclusion.

What is the relevance of this finding for our understanding and description of fission dynamics?

Including dissipation and fluctuations

Classically, Langevin equation:

$$m\ddot{x}(t) = F - \gamma m\dot{x}(t) + m\xi(t),$$
$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \Gamma\delta(t-t'),$$
$$\dot{x}(t) = \mathrm{v}(0)\exp(-\gamma t) + \frac{F}{m\gamma}\left(1-\exp(-\gamma t)\right) + \int_0^t dt'\xi(t)\exp(-\gamma(t-t')),$$
$$\langle \mathrm{v}(t) \rangle \to \frac{F}{m\gamma}, \quad \langle\langle \mathrm{v}^2(t) \rangle\rangle \to \frac{\Gamma}{2\gamma} = \frac{T}{m}$$

Quantum mechanically, Lindblad equation:

$$i\hbar\dot{\rho} = \left[H,\rho\right] - i\left(W\rho + \rho W\right) + i\sum_{k,l} h_{kl} A_k \rho A_l^\dagger,$$
$$W = W^\dagger = \frac{1}{2}\sum_{k,l} h_{kl} A_l^\dagger A_k, \quad h_{kl} = h_{lk}^*, \quad \mathrm{Tr}\dot{\rho} = 0.$$

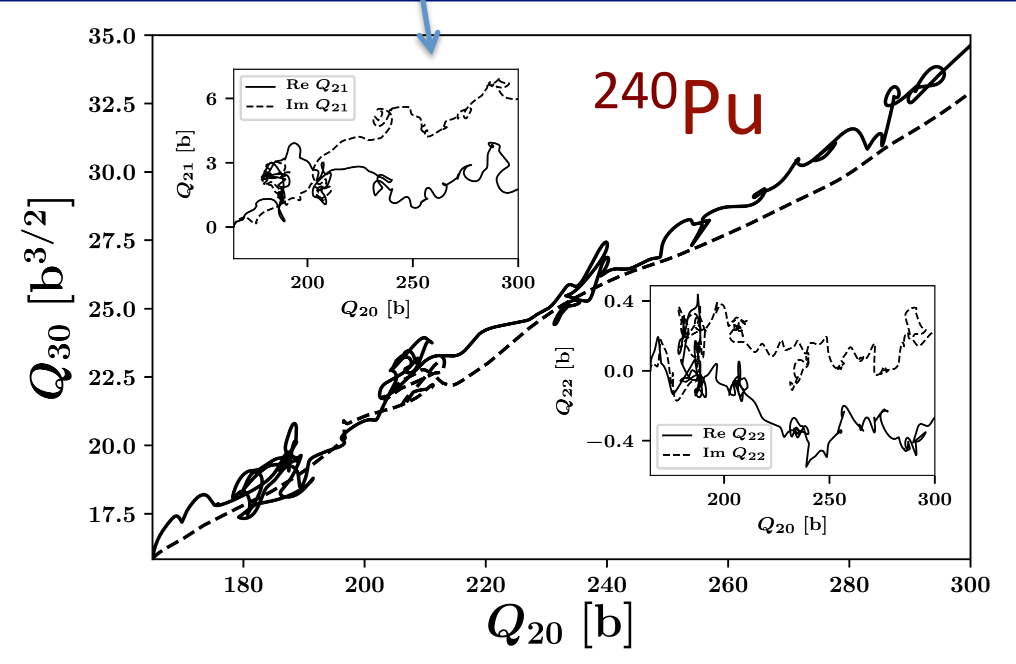
A much better and simpler solution:
A quantum Hermitian “Langevin” equation

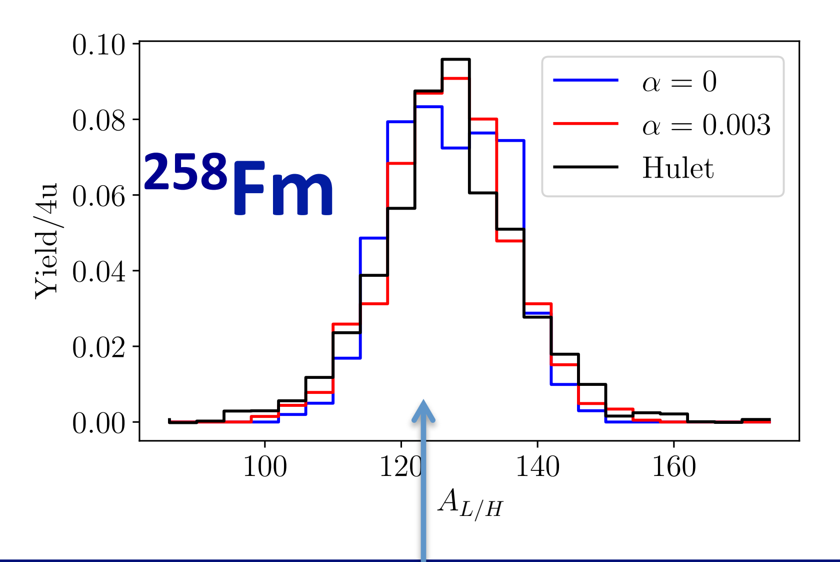
Quantum friction

$$i\hbar\dot{\psi}_k(\vec{r},t) = h\left[n(\vec{r},t)\right]\psi_k(\vec{r},t) + \gamma\left[n(\vec{r},t)\right]\dot{n}(\vec{r},t)\psi_k(\vec{r},t)$$

$$-\frac{1}{2}\left[\vec{u}(\vec{r},t)\cdot\vec{p} + \vec{p}\cdot\vec{u}(\vec{r},t)\right]\psi_k(\vec{r},t) + \varsigma(\vec{r},t)\psi_k(\vec{r},t)$$

“Stochastic fields”





Mass yields
Without shell corrections

Summary

- While pairing is not the engine driving the fission dynamics, pairing provides the essential lubricant, without which the evolution may arrive quickly to a screeching halt.

- TDDFT will offer insights into nuclear processes and quantities which are either not easy or impossible to obtain in the laboratory: fission fragments excitation energies and angular momenta distributions prior to neutron and γ emission, element formation in astrophysical environments, and other nuclear reactions in a parameter free approach …

- The quality of the agreement with experimental observations is surprisingly good, especially taking into account the fact that we made no effort to reproduce any fission measured data. No fitting of parameters!

- It has been now firmly established microscopically that large amplitude collective motion is strongly dissipative and overdamped and phenomenological models would have to be altered accordingly.

- The fissioning nucleus behaves superficially as a very viscous system.

- The “temperatures” of the fission fragments are not equal.