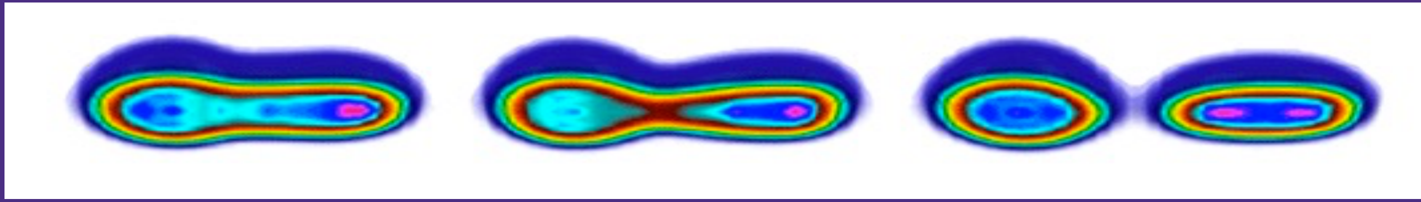
Final Exam

Fission Dynamics in a Microscopic Theory



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05/29/2019

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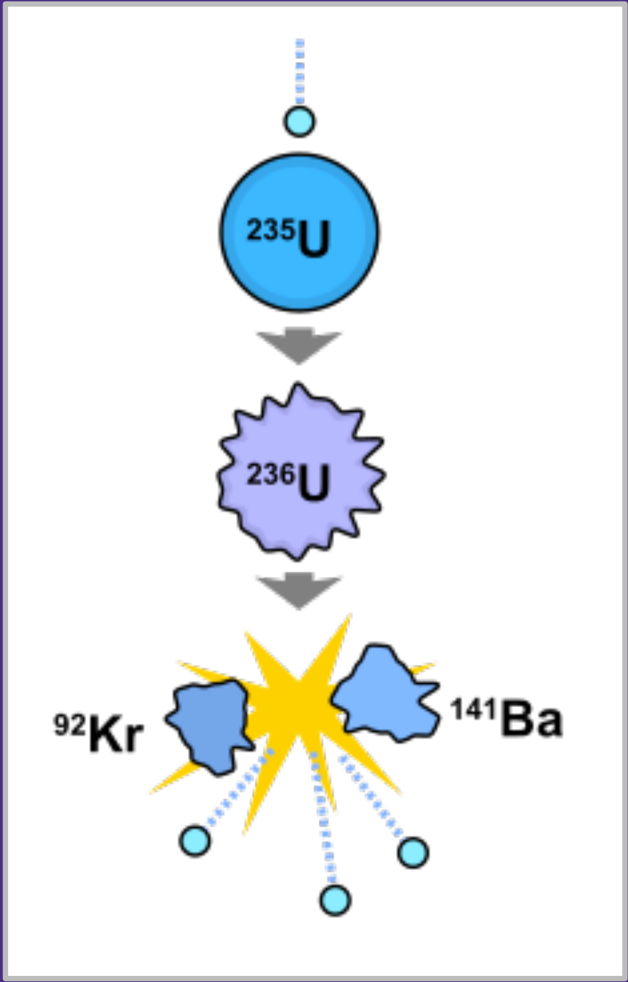
History and Background

Discovery

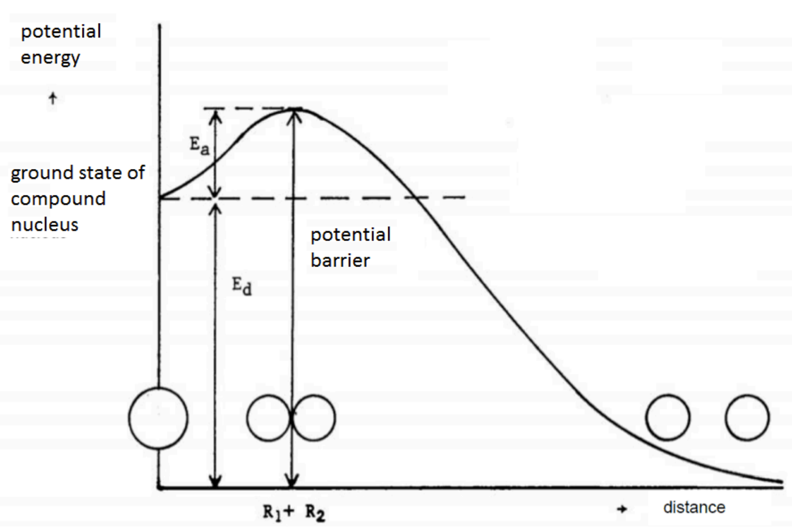
- Nuclear fission was observed by Hahn and Strassmann in 1938-1939.
- Experiment on the bombardment of Uranium atoms with neutrons.
- Lighter elements akin to Barium (Z = 56) were formed in the reaction



History and Background

Interpretation based on liquid drop model

- Fission was interpreted by Meitner and Frisch and Bohr and Wheeler in 1939 based on the liquid drop model (LDM).
- In LDM, fission is described as the Coulomb-driven division of a classically charged liquid drop in competition with the surface tension of the liquid drop.

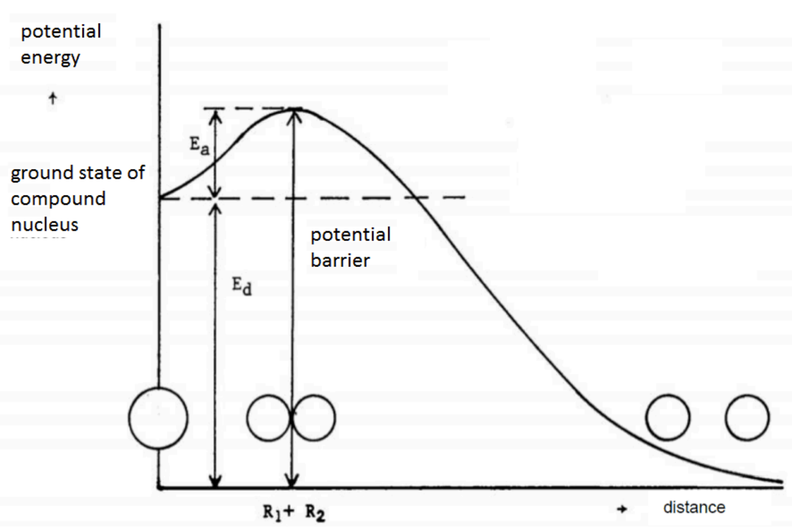


Potential Energy Surface (PES)

History and Background

Interpretation based on liquid drop model

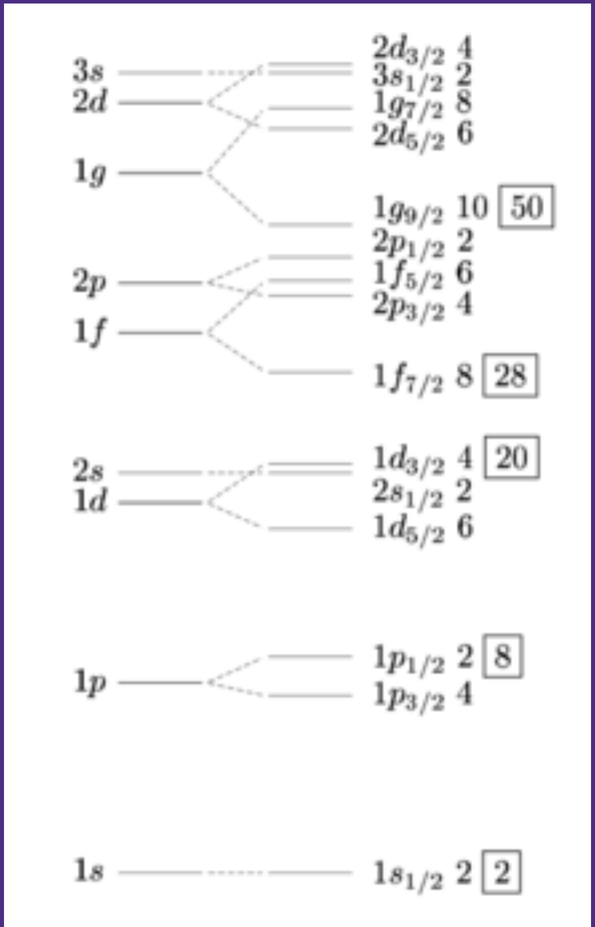
- Limitation
  - It can only predict a symmetric fission where two fragments have the same mass.
  - It is a classical theory and it ignores the quantum effects, i.e. the individual behaviors of nucleons.



History and Background

Shell Model

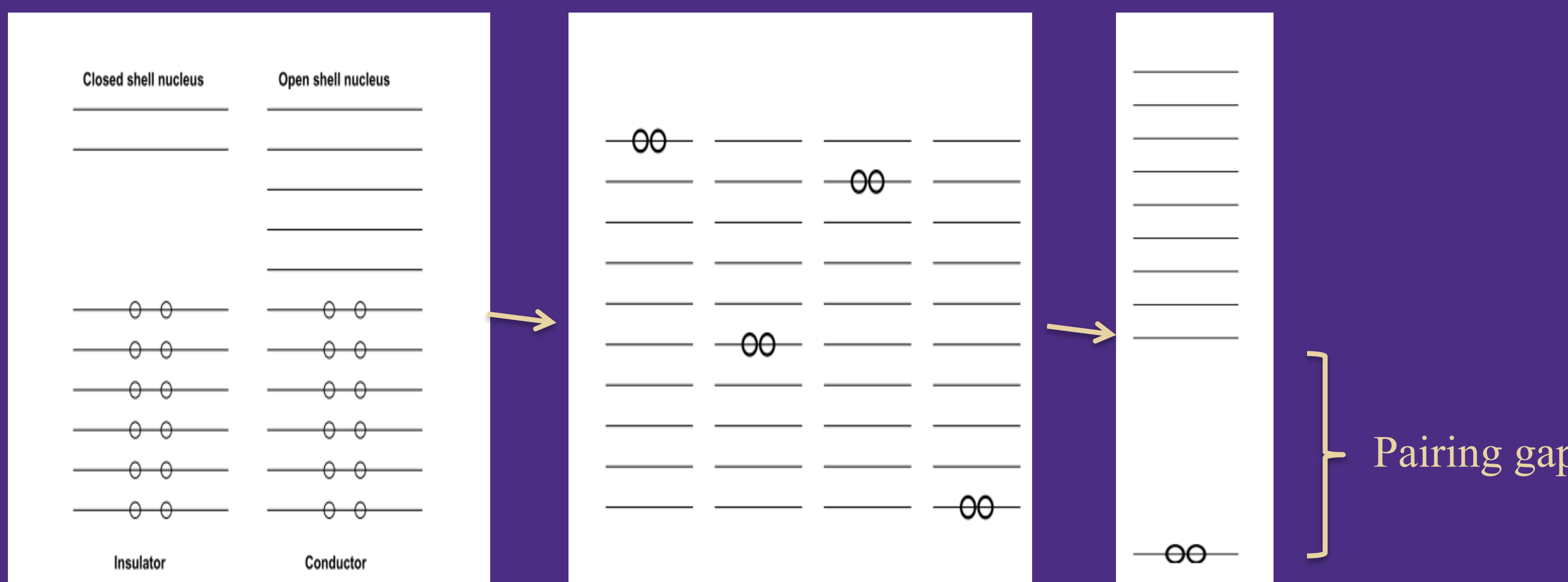
- The evidence from the scattering experiments shows that the mean free path of the nucleon is at least the order of the size of the nucleus.
- In a good approximation, the nucleons in the nucleus can be treated as independent particles.
- In shell model, nucleons occupy quantized orbits and the strong spin-orbit interaction in the nucleus leads the energy levels in a shell structure and the formation of magic numbers.



History and Background

Pairing Correlations

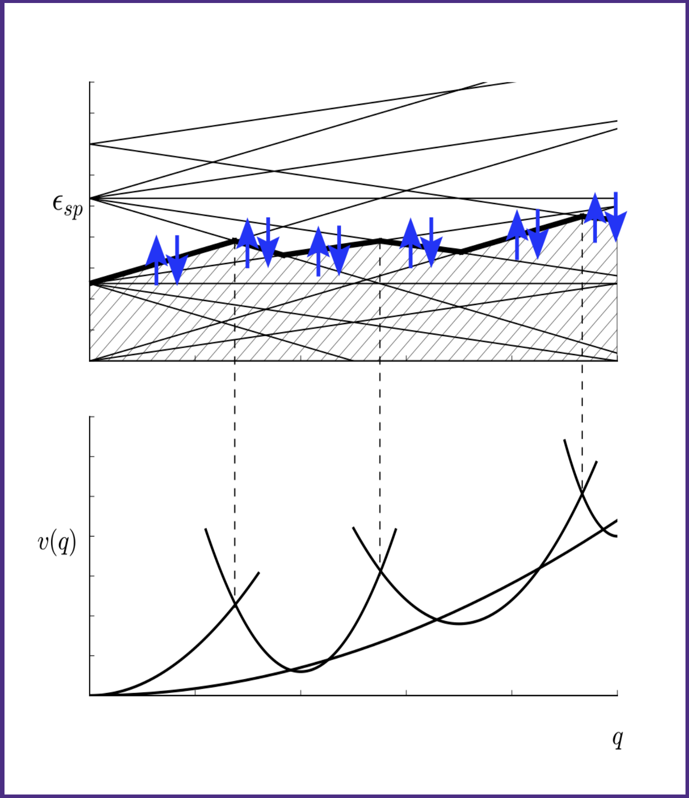
- Analogous to the BCS theory of superconductivity, in open shell nuclei, nucleons near the Fermi surface with opposite momenta and spins form “Cooper pairs” (m, -m).



History and Background

Deformation energy in a picture of individual particles

- While a nucleus elongates, the Fermi surface becomes oblate. Its sphericity can be restored only by redistributing the nucleons on different energy levels.
- Each single-particle doublet is occupied by particles with time reversed quantum numbers (Kramers degeneracy).
- At each crossing two nucleons change their angular momenta $(m_1, -m_1) \Rightarrow (m_2, -m_2)$: "Cooper pair" => "Cooper pair".
- Pairing interactions are the most effective mechanism at performing such transitions.

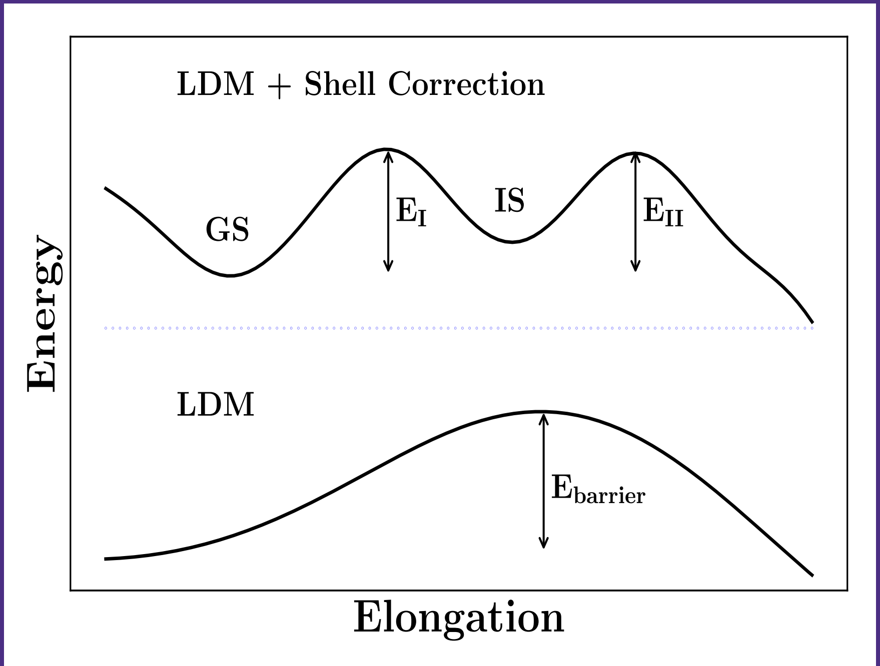


History and Background

Shell correction

- Strutinsky proposed a method to calculate the shell correction energy of the LDM by identifying the fluctuations of the single particle energies.

- The PES has a double-humped shape, with a second minimum named the fission isomer (IS).



History and Background

Several recent developments have radically changed our prospects of attaining a microscopic description of nuclear fission.

- **THEORY:**
  - The extension of the Local Density Approximation (LDA) formulation of DFT due to Kohn and Sham, to superfluid time-dependent phenomena, the Time-dependent Superfluid Local Density Approximation (TDSLDA).
  - Validation and verification of (TD)SLDA against a large set of theoretical and experimental data for systems of strongly interacting fermions.
- **HIGH PERFOMANCE COMPUTING:**
  - Emergence of very powerful computational resources
  - Non-trivial numerical implementation of TDSLDA
  - Advanced capabilities of leadership class computers, in particular tens of thousands of GPUs.

Theoretical Tool

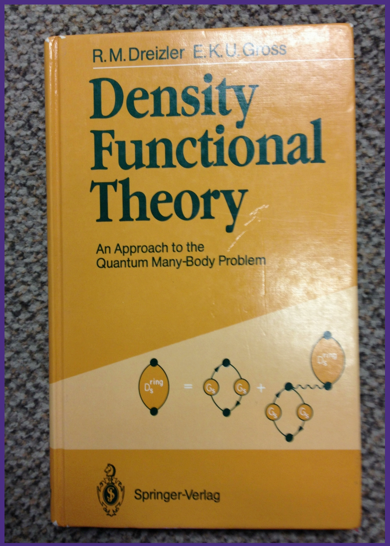
Microscopically a nucleus is described by the (static) many-body Schrödinger equation:

$$H\Psi(1,\cdots,A) = E\Psi(1,\cdots,A),$$

$$H = \overbrace{\sum_{i}^{A} -\frac{\hbar^2}{2m}\Delta_i}^{\hat{T}} + \overbrace{\sum_{i<j}^{A} \hat{V}_{ij} + \sum_{i<j<k}^{A} \hat{V}_{ijk}}^{\hat{W}} + \overbrace{\sum_{i}^{A} \hat{V}_{\mathrm{ext},i}}^{\hat{V}_{\mathrm{ext}}}$$

- $(i) = (\mathbf{r}_i, s_i, t_i)$: spatial coordinates (x, y, z), spin (up and down), isospin (neutron and proton).
- A heavy nucleus, e.g. ^{240}Pu: $\Psi(1,\cdots,A)$ has N^{240} spatial components and $2^{240} \approx 1.77 \times 10^{72}$ spin components. $N = N_x N_y N_z$ is the number of lattice points in 3D space.
- A direct solution of the many-body SE is not possible within current computing resources, if ever.

Theoretical Tool



Density Functional Theory (DFT)

- The wavefunction has a one-to-one correspondence to the one-body local density (Hohenberg and Kohn, 1964)

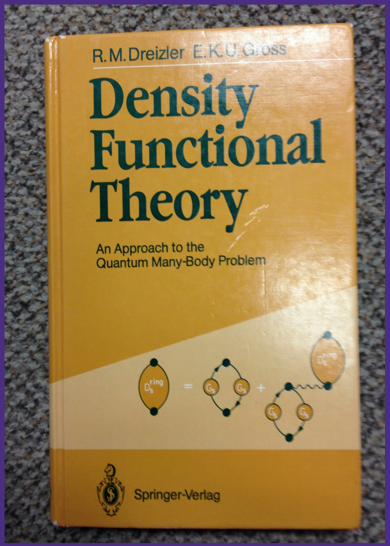
$$\Psi(1, ..., A) \Leftrightarrow \Psi[n] \Leftrightarrow V_{\rm ext}(\boldsymbol{r}) \Leftrightarrow n(\mathbf{r})$$

$$n(\boldsymbol{r}) = \langle \Psi | \sum_s \hat{\psi}_s^\dagger(\boldsymbol{r})\hat{\psi}_s(\boldsymbol{r}) | \Psi \rangle$$

$$E_0 = \langle \Psi[n] | \hat{H} | \Psi[n] \rangle = \min_{n(\boldsymbol{r})} \int d^3r \left(\mathcal{E}[n(\boldsymbol{r})] + V_{\rm ext}(\boldsymbol{r}) n(\boldsymbol{r}) \right)$$

$$\mathcal{E}[n(\boldsymbol{r})] = \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle$$ is independent of $V_{\rm ext}(\boldsymbol{r})$

Theoretical Tool



Density Functional Theory (DFT)

- For any interacting system, there exists a non-interacting system that has the same ground state density (Kohn and Sham, 1965).

Schrödinger equation

$$H\Psi = E\Psi$$

$$n(\boldsymbol{r}) = \langle\Psi|\sum_s \hat{\psi}_s^\dagger(\boldsymbol{r})\hat{\psi}_s(\boldsymbol{r})|\Psi\rangle$$

Kohn and Sham (KS) equation

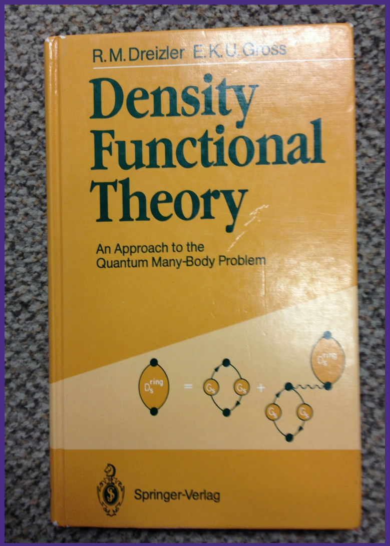
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) + V_{\text{ext}}(\boldsymbol{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$n_{\text{ks}}(\boldsymbol{r}) = \sum_i |\phi_i(\boldsymbol{r})|^2$$

$$n(\boldsymbol{r}) = n_{\text{ks}}(\boldsymbol{r})$$

Theoretical Tool

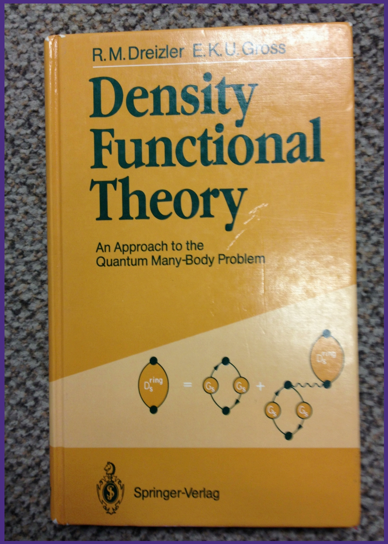
Nuclear DFT



- HK theorem proves there exists a universal energy density functional (EDF) for all many-fermion systems.
- But it does not provide a recipe of constructing the EDF.
- Since a nucleus is a superfluid system with spins, a generic nuclear EDF (NEDF) should contain the following ingredients (for each neutron and proton)
  - number density $n(\vec{r})$
  - anomalous density $\kappa(\vec{r})$
  - spin density $\vec{s}(\vec{r})$
  - kinetic density $\tau(\vec{r})$
  - current density $\vec{j}(\vec{r})$
  - spin current density $\vec{J}(\vec{r})$

$\kappa(\vec{r}) \sim \langle \Psi | \hat{\psi}_\uparrow(\vec{r}) \hat{\psi}_\downarrow(\vec{r}) | \Psi \rangle$ signals the presence of Cooper pairs

Theoretical Tool



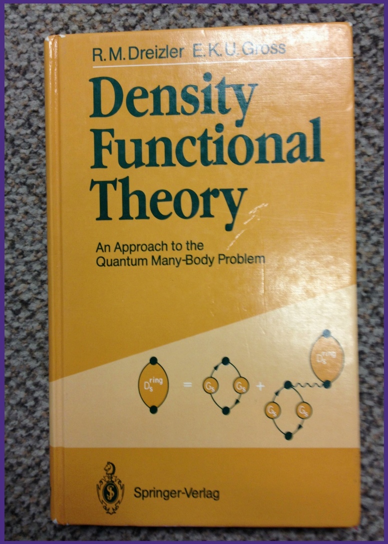
Nuclear DFT

Quasi-particle wavefunctions (qpwfs)

$$\phi_k(\boldsymbol{r}) \Rightarrow [u_{k\uparrow}(\boldsymbol{r}), u_{k\downarrow}(\boldsymbol{r}), v_{k\uparrow}(\boldsymbol{r}), v_{k\downarrow}(\boldsymbol{r})]^T$$

- number density: $n(\vec{r}) = \sum_{k,s} v^*_{k,s}(\vec{r}) v_{k,s}(\vec{r})$
- kinetic density: $\tau(\vec{r}) = \sum_{k,s} \vec{\nabla} v^*_{k,s}(\vec{r}) \cdot \vec{\nabla} v_{k,s}(\vec{r})$
- anomalous density: $\kappa(\vec{r}) = \sum_{k} v^*_{k\uparrow}(\vec{r}) u_{k\downarrow}(\vec{r})$
- current density: $\vec{j}(\vec{r}) = \frac{1}{2i} \sum_{k,s} \left[v_{k,s}(\vec{r}) \vec{\nabla} v^*_{k,s}(\vec{r}) - v^*_{k,s}(\vec{r}) \vec{\nabla} v_{k,s}(\vec{r}) \right]$
- spin density: $\vec{s}(\vec{r}) = \sum_{k,s,s'} \vec{\sigma}_{ss'} v^*_{k,s}(\vec{r}) v_{k,s'}(\vec{r})$
- spin current density: $\vec{J}(\vec{r}) = \frac{1}{2i} (\vec{\nabla} - \vec{\nabla}') \times \vec{s}(\vec{r}, \vec{r}') \Big|_{\vec{r}=\vec{r}'}$

Theoretical Tool



Nuclear DFT

- A generic NEDF is represented as a sum of the kinetic, the interaction, the Coulomb, and the pairing contributions.

$$\mathcal{E} = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{interaction}} + \mathcal{E}_{\text{Coul}} + \mathcal{E}_{\text{pair}}.$$

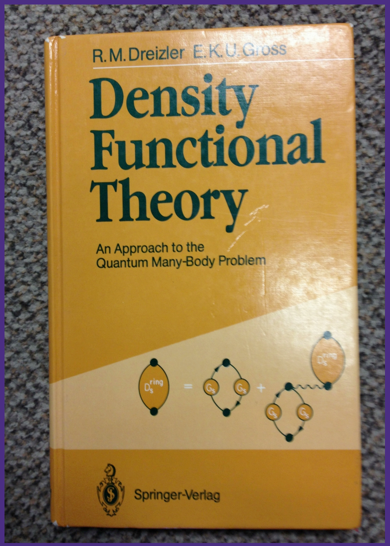
- kinetic energy density

$$\mathcal{E}_{\text{kin}} = \frac{\hbar^2}{2m}(\tau_n + \tau_p), \quad m = \frac{m_n + m_p}{2}$$

- Coulomb energy density

$$\mathcal{E}_{\text{Coul}} = \frac{1}{2}\int d^3r' \frac{e^2 n_p(\boldsymbol{r}) n_p(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} - \frac{3e^2}{4}\left(\frac{n_p(\boldsymbol{r})}{3\pi}\right)^{4/3}$$

Theoretical Tool



Nuclear DFT

- Pairing energy density

$$\mathcal{E}_{\text{pair}}(\vec{r}) = \sum_{q=n,p} g_{\text{eff}}(\vec{r})|\kappa_q(\vec{r})|^2$$

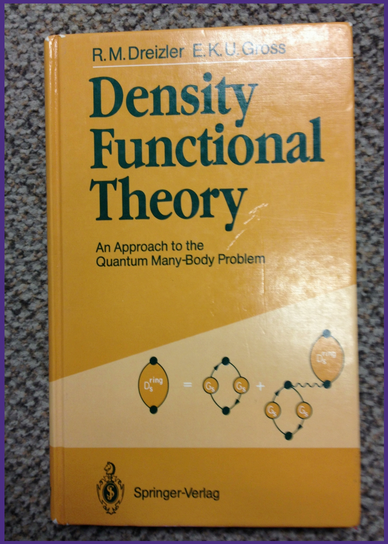
- Superfluid local density approximation (SLDA)

- The effective pairing coupling $g_{\text{eff}}(\vec{r})$ is obtained via a renormalization of the bare pairing strength

$$g_0(\vec{r}) = g_0\left(1 - \alpha\frac{n(\vec{r})}{n_0}\right),$$

- $n_0 = 0.16\ \text{fm}^{-3}$ is the saturation density.
- The parameter $\alpha = 0, 1, 1/2$ corresponds to volume, surface, and mixed pairing respectively.

Theoretical Tool



Nuclear DFT

- Interaction energy density
- Skyrme family NEDFs (SLy4, SkM*, SkP etc.)

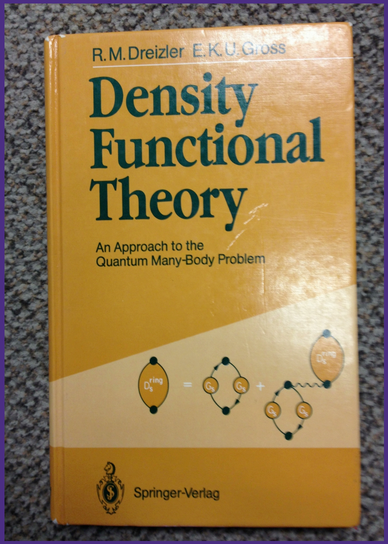
$$\begin{aligned}\mathcal{E}_{\text{Skyrme}} &= \mathcal{E}_{n^2} + \mathcal{E}_{n^\gamma} + \mathcal{E}_{n\Delta n} + \mathcal{E}_{n\tau} + \mathcal{E}_{n\nabla J} \\ &= \sum_{t=0,1} C_t^n n_t^2 + C_t^\gamma n_t^2 n_0^\gamma + C_t^{n\Delta n} n_t \Delta n_t \\ &+ C_t^\tau (n_t \tau_t - \vec{j}_t \cdot \vec{j}_t) + C_t^{\nabla J} \left(n_t \vec{\nabla} \cdot \vec{J}_t + \vec{s}_t \cdot (\vec{\nabla} \times \vec{j}_t) \right)\end{aligned}$$

- SeaLL1 NEDF (Bulgac, Forbes, **Shi,** *et al.*, Phys. Rev. C 97, 044313 (2018))

$$\begin{aligned}\mathcal{E}_{\text{SeaLL1}} &= \mathcal{E}_{\text{vol}} + \mathcal{E}_{n\Delta n} + \mathcal{E}_{n\nabla J} \\ &= \sum_{j=0}^{2} (a_j n_0^{5/3} + b_j n_0^2 + c_j n_0^{7/3}) \left(\frac{n_1}{n_0} \right)^j \\ &+ \sum_{t=0,1} C_t^{n\Delta n} n_t \Delta n_t + C_t^{\nabla J} \left(n_t \vec{\nabla} \cdot \vec{J}_t + \vec{s}_t \cdot (\vec{\nabla} \times \vec{j}_t) \right)\end{aligned}$$

Theoretical Tool

Nuclear DFT



qpwfs $\phi_k(\boldsymbol{r}) \Rightarrow [u_{k\uparrow}(\boldsymbol{r}), u_{k\downarrow}(\boldsymbol{r}), v_{k\uparrow}(\boldsymbol{r}), v_{k\downarrow}(\boldsymbol{r})]^T$

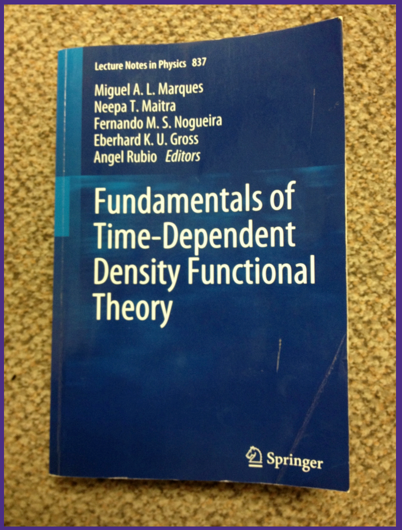
are obtained by solving the Hartree-Fock-Bogoliubov (HFB) equation

$$\begin{pmatrix} h_{\uparrow\uparrow}(\vec{r}) - \mu & h_{\uparrow\downarrow}(\vec{r}) & 0 & \Delta(\vec{r}) \\ h_{\downarrow\uparrow}(\vec{r}) & h_{\downarrow\downarrow}(\vec{r}) - \mu & -\Delta(\vec{r}) & 0 \\ 0 & -\Delta^*(\vec{r}) & -h^*_{\uparrow\uparrow}(\vec{r}) + \mu & -h^*_{\uparrow\downarrow}(\vec{r}) \\ \Delta^*(\vec{r}) & 0 & -h^*_{\downarrow\uparrow}(\vec{r}) & -h^*_{\downarrow\downarrow}(\vec{r}) + \mu \end{pmatrix} \begin{pmatrix} u_{k\uparrow}(\vec{r}) \\ u_{k\downarrow}(\vec{r}) \\ v_{k\uparrow}(\vec{r}) \\ v_{k\downarrow}(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} u_{k\uparrow}(\vec{r}) \\ u_{k\downarrow}(\vec{r}) \\ v_{k\uparrow}(\vec{r}) \\ v_{k\downarrow}(\vec{r}) \end{pmatrix}$$

$$h(\vec{r}) = \frac{\delta E}{\delta n(\vec{r})}, \quad \Delta(\vec{r}) = -\frac{\delta E}{\delta \nu^*(\vec{r})}$$

$$E = \int d^3r \mathcal{E}[n(\vec{r}), \tau(\vec{r}), \vec{J}(\vec{r}), \vec{s}(\vec{r}), \kappa(\vec{r}), \vec{j}(\vec{r})]$$

Theoretical Tool



Time-dependent Density Functional Theory (TDDFT)

- The conceptual and computational foundations are analogous to DFT's.

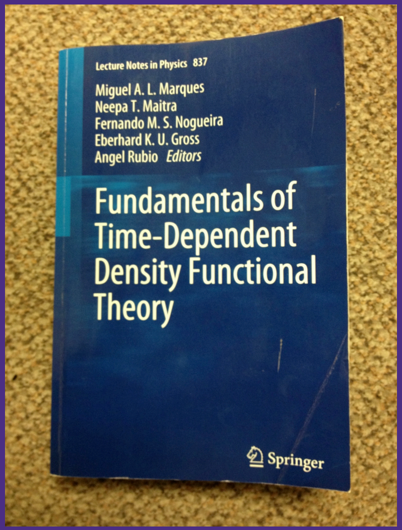
- TD Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(1,\cdots,A,t) = \left\{\sum_{i=1}^{A} -\frac{\hbar^2}{2m}\Delta_i + V(1,\cdots,A,t)\right\}\Psi(1,\cdots,A,t)$$

- The (TD) wavefunction still has a one-to-one correspondence to the one-body local density (Runge and Gross, 1984):

$$\Psi(1,...,A,t) \Leftrightarrow \Psi[n] \Leftrightarrow n(\mathbf{r},t) = \sum_k |\phi_k(\mathbf{r},t)|^2$$

Theoretical Tool



Time-dependent Density Functional Theory (TDDFT)

- Time-dependent KS equation

$$i\hbar\frac{\partial}{\partial t}\phi_i(\vec{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ks}}(\vec{r},t)\right]\phi_i(\vec{r})$$

- Time-dependent SLDA (TDSLDA) equation

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\vec{r},t) \\ u_{k\downarrow}(\vec{r},t) \\ v_{k\uparrow}(\vec{r},t) \\ v_{k\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow}(\vec{r},t)-\mu & h_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ h_{\downarrow\uparrow}(\vec{r},t) & h_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -h^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -h^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -h^*_{\downarrow\uparrow}(\vec{r},t) & -h^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{k\uparrow}(\vec{r},t) \\ u_{k\downarrow}(\vec{r},t) \\ v_{k\uparrow}(\vec{r},t) \\ v_{k\downarrow}(\vec{r},t) \end{pmatrix}$$

Computational Implementation

Highly-efficient GPU code

Simulation box: $30 \times 30 \times 60\ \mathrm{fm}^3, \quad dx = 1.25\ \mathrm{fm}$

Time step: $\Delta t \approx 0.03\ \mathrm{fm/c}$

Number of PDEs: $\approx 5 \times 10^5$

number of GPUs: 720 (on Summit, NVIDIA V100)

Wall time (on Summit) : 1.4 h / (1000 fm/c)

Benchmarked on leadership-class supercomputers

Titan

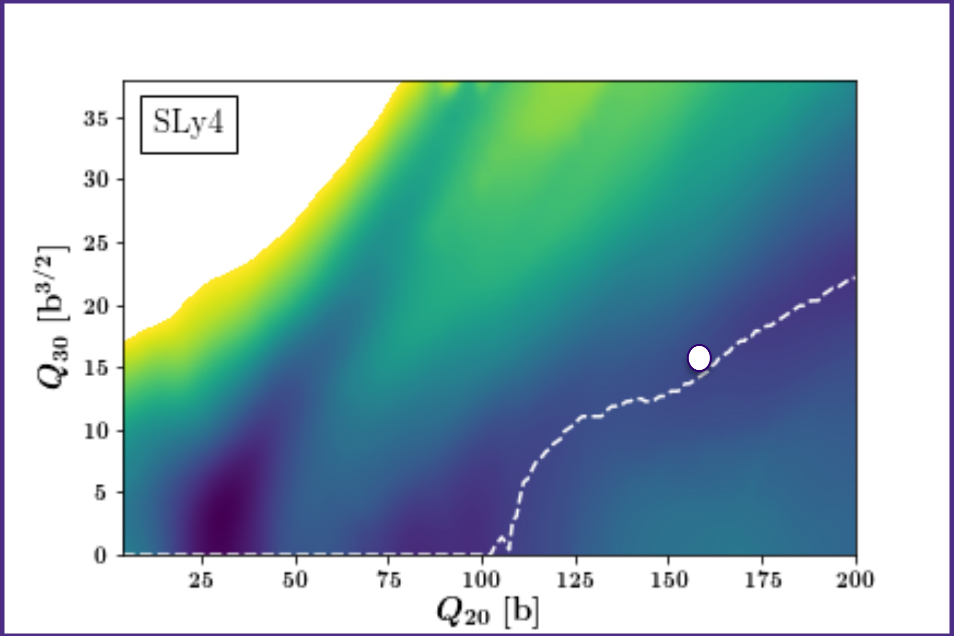
Piz-Daint (Switzerland)

Summit

Fission Dynamics

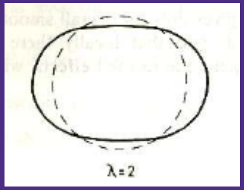
Benchmark Work

A. Bulgac, P. Magierski, K.J. Roche, I. Stetcu, *Induced Fission of ^{240}Pu within a Real-Time Microscopic Framework*, Phys. Rev. Lett. 116, 122504 (2016)

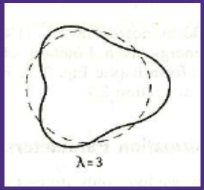


- EDF: SLy4
- Pairing coupling: -233 MeV
- Simulation box: $22.5 \times 22.5 \times 45 \text{ fm}^3, \quad dx = 1.25 \text{ fm}$
- Time step: $\Delta t \approx 0.119 \text{ fm/c}$

Q_{20}



Q_{30}



Fission Dynamics

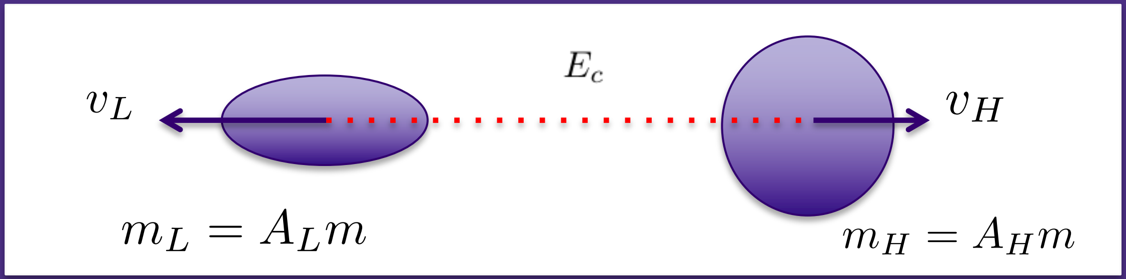
- The properties of fission fragments agree well with experimental observations.

t_{sc}	TKE ^{syst}	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L
12259	177.26	173.42	100.55	101.7	60.69	61.3	39.81	40.4

t_{sc} : (fm/c), TKE: (MeV)

Total kinetic energy (TKE):

$$\text{TKE} = \frac{1}{2} m_L v_L^2 + \frac{1}{2} m_H v_H^2 + E_c$$



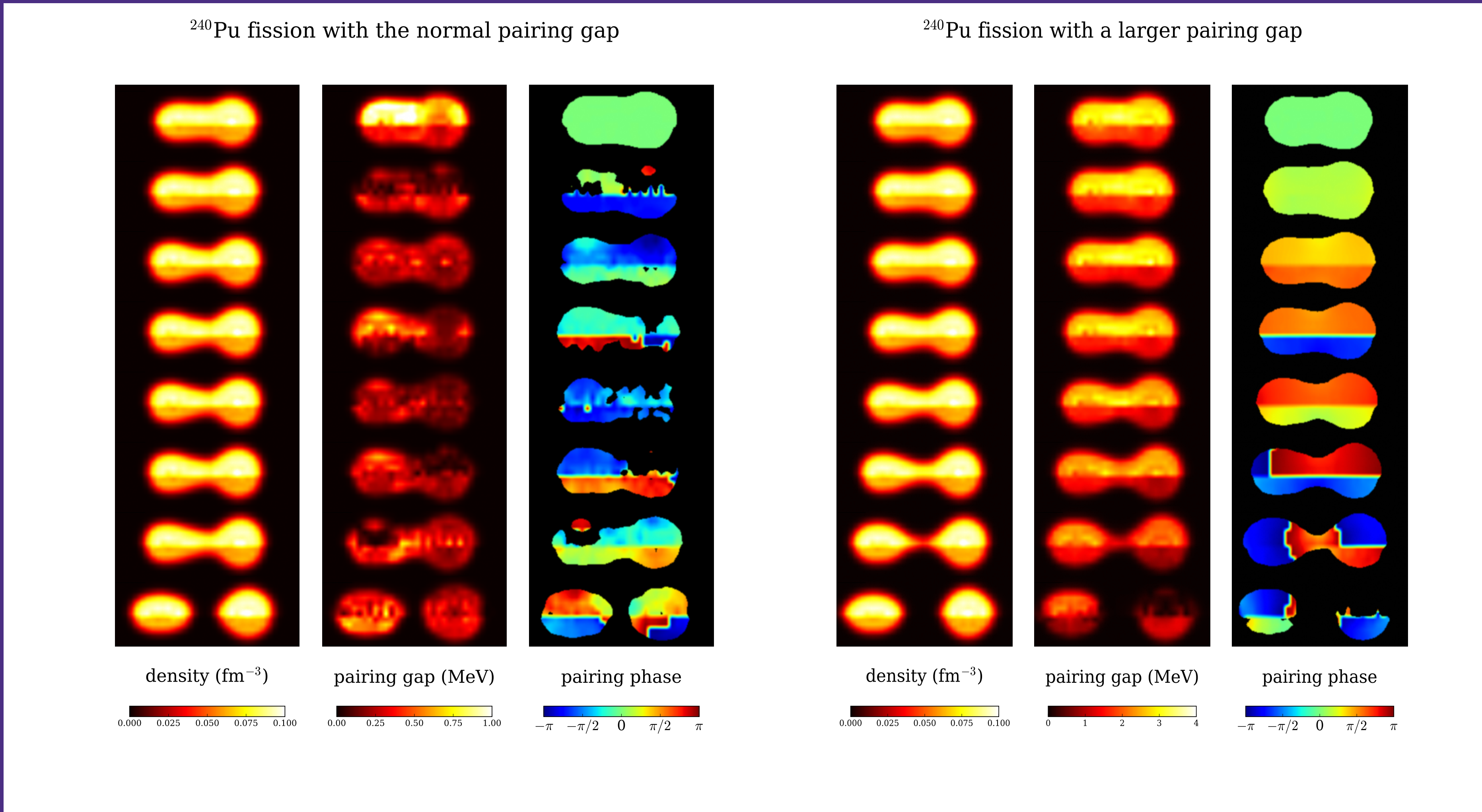
Fission Dynamics

Questions to be answered

- How do various input parameters influence the dynamics and the fission fragments (FFs) properties?
  - Pairing correlations
  - NEDF
  - Initial configurations

- How is the excitation energy shared between FFs?

- How many neutrons (if any) are emitted?



Normal pairing strength, saddle to scission 14,000 fm/c

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

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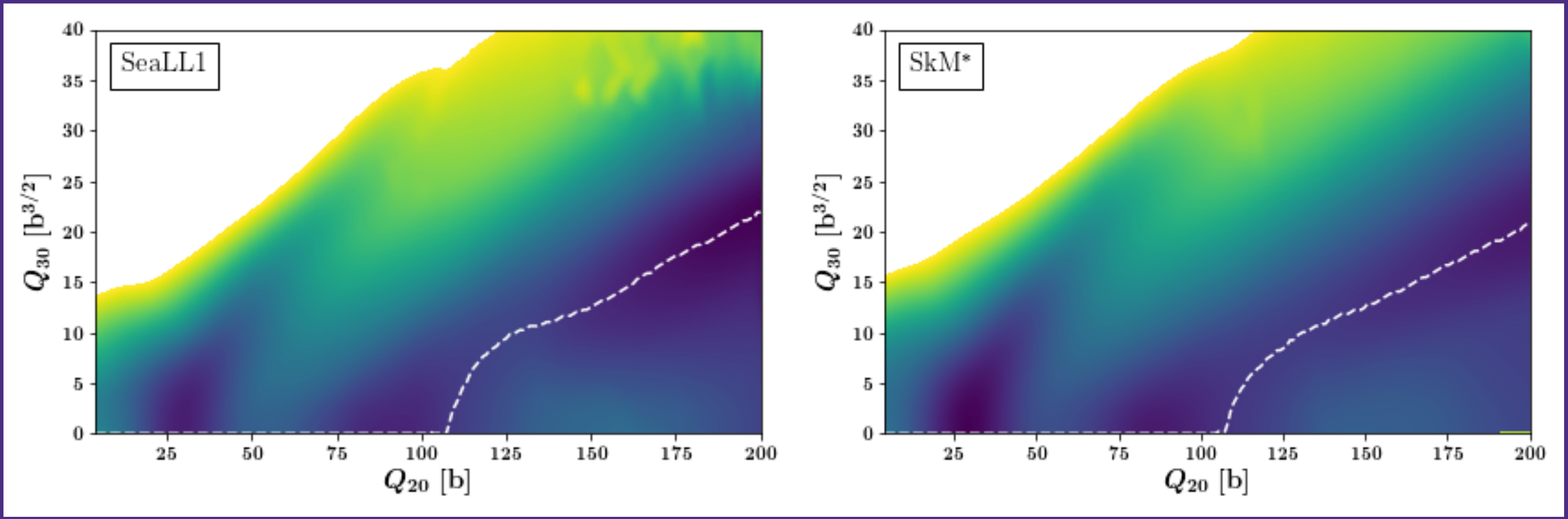
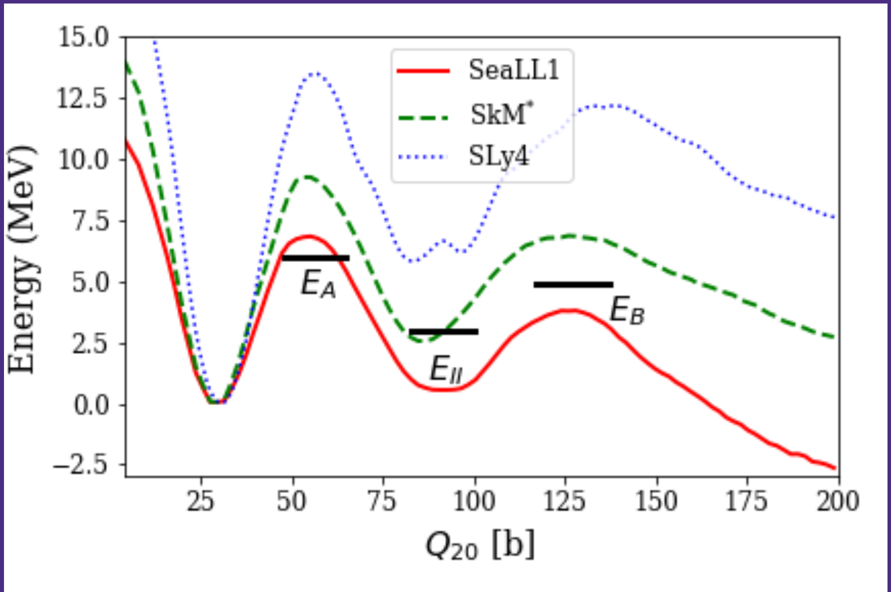
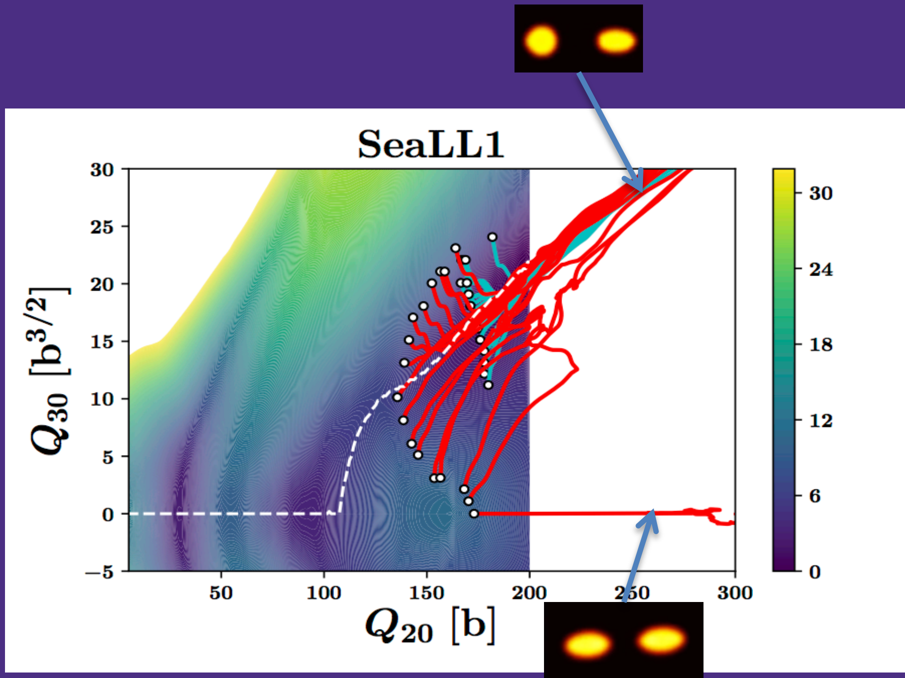
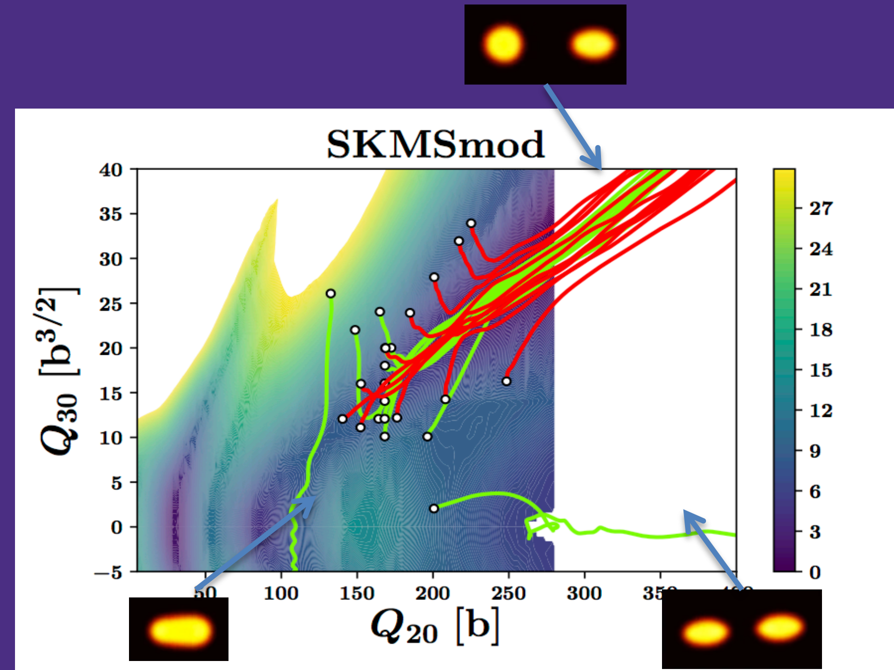


SeaLL1
SkM*
Q_{30} [$b^{3/2}$]
Q_{20} [b]



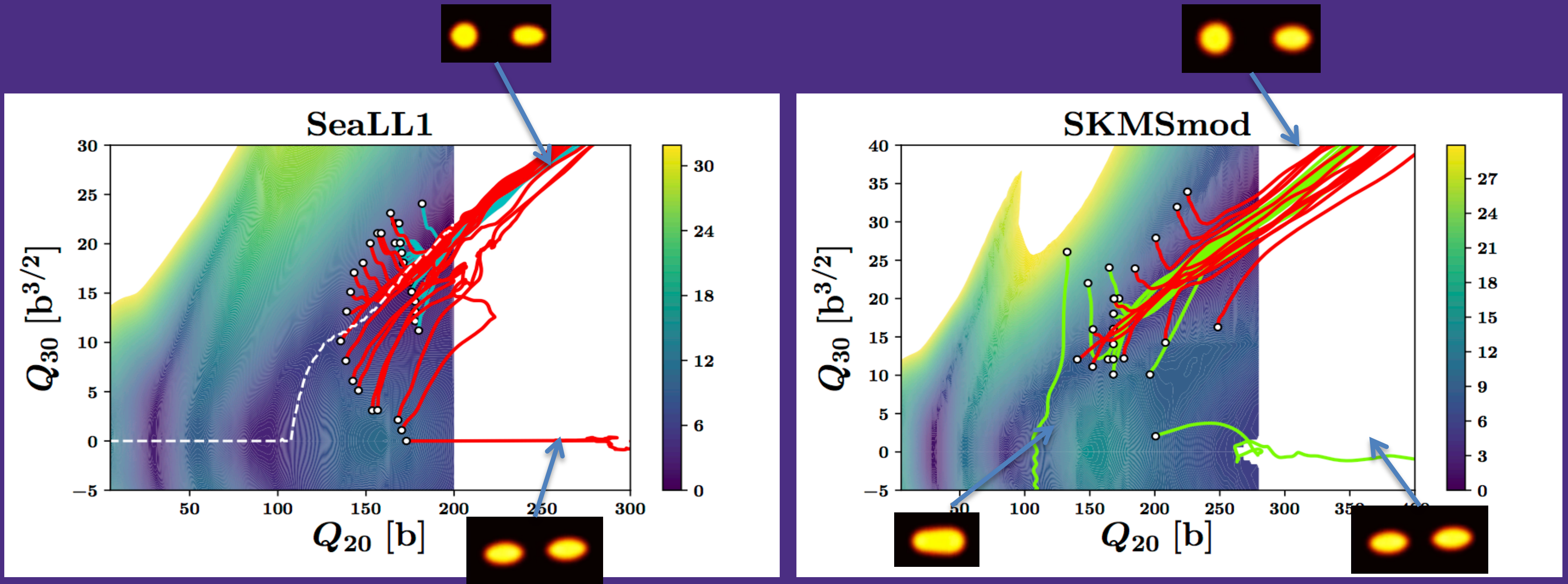
SeaLL1
SkM*
SLy4
Energy (MeV)
Q_{20} [b]
E_A
E_{II}
E_B





NEDF	$E^*_{\rm ini}$	TKE	$N_{\rm H}$	$Z_{\rm H}$	$N_{\rm L}$	$Z_{\rm L}$	$E^*_{\rm H}$	$E^*_{\rm L}$	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*-1asy	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*-1sy	9.6	149.0	73.4	47.2	72.6	46.7	29.4	28.5	57.9	206.9	3673
SkM*-2asy	8.1(0.2)	182.8(4.4)	82.6(1.0)	52.4(0.6)	63.6(1.0)	41.7(0.5)	14.3(3.9)	13.0(3.0)	27.3(3.4)	210.1(1.8)	1349(309)

$$N_{\rm L}{}^{\rm syst} \approx 61, N_{\rm H}{}^{\rm syst} \approx 85, Z_{\rm L}{}^{\rm syst} \approx 40, N_{\rm L}{}^{\rm syst} \approx 54, {\rm TKE}^{\rm syst} \approx 177 \cdots 178\ {\rm MeV}$$



NEDF	T_L [MeV]	T_H [MeV]	Q_{20}^L [b]	Q_{20}^H [b]	Q_{30}^L [$b^{3/2}$]	Q_{30}^H [$b^{3/2}$]	$(c/a)_H$	$(c/a)_L$	$\tau_{s\to s}$ [fm/c]
SeaLL1-1	1.40(0.07)	1.11(0.08)	15.7(0.9)	2.6(0.5)	0.08(0.17)	−0.20(0.06)	1.06(0.01)	1.59(0.03)	2392(800)
SeaLL1-2	1.15(0.08)	1.19(0.12)	17.1(1.1)	2.6(0.6)	0.23(0.08)	−0.19(0.06)	1.06(0.01)	1.63(0.03)	1460(176)
SeaLL1-sy	1.54	1.99	27.4	27.0	0.9	-1.1	1.87	1.73	10103
SkM*-1asy	1.20(0.09)	1.10(0.10)	11.3(1.3)	3.5(0.9)	0.1(0.1)	−0.4(0.1)	1.08(0.02)	1.42(0.04)	1214(448)
SkM*-1sy	1.56	1.55	24.2	25.6	0.9	-1.0	1.72	1.75	3673
SkM*-2asy	1.11(0.14)	1.02(0.14)	14.5(1.7)	2.3(0.7)	0.09(0.08)	−0.3(0.1)	1.05(0.02)	1.53(0.06)	1349(309)

$$E_f^* = \frac{A_f}{a} T_f^2, \quad a \approx 10$$

Adiabaticity of Fission Dynamics

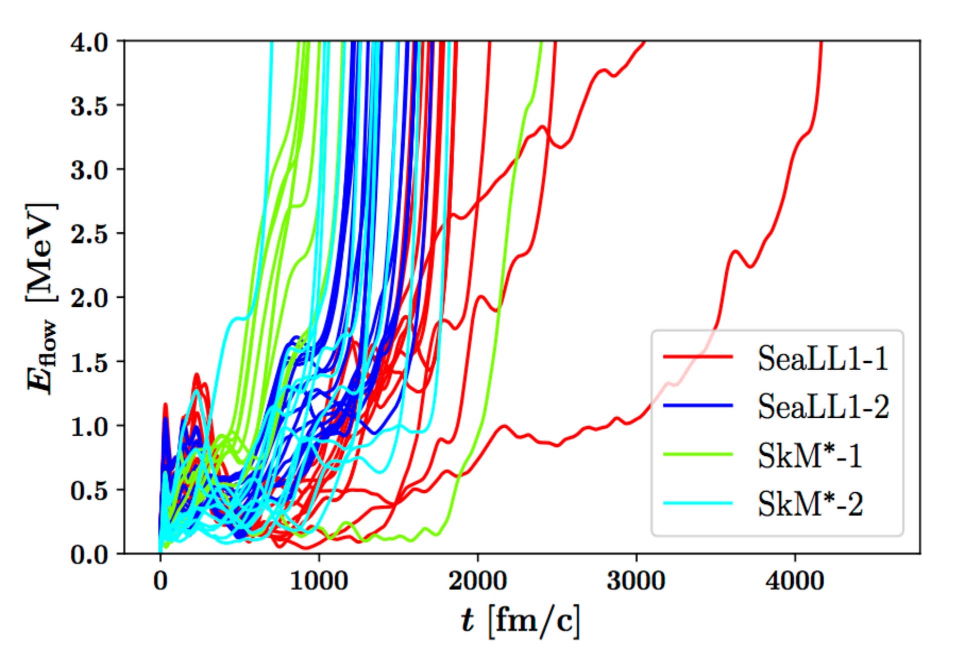
Is fission dynamics adiabatic?

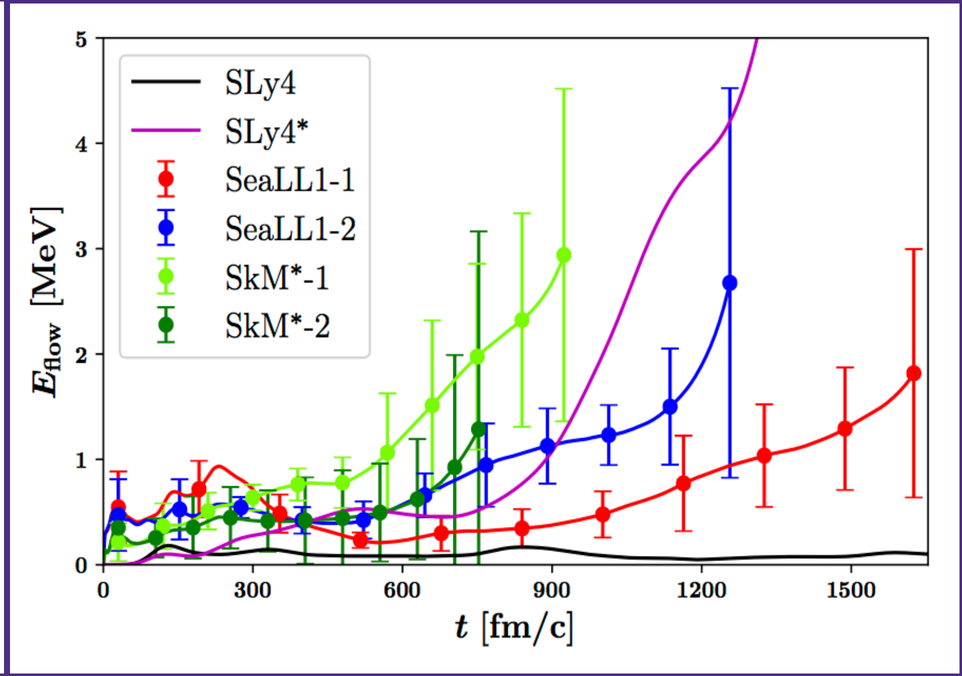
If it is adiabatic, then ....

- No intrinsic entropy is produced.
- The potential energy difference will be entirely transferred to the collective flow energy

$$E_{\text{flow}}(t) = \sum_{q=n,p} \int d^3r \, \frac{\hbar^2}{2m} \frac{\vec{j}_q^{\,2}(\vec{r},t)}{n_q(\vec{r},t)}$$

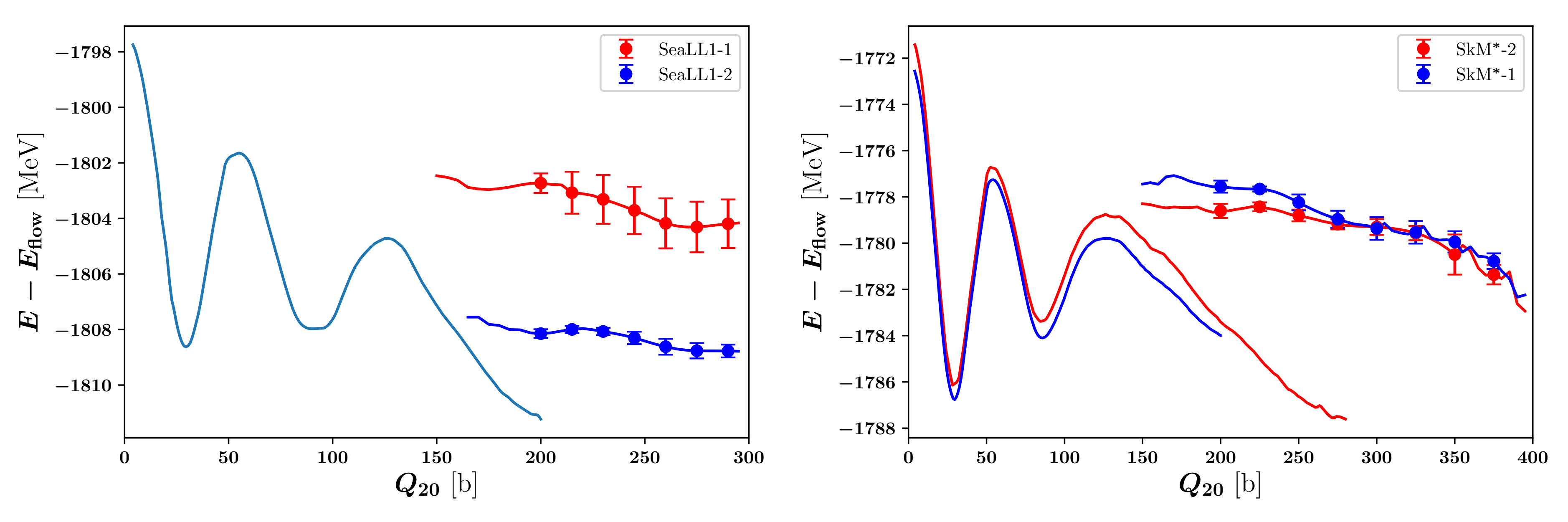
- For ^{240}Pu the potential energy difference is 15 ... 20 MeV.





However …….

- **The collective flow energy remains a very small value ~ 1 … 2 MeV before scission!**
- **Fission dynamics is quasi-static and over-damped, but not adiabatic !**



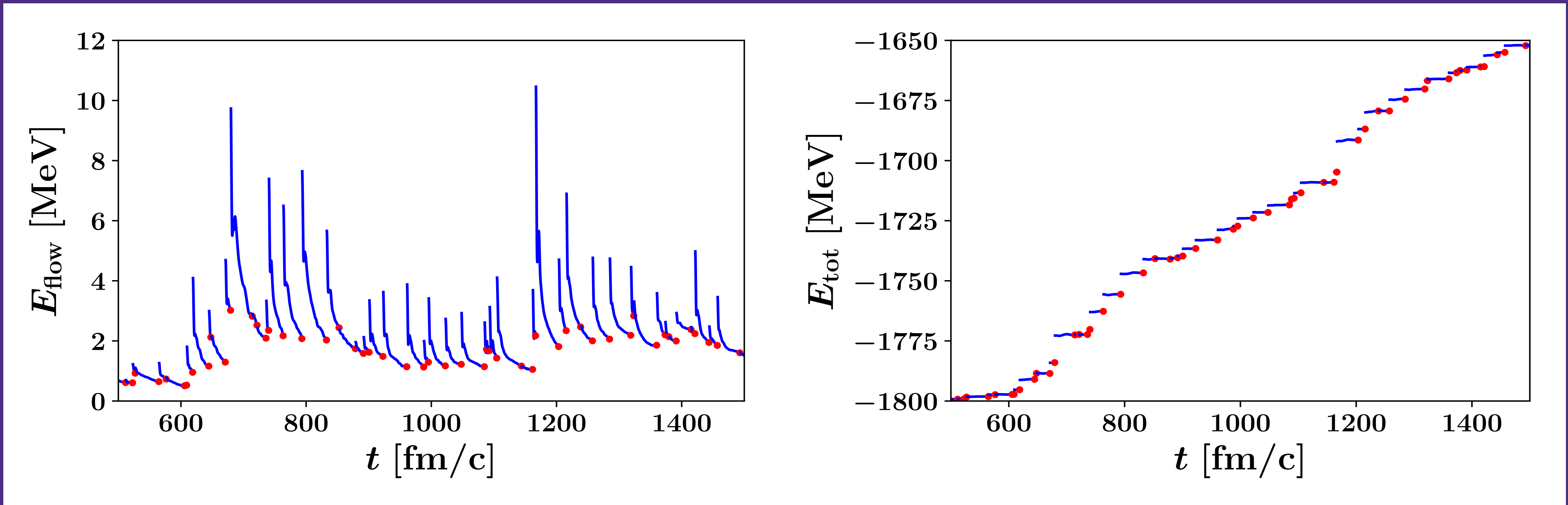
- The internal energy

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

remains almost constant as potential energy drops!

- The driving force of the collective dynamics is determined by the free energy gradient

$$\boldsymbol{F_Q} = -\boldsymbol{\nabla_Q}[E_{\text{int}}(\boldsymbol{Q},T) - TS(\boldsymbol{Q},T)]$$



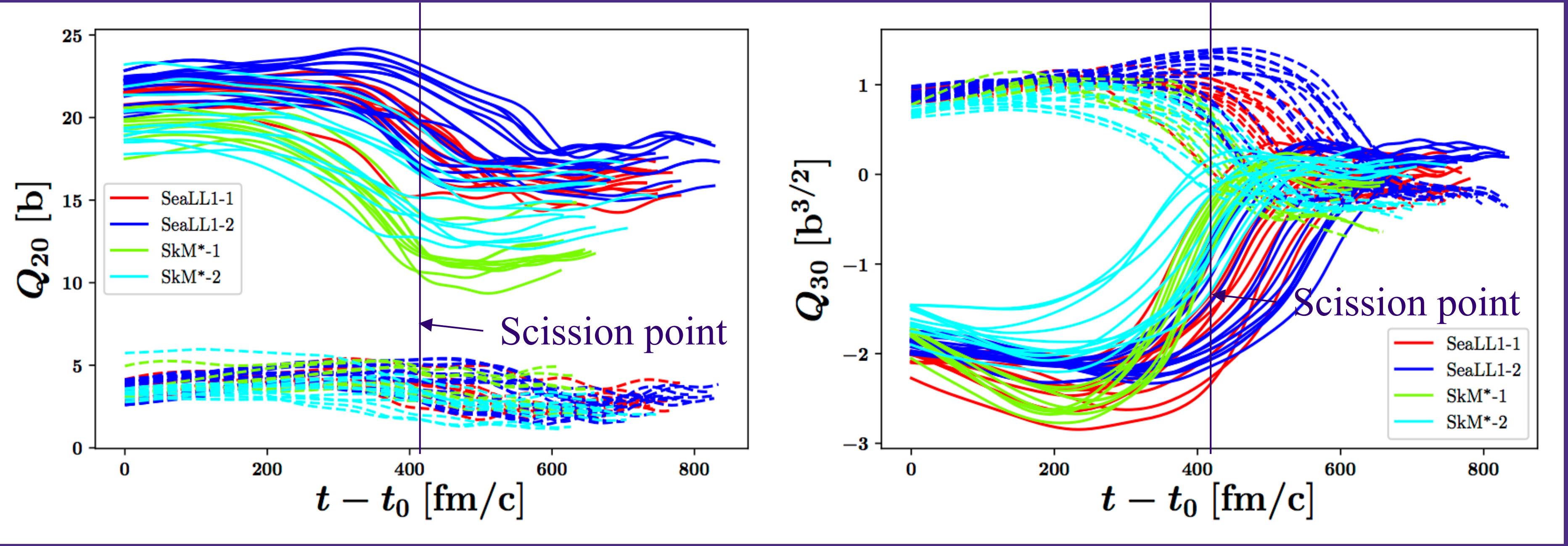
Another theoretical experiment

- We applied at random times collective kicks to the nucleus of random intensities η

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

- At each kick, collective flow energy is rapidly absorbed into internal energy.

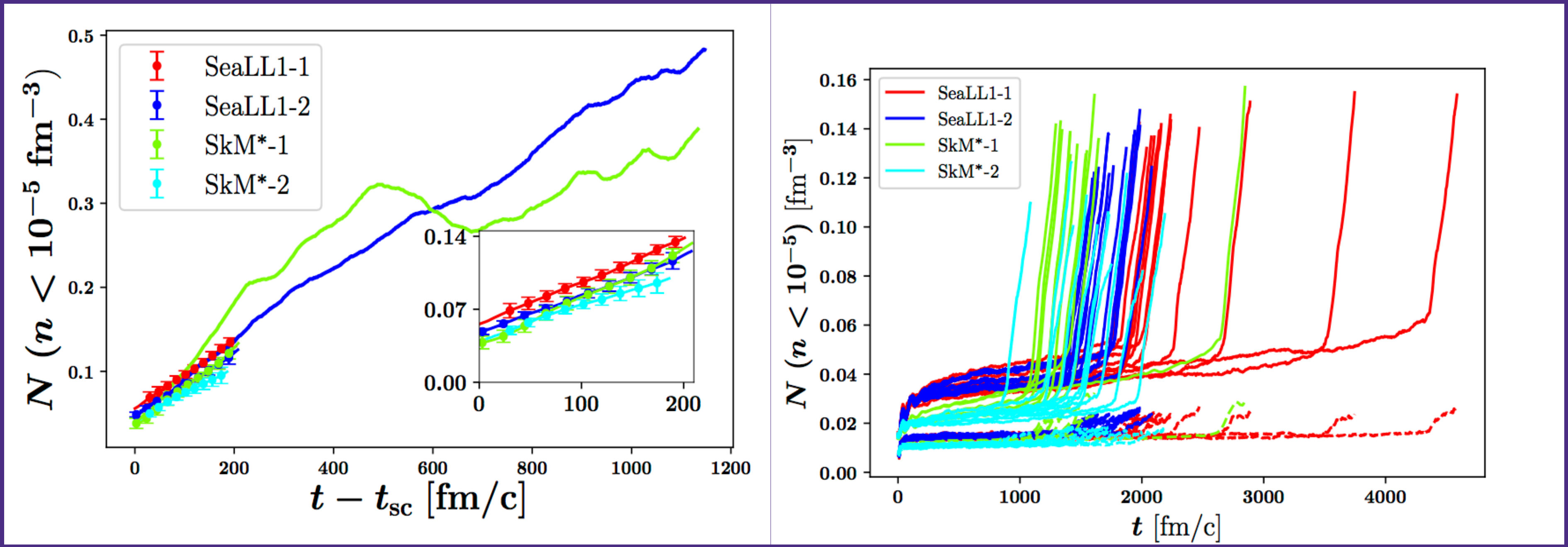
- The absorption rate doesn't change as the intrinsic energy increases by ~ 150 MeV.



Shape relaxation of fission fragments

- At scission, the multiple moments of both fragments are very different from the corresponding ones in the ground state.

- After scission, all these moments relaxed rapidly to the values very close to the ground state values, without performing any oscillations.



Neutrons emitted by fission fragments

- Stable rate 4×10^{-4} neutrons/(fm/c), regardless of the initial conditions or EDF.
- By the time the FFs reach a separation of ~ 60 fm, about 0.4 neutrons are emitted on average.

Discussion

The main results we presented so far show that:

- The difference in initial conditions is largely washed out during the evolution of TDDFT due to the strong one-body dissipation.
- It leads to very small distribution widths of various observables.
- One of the limitations of DFT: it lacks the two-body correlation in the formalism.

Discussion

Path integral method

$$\Psi(t) = \int \mathcal{D}[\sigma(t)] W[\sigma(t)] \exp\left(-\frac{i}{\hbar} \int_{t_i}^{t_f} \hat{h}[\sigma(t)] \right) \Psi(0).$$

- $\sigma(t)$: one-body auxiliary fields
- $\mathcal{D}[\sigma(t)]$: an appropriate measure
- $W[\sigma(t)]$: a Gaussian weight function
- $\hat{h}[\sigma(t)]$: a one-body hamiltonian built with $\sigma(t)$.

- One can evolve a linear superposition of many (time-dependent) many-body wavefunctions.
- Similar to time-dependent generator coordinate method (TDGCM)

Discussion

Mean-field trajectory

- Writing $\sigma(t) = \bar{\sigma}(t) + \eta(t)$

Fluctuations

$$\Psi(t) = \int \mathcal{D}[\eta(t)]\tilde{W}[\eta(t)] \exp\left(-\frac{i}{\hbar}\hat{h}[\bar{\sigma}(t) + \eta(t)]\right)\Psi(0)$$

- One can treat fluctuations around the mean field trajectory with the classical Langevin description of the nuclear collective motion.

Fluctuations and Dissipation

Brownian Motion

- Langevin equation

$$m\ddot{x}(t) = F(x(t)) - \overbrace{m\gamma\dot{x}(t)}^{\text{friction term}} + \underbrace{m\xi(t)}_{\text{stochastic term}} .$$

- $\xi(t)$ is a Gaussian white noise

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \Gamma\delta(t - t')$$

- Einstein dissipation fluctuation theorem

$$m\Gamma = 2\gamma T$$

where T is the temperature.

Fluctuations and Dissipation

In fission dynamics ....

- Langevin equation in phase space

$$\frac{dp_i}{dt} = -\frac{p_j p_k}{2}\frac{\partial}{\partial x_i}(\mathcal{M}^{-1})_{jk} - \frac{\partial V}{\partial x_i} - \eta_{ij}(\mathcal{M}^{-1})_{jk}p_k + g_{ij}\Gamma_j(t)$$
$$\frac{dx_i}{dt} = (\mathcal{M}^{-1})_{ij}p_j$$

- x_i: collective coordinate
- p_i: momentum conjugate to x_i
- V: The potential energy, obtained from the macroscopic-microscopic method or self-consistent mean-field method.
- $\mathcal{M}_{ij}$: The inertia tensor, derived from phenomenological models or the generator coordinate method (GCM).

Fluctuations and Dissipation

In fission dynamics ....

- Langevin equation in phase space

$$\frac{dp_i}{dt} = -\frac{p_j p_k}{2}\frac{\partial}{\partial x_i}(\mathcal{M}^{-1})_{jk} - \frac{\partial V}{\partial x_i} - \eta_{ij}(\mathcal{M}^{-1})_{jk}p_k + g_{ij}\Gamma_j(t)$$
$$\frac{dx_i}{dt} = (\mathcal{M}^{-1})_{ij}p_j$$

- η_{ij}: the dissipation tensor
- $g_{ij}\Gamma_j(t)$: the random (Langevin) force;
  - $\Gamma(t)$: a time-dependent stochastic variable with a Gaussian distribution
  - g_{ij}: the random-force strength tensor.

Fluctuations and Dissipation

How to implement fluctuations/dissipations in TDDFT?

- We need an additional term

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

- Introducing stochastic vector field in the kinetic term

$$\frac{(\hat{\vec{p}} - m\vec{u})^2}{2m} = \frac{\hat{\vec{p}}^2}{2m} - \frac{1}{2}(\vec{u}\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\vec{u}) + \frac{m\vec{u}^2}{2}.$$

- Resulting TDDFT equations

$$i\hbar\dot{\psi}_k(\vec{r},t) = h[n]\psi_k(\vec{r},t) - \frac{1}{2}(\vec{u}\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\vec{u})\psi_k(\vec{r},t) + \frac{m\vec{u}^2}{2}\psi_k(\vec{r},t)$$

Fluctuations and Dissipation

Another way ....

- Gauge transformation

$$\psi_k(\vec{r},t) = \phi_k(\vec{r},t)\exp[i\chi(\vec{r},t)].$$

Then $\phi_k(\vec{r},t) = \psi_k(\vec{r},t)\exp[-i\chi(\vec{r},t)]$ satisfies the equation

$$i\hbar\dot{\phi}_k(\vec{r},t) = \frac{[\vec{p} - \hbar\vec{\nabla}\chi(\vec{r},t)]^2}{2m}\phi_k(\vec{r},t) + [U(\vec{r},t) + \hbar\dot{\chi}(\vec{r},t)]\phi_k(\vec{r},t)$$

- Assuming the vector field is irrotational $\vec{\nabla}\times\vec{u}(\vec{r},t) = 0$, then if

$$m\vec{u}(\vec{r},t) = \hbar\vec{\nabla}\chi(\vec{r},t)$$

- One eliminates the vector field terms and gets

$$i\hbar\dot{\phi}_k(\vec{r},t) = h[n]\phi_k(\vec{r},t) + \hbar\dot{\chi}(\vec{r},t)\phi_k(\vec{r},t).$$

Fluctuations and Dissipation

In general ....

- One could include both vector and scalar channels of fluctuations

$$i\hbar\dot{\psi}_k(\vec{r},t) = h[n]\psi_k(\vec{r},t) - \frac{1}{2}\left[\vec{u}(\vec{r},t)\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\vec{u}(\vec{r},t)\right]\psi_k(\vec{r},t) + u_0(\vec{r},t)\psi_k(\vec{r},t)$$

to produce both rotational and irrotational velocity field!

- Then $\vec{u}(\vec{r},t)$ and $u_0(\vec{r},t)$ can be treated as independent components of the 4-vector field

$$u_\nu(\vec{r},t), \quad \nu = 0,1,2,3$$

Fluctuations and Dissipation

Form of $u_\nu(\vec{r}, t)$

Superposition of Gaussian functions in both spatial and temporal dimensions.

$$u_\nu(\vec{r}, t) = \sqrt{\Gamma} \sum_{k=1}^{N_k} F(t - t_k, \tau_k) \eta_k(\vec{r}),$$

$$F(t - t_k, \tau_k) = \frac{1}{(\pi \tau_k^2)^{1/4}} \exp\left[-\frac{(t - t_k)^2}{2\tau_k^2} \right]$$

$$\langle t_k - t_{k-1} \rangle \propto \langle \tau_k \rangle,$$

$$\langle \tau_k \rangle = \mathcal{O}\left(\frac{m R_A}{\hbar k_F} \right), \langle \tau_k \tau_l \rangle \propto \delta_{kl}$$

Fluctuations and Dissipation

Form of $u_\nu(\vec{r}, t)$

$$u_\nu(\vec{r}, t) = \sqrt{\Gamma} \sum_{k=1}^{N_k} F(t - t_k, \tau_k)\eta_k(\vec{r}),$$

$$\eta_k(\vec{r}) = \sqrt{\frac{1}{N_{kb}} \sum_{l=1}^{N_{kb}} \frac{s_{kl}}{(\pi a_{kl}^2)^{3/4}} \exp\left[-\frac{(\vec{r} - \vec{r}_{kl})^2}{2a_{kl}^2}\right]},$$

$$\langle N_{kb} \rangle = \mathcal{O}(A), \langle N_{kb} N_{lc} \rangle \propto \delta_{kl}\delta_{bc}$$

$$\langle s_{kl} \rangle = 0, \quad \langle s_{kl} s_{mn} \rangle = \delta_{km}\delta_{ln},$$

$$\langle |\vec{r}_{kl}| \rangle = \mathcal{O}(R_A), \langle \vec{r}_{kl} \vec{r}_{mn} \rangle \propto \delta_{km}\delta_{ln},$$

$$\langle a_{kl} \rangle = \mathcal{O}\left(\frac{\pi}{k_F}\right), \langle a_{kl} a_{mn} \rangle \propto \delta_{km}\delta_{ln}$$

Fluctuations and Dissipation

Dissipation

- Quantum friction (Bulgac et al, arXiv:1305.6891)

$$V_{\text{fric}}(\vec{r},t) \propto \gamma \dot{n}(\vec{r},t) = -\gamma \vec{\nabla} \cdot \vec{j}(\vec{r},t)$$

- One can show that in the presence of this ``quantum friction" term alone the system will be cooled $\dot{E}_{\text{tot}} \leq 0$ and the collective velocity $\lim_{t\to\infty} \vec{v}(\vec{r},t) = 0$

- Finally, the TDDFT evolution equations augmented to incorporate dissipation and fluctuations we introduce have the form

$$i\hbar\dot{\psi}_k(\vec{r},t) = h[n]\psi_k(\vec{r},t) + \gamma\dot{n}(\vec{r},t)\psi_k(\vec{r},t)$$
$$-\frac{1}{2}\left[\vec{u}(\vec{r},t)\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\vec{u}(\vec{r},t)\right]\psi_k(\vec{r},t) + u_0(\vec{r},t)\psi_k(\vec{r},t).$$

Fluctuations and Dissipation

Test case: 1D harmonic oscillator

$$i\hbar\frac{\partial}{\partial t}\dot{\psi}(x,t) = -\frac{\hbar^2}{2m}\psi(x,t) + \frac{1}{2}m\omega^2 x^2\psi(x,t)$$
$$+\gamma\dot{n}(x,t)\psi(x,t) + \Gamma(x,t)\psi(x,t)$$

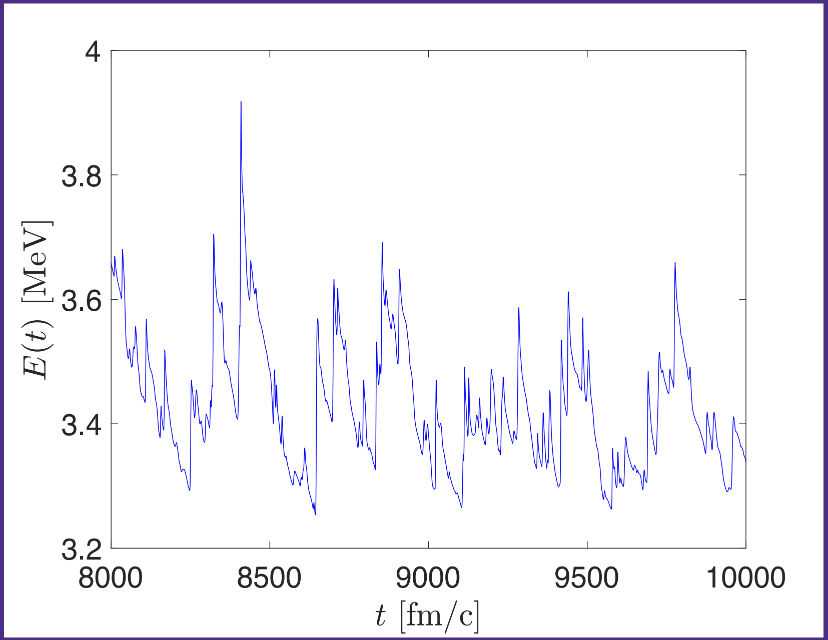
$$\frac{1}{\tau}\int_0^\tau dt E(t) = \frac{1}{Z(\beta)}\sum_{n=0}^{\infty} e^{-\beta\varepsilon_n}\varepsilon_n,$$

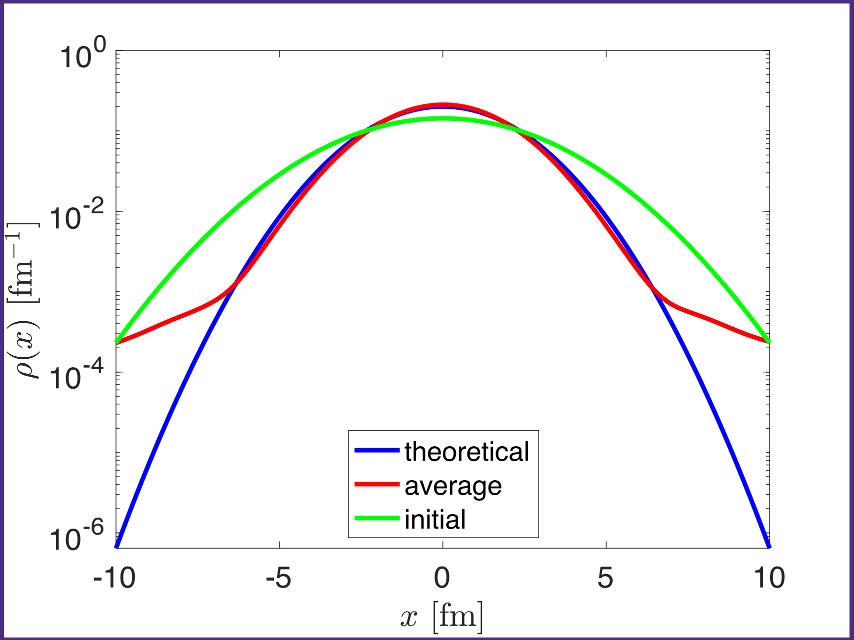
$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta\varepsilon_n}, \quad \varepsilon = \hbar\omega\left(n+\frac{1}{2}\right),$$

$$\rho(x) = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt|\psi(x,t)|^2 \approx \frac{1}{Z(\beta)}\sum_{n=0}^{\infty} e^{-\beta\varepsilon_n}|\phi_n(x)|^2,$$

Fluctuations and Dissipation

Test case: 1D harmonic oscillator





Fluctuations and Dissipation

Fission of ^{258}Fm: quantum hydrodynamics

- The Langevin approach usually requires a considerable number of random trajectories for each initial conditions.
- For full TDDFT approach, the time cost for each trajectory is expensive.
- Alternative: nuclear hydrodynamics
  - Landau's two-fluid model: normal components and superfluid components.
  - At zero temperature, only the superfluid one survives.
  - The dynamics reduces to that of a neutron and a proton perfect fluids.

Fluctuations and Dissipation

Fission of ^{258}Fm: quantum hydrodynamics

- In hydrodynamics, the complex "wavefunction" has the form (for each neutron and proton)

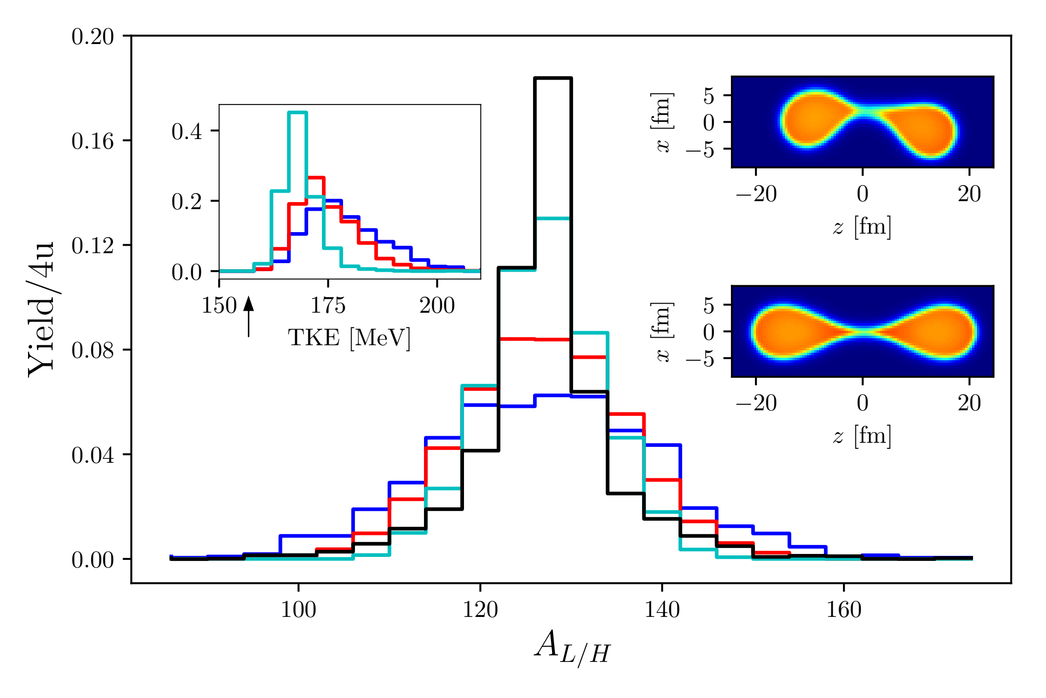
$$\psi_q(\vec{r}) = \sqrt{n_q(\vec{r})}\exp(i\phi_q(\vec{r})), \quad \vec{v}_q(\vec{r}) = \frac{\hbar}{m}\vec{\nabla}\phi_q(\vec{r}).$$

- Nuclear hydrodynamics equation

$$i\hbar\dot{\psi}_q(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi_q(\vec{r},t) + \frac{\delta\mathcal{E}_{\text{int}}}{\delta n(\vec{r},t)}\psi_q(\vec{r},t) + \gamma[n]\dot{n}(\vec{r},t)\psi_q(\vec{r},t) + u_0(\vec{r},t)\psi_q(\vec{r},t).$$

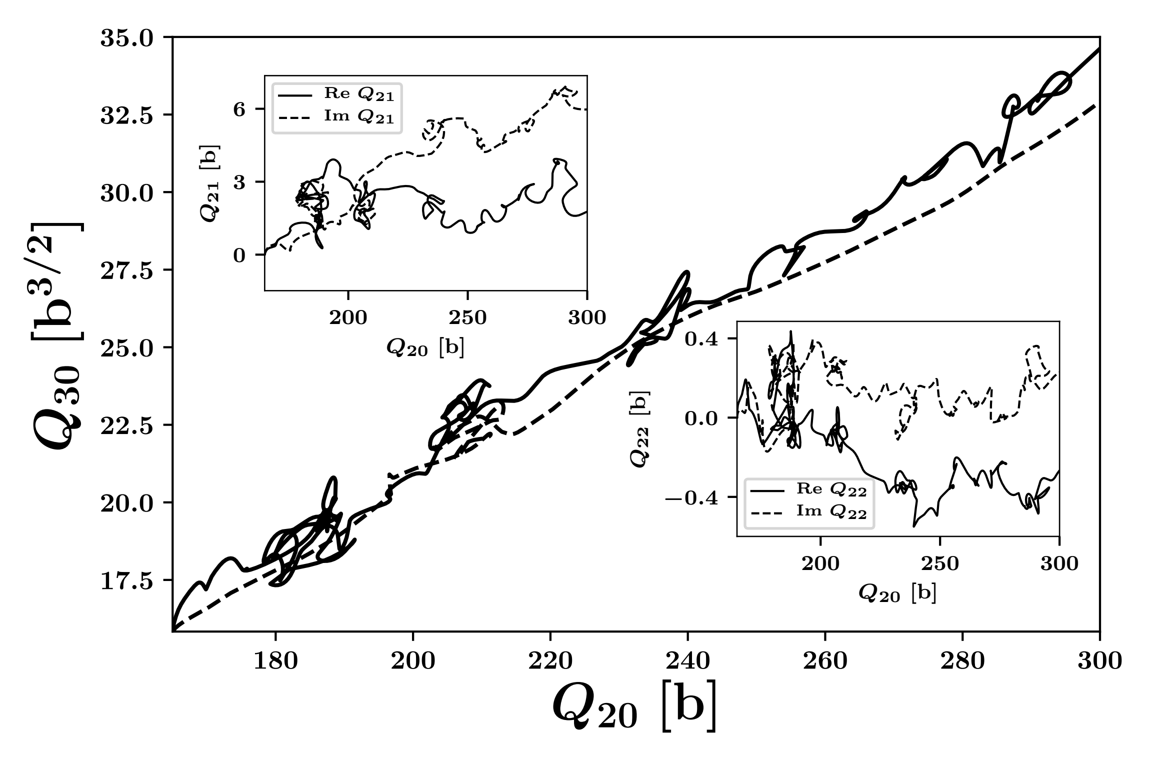
Fluctuations and Dissipation

Fission of ^{258}Fm: quantum hydrodynamics



Fluctuations and Dissipation

Exploration of fluctuation-dissipation in TDSLDA



Conclusions

- Nuclear fission is one of the most complicated quantum many-body problem. Pairing interaction plays an important role in the shape evolution from saddle to scission.
- TDSLDA can reliably predict the most probable fission fragments (FFs) properties.
- The dynamics from saddle to scission is non-adiabatic and over-damped.
- The fluctuations of FFs properties are absent in TDSLDA and have to be included. The fluctuations of FFs properties can be reproduced by introducing stochasticity into TDSLDA.

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