Induced Fission of ^{240}Pu with time-dependent density functional theory

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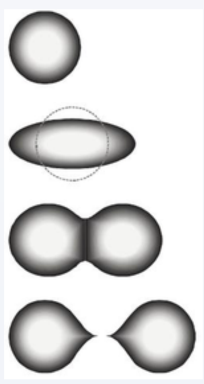
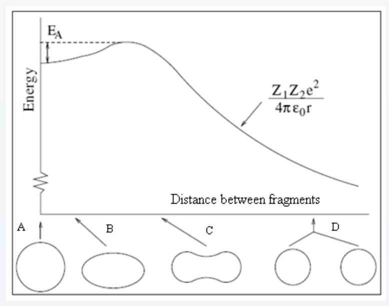
Introduction

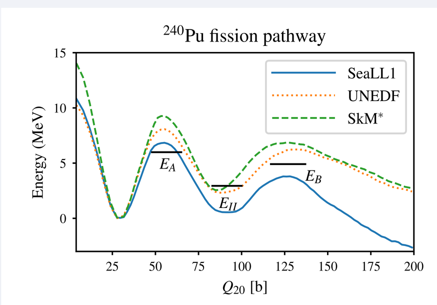
Meitner and Frisch, Bohr and Wheeler (1939) interpreted the neutron induced fission of uranium observed by Hahn and Strassmann as the Coulomb-driven division of a classically charged liquid drop in competition with the surface tension of the liquid drop.



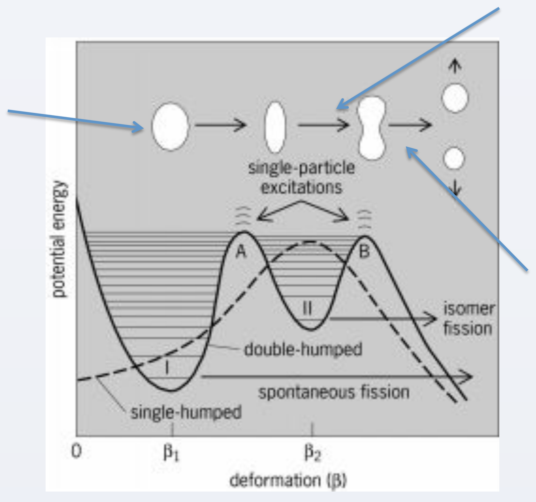


The basic mechanism of induced fission of ^{240}Pu is the following:

The impinging neutron on ^{239}Pu, leads to the formation of an excited state, the compound nucleus (^{240}Pu) .



Quantum shell effects lead to a double-humped fission barrier.



The nucleus evolves for a very long time from its ground state shape towards the top of the fission.

$$t_1 \approx 10^9 \text{ fm/c}$$

The Coulomb repulsion overcomes surface tension and the nucleus starts its descent to scission, where the two fission fragments are formed.

$$t_2 \approx 10^3 \sim 10^4 \text{ fm/c}$$

Fission dynamics is a very complex process. From saddle to scission, fission dynamics is a non-adiabatic, large amplitude collective motion. It still did not reach a microscopic description for 80 years after the discovery.

Theoretical formalism

Density functional theory (DFT)

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

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

Hohenberg and Kohn (HK) theorem:

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

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

$$E_0 = \langle\Psi[n]|\hat{H}|\Psi[n]\rangle = \min_{n(\boldsymbol{r})} \int d^3r\,(\mathcal{E}[n(\boldsymbol{r})] + V_{\text{ext}}(\boldsymbol{r})n(\boldsymbol{r})) \qquad \mathcal{E}[n(\boldsymbol{r})] = \langle\Psi|\hat{T}+\hat{W}|\Psi\rangle$$

The total energy of a superfluid nucleus is a functional of various one-body local densities (for neutron and proton respectively)

$$E = \int d^3r\mathcal{E}[n(\boldsymbol{r}), \tau(\boldsymbol{r}), \boldsymbol{J}(\boldsymbol{r}), \boldsymbol{\nabla}n(\boldsymbol{r}), \nu(\boldsymbol{r})]$$

All the local densities are calculated from the 4-component quasi-particle wavefunctions (qpwfs)

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

normal density: $n(\boldsymbol{r}) = \sum_{k,s} v_{k,s}^*(\boldsymbol{r})v_{k,s}(\boldsymbol{r}),$

kinetic density: $\tau(\boldsymbol{r}) = \sum_{k,s} \boldsymbol{\nabla}v_{k,s}^*(\boldsymbol{r}) \cdot \boldsymbol{\nabla}v_{k,s}(\boldsymbol{r}),$

spin-orbit density: $\boldsymbol{J}(\boldsymbol{r}) = -i\sum_{k,s,s'} v_{k,s}^*(\boldsymbol{r})\,[\boldsymbol{\nabla}v_{k,s}(\boldsymbol{r}) \times \boldsymbol{\sigma}_{s,s'}]$

anomalous density: $\nu(r) = \sum_k v_{k\uparrow}^*(\boldsymbol{r})u_{k\downarrow}(\boldsymbol{r})$

Hartree-Fock-Bogoliubov (HFB) - like equation for each qpwfs

$$\begin{pmatrix} h_{\uparrow\uparrow}-\mu & h_{\uparrow\downarrow} & 0 & \Delta \\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow}-\mu & -\Delta & 0 \\ 0 & -\Delta^* & -h_{\uparrow\uparrow}^*+\mu & -h_{\uparrow\downarrow}^* \\ \Delta^* & 0 & -h_{\downarrow\uparrow}^* & -h_{\downarrow\downarrow}^*+\mu \end{pmatrix} \begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix} = E_k \begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix} \qquad hv_{k\uparrow} = \frac{\delta E}{\delta v_{k\uparrow}^*}, \quad \Delta v_{k\uparrow} = \frac{\delta E}{\delta u_{k\uparrow}^*}$$

Time-dependent density functional theory (TDDFT)

$$i\hbar\frac{\partial}{\partial t}\Psi(1,\cdots,A,t) = \left\{\sum_{i=1}^A -\frac{\hbar^2}{2m}\Delta_i + V(1,\cdots,A,t)\right\}\Psi(1,\cdots,A,t) \quad \Psi(1,...,A,t) \Leftrightarrow \Psi[n] \Leftrightarrow n(\mathbf{r},t) = \sum_k |\phi_k(\mathbf{r},t)|^2$$

Time-dependent superfluid local density approximation (TDSLDA) equation:

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

$$h(\boldsymbol{r},t) = h[n(\boldsymbol{r},t), \tau(\boldsymbol{r},t), \boldsymbol{J}(\boldsymbol{r},t), \boldsymbol{\nabla}n(\boldsymbol{r},t), \boldsymbol{j}(\boldsymbol{r},t)], \quad \Delta(\boldsymbol{r},t) = \Delta[\nu(\boldsymbol{r},t)]$$

current density: $\boldsymbol{j}(r,t) = \sum_k \text{Im}\,\left(v_{k\uparrow}(\boldsymbol{r},t)\boldsymbol{\nabla}v_{k\uparrow}^*(\boldsymbol{r},t) + v_{k\downarrow}(\boldsymbol{r},t)\boldsymbol{\nabla}v_{k\downarrow}^*(\boldsymbol{r},t)\right)$

Numerical simulation

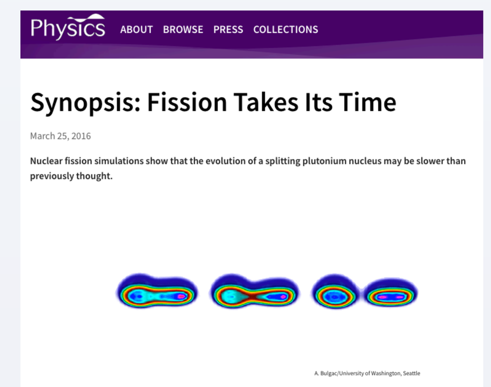
Simulation box: $30 \times 30 \times 60\ \text{fm}^3, \quad dx = 1.25$ fm

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

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

number of GPUs: 1730 (on Titan, Tesla K20)

Wall time: 3.7 h / (1000 fm/c)



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: $g_0 = -233$ MeV

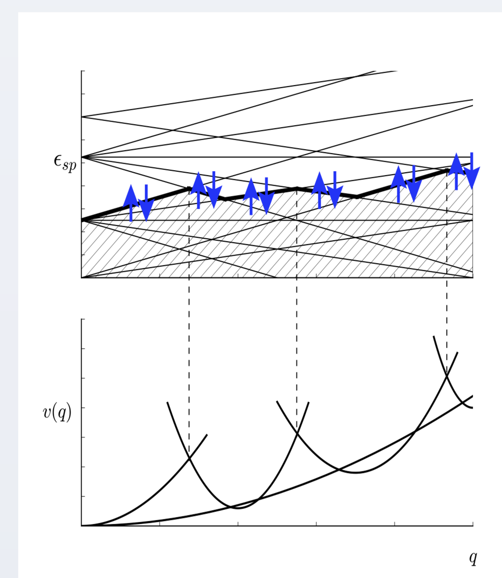
The properties of fission fragments agree surprisingly well with experimental observations.

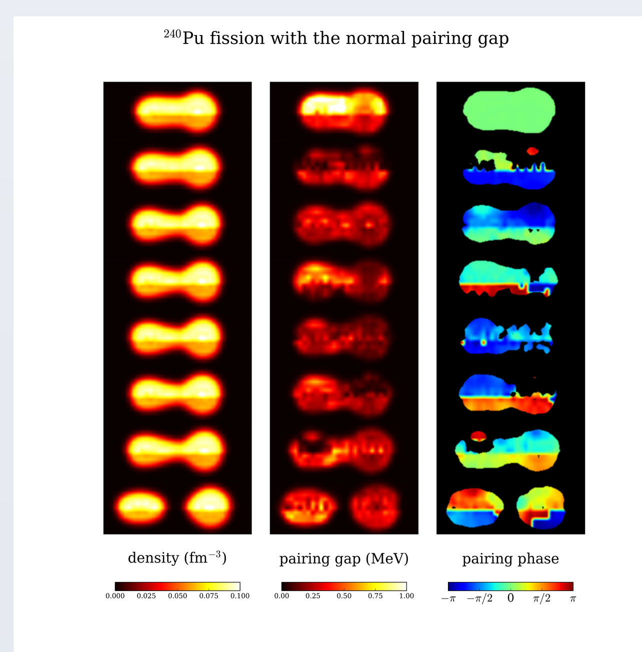
t_{sc}	TKE ^{syst}	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L
12259	177.26	173.42	100.55	101.7	60.69	61.3	39.81	40.4

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

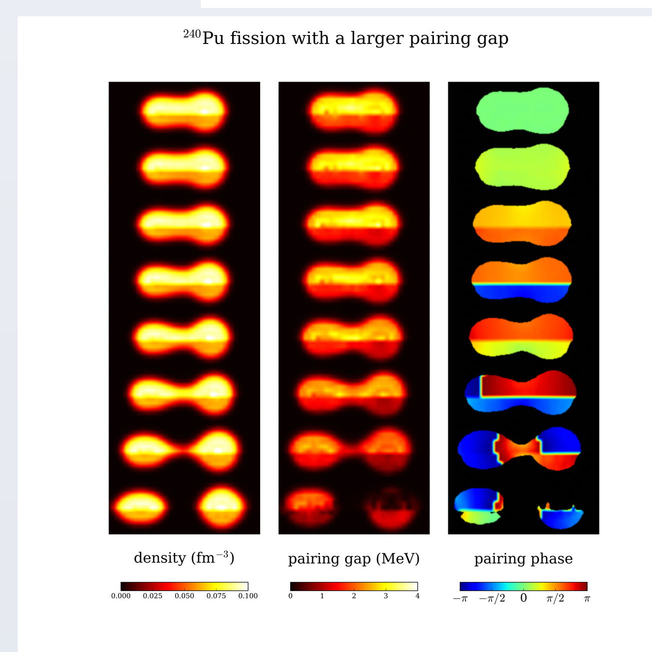
Importance of pairing interaction

- 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 level doublet is occupied with time reversed quantum numbers (in the shaded area).
- At each crossing two nucleons change their angular momenta (m, -m) => (m', -m') : "Cooper pair" => "Cooper pair".
- Pairing interactions is the most effective mechanism at performing such transitions.



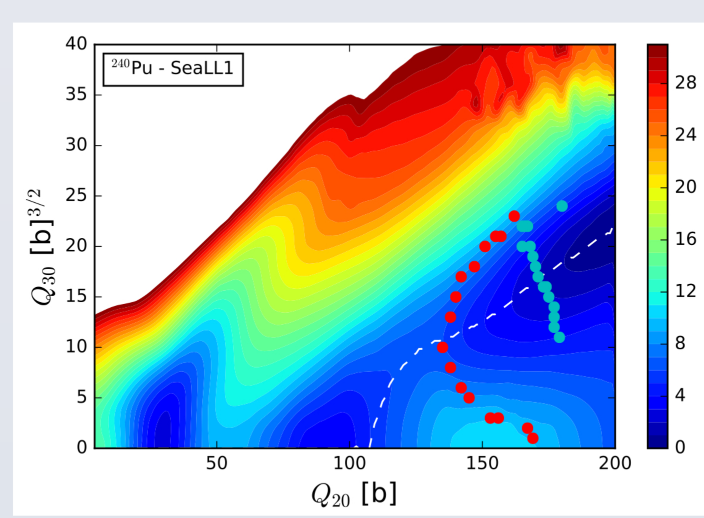


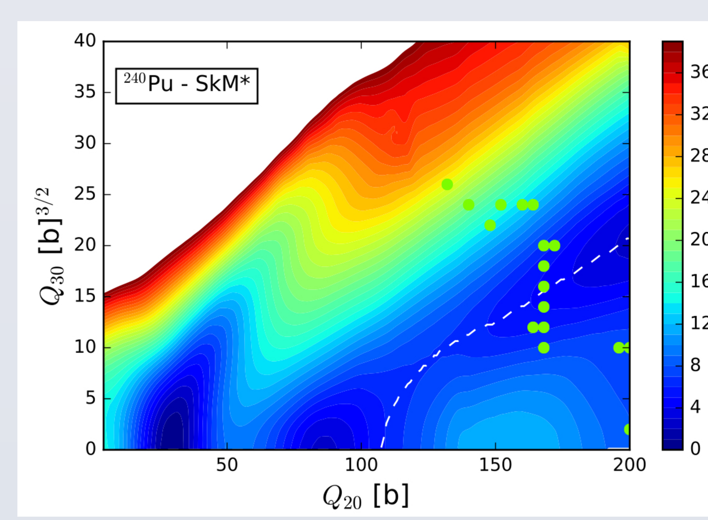
Normal pairing strength, saddle to scission 14000 fm/c

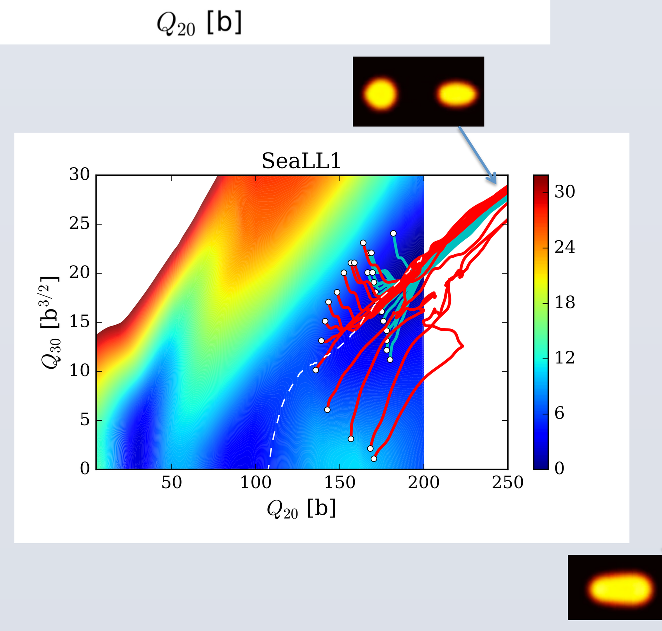


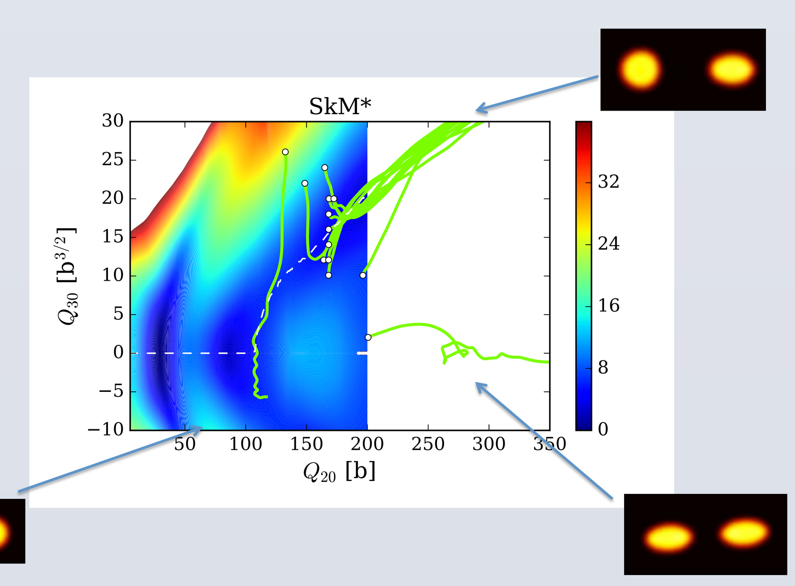
Enhanced pairing strength, saddle to scission 1400 fm/c !!!

Different initial conditions and EDFs









Label	E_{ini}^*	TKE	N_H	Z_H	N_L	Z_L	E_H^*	E_L^*
SeaLL1-1	7.9(1.7)	177.8(2.8)	83.5(0.4)	53.2(0.4)	62.8(0.5)	41.1(0.4)	17.0(2.4)	20.1(2.0)
SeaLL1-2	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)
SkM*-a	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)
SkM*-s	9.6	149.0	73.4	47.2	72.6	46.7	29.4	28.5

number in the parenthesis represents the standard deviation of the quantity

References

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4. A. Bulgac, S. Jin, P. Magierski, K.J. Roche, and I. Stetcu, *Microscopic theory of nuclear fission* , PoS(INPC2016)225