A roadmap of the microscopic theory for spontaneous fission

Jhilam Sadhukhan
Variable Energy Cyclotron Centre
Kolkata, India

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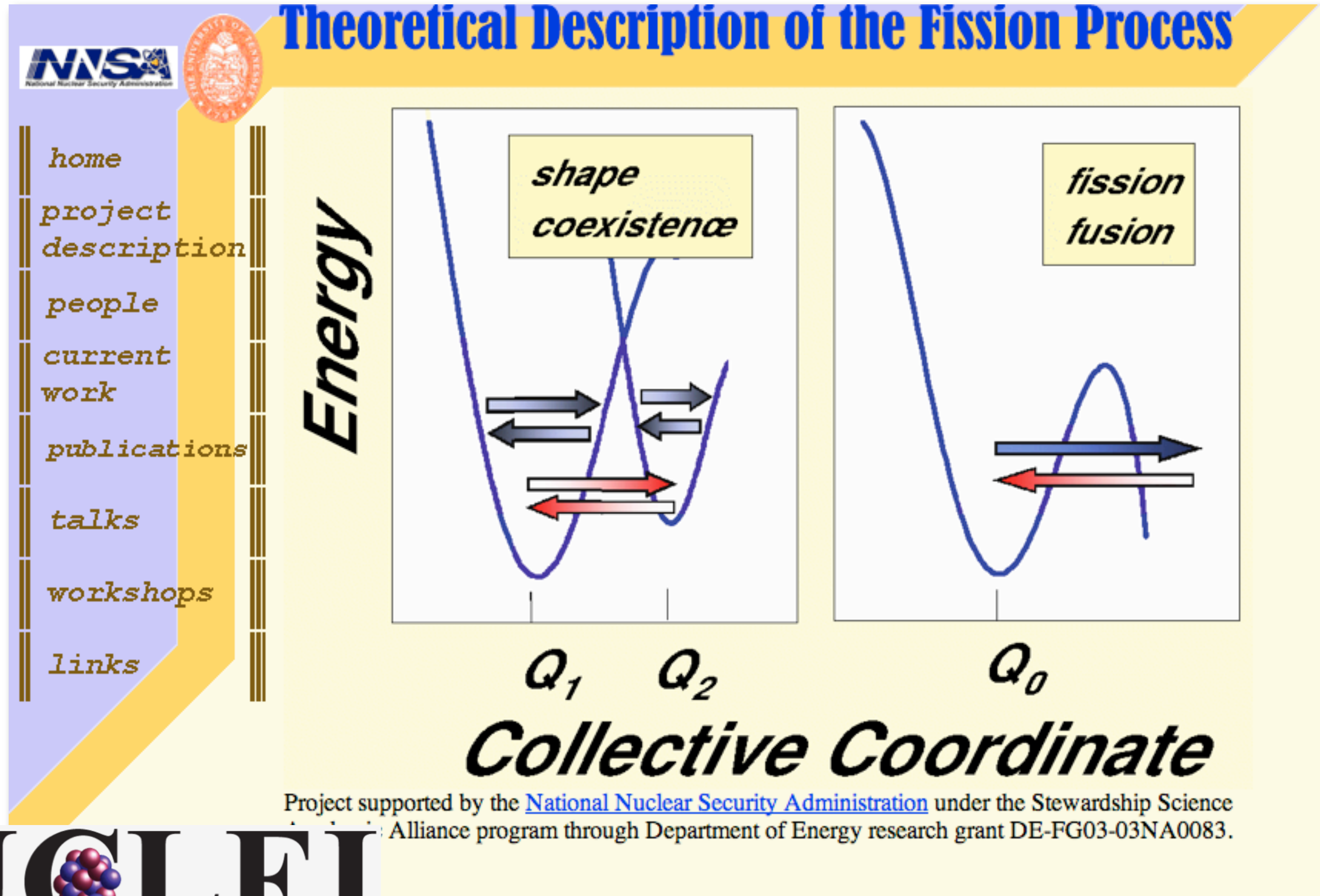
Team

https://people.nscl.msu.edu/~witek/fission/fission.html

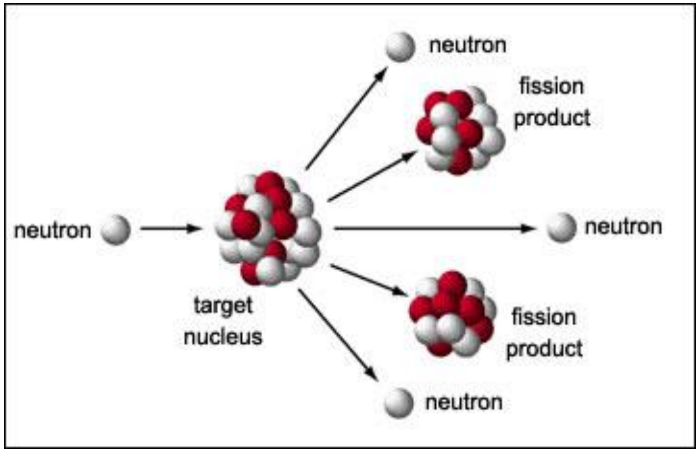


NUCLEI
Nuclear Computational Low-Energy Initiative

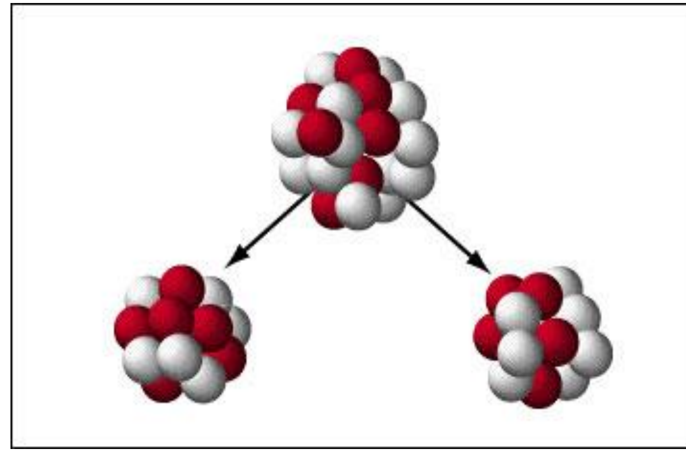
Progress in Spontaneous Fission studies in last 2-3 years will be discussed

Fission mechanisms

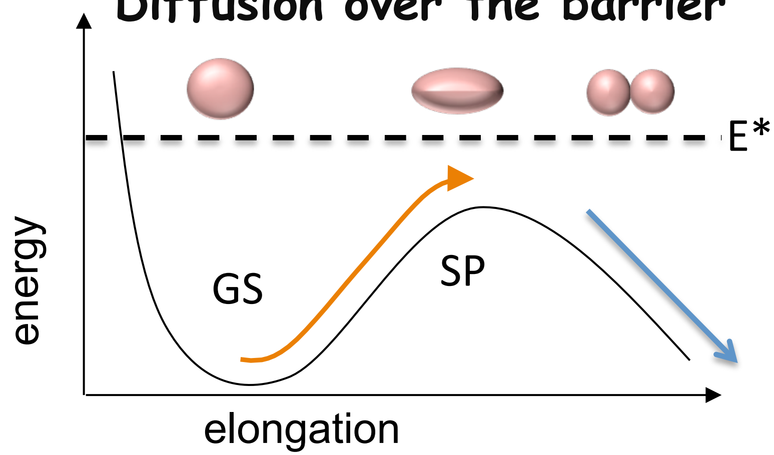
Induced fission



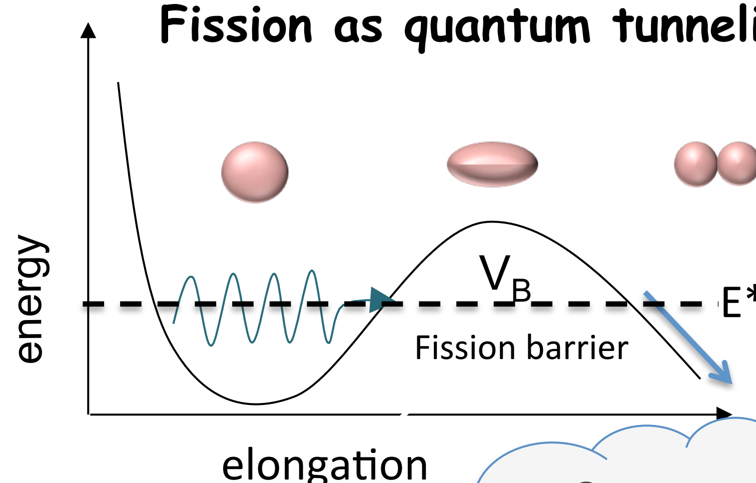
Spontaneous fission



Diffusion over the barrier



Fission as quantum tunneling

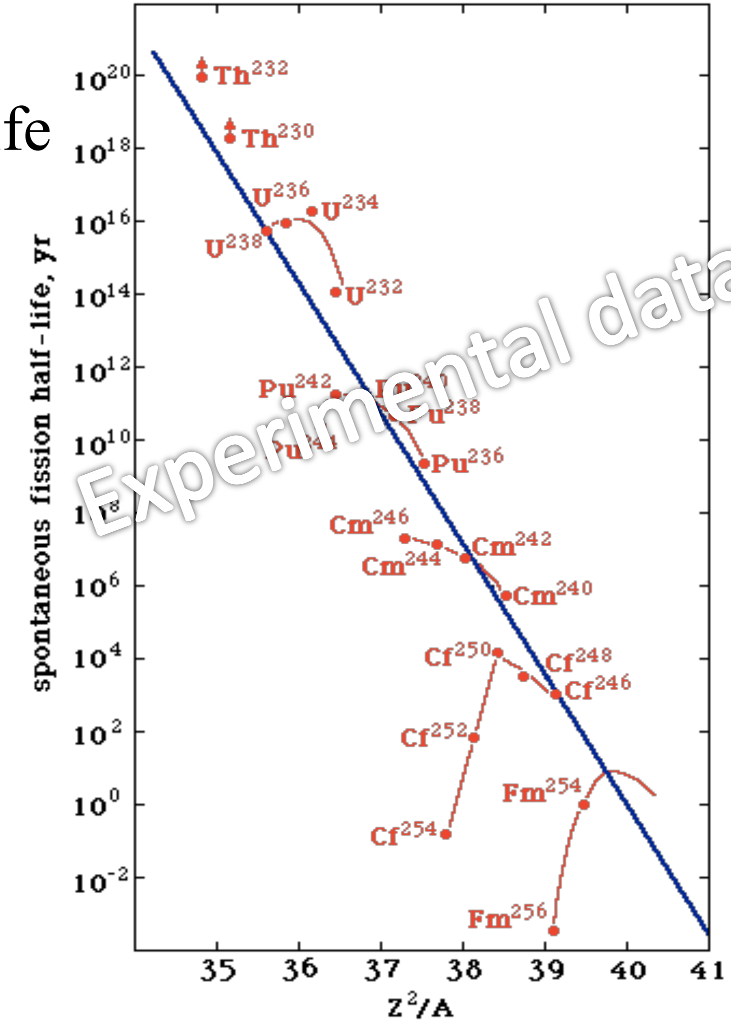


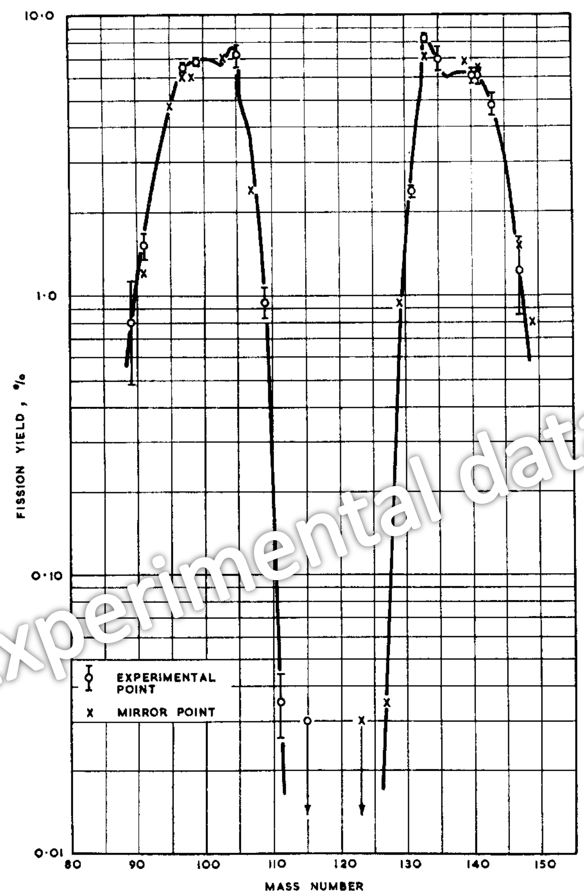
Dynamics can be treated classically……..

Quantum many-body problem

Spontaneous fission observables

- Spontaneous fission half-life





- Fission fragment yields

Spontaneous fission half-life

*A. Baran, Phys. Lett. B **76**, 8 (1978)*

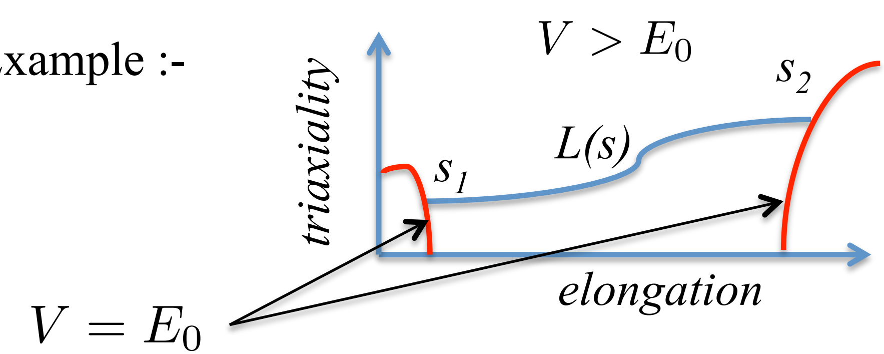
$$T_{1/2} = \frac{\ln 2}{nP}$$

n is the number of assaults on the fission barrier per unit time

Penetration probability → $P = (1 + \exp 2S(L))^{-1}$ (WKB)

Action integral along the fission path *L(s)* → $S(L) = \int_{s_1}^{s_2} \frac{1}{\hbar} \left[2\mathcal{M}_{\text{eff}}(s)\,(V_{\text{eff}}(s) - E_0)\right]^{1/2} ds$

Example :-



$V_{\text{eff}}(s) = V$ along $L(s)$

$\mathcal{M}_{\text{eff}}(s) =$ effective $\mathcal{M}$ along $L(s)$

$E_0 =$ ground state vibrational energy

Most probable fission path = Minimum action path

We need $V(q_1, q_2 \ldots.), \mathcal{M}(q_1, q_2 \ldots.)$ ← **Self-consistent DFT**

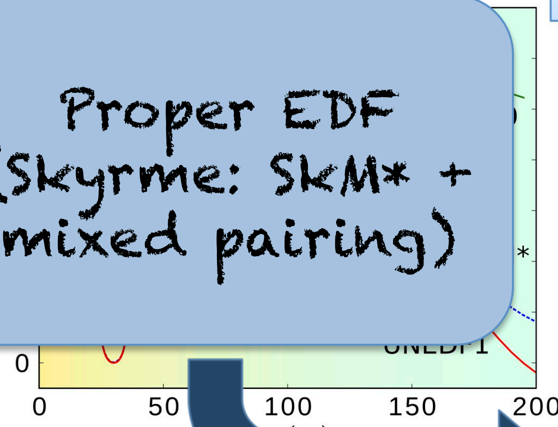
Our Strategy

Quality Input

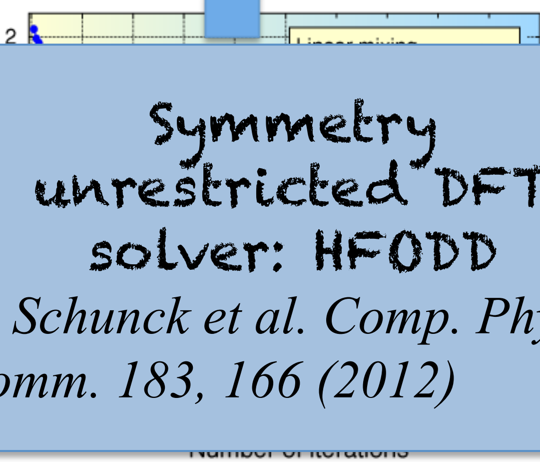
Large-scale Simulations on Leadership-class Computers

Dynamics

Proper EDF (Skyrme: SkM* + mixed pairing)



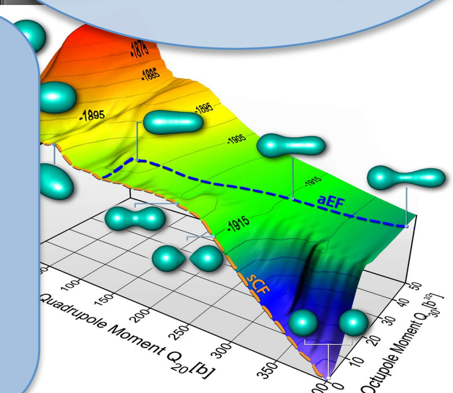
Numeric



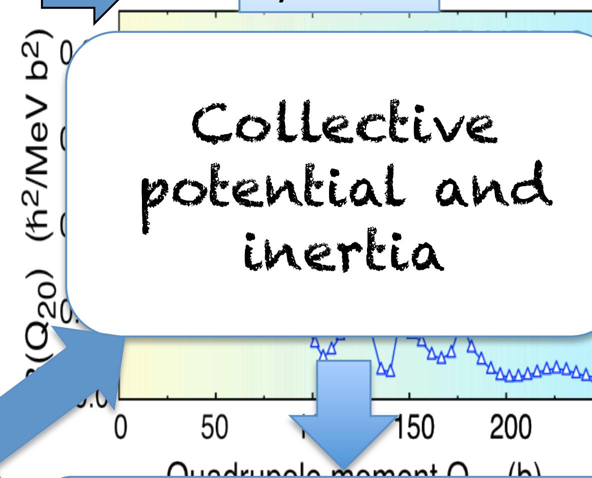
Symmetry unrestricted DFT solver: HFODD

N. Schunck et al. Comp. Phys. Comm. 183, 166 (2012)

Solve HFB Equations

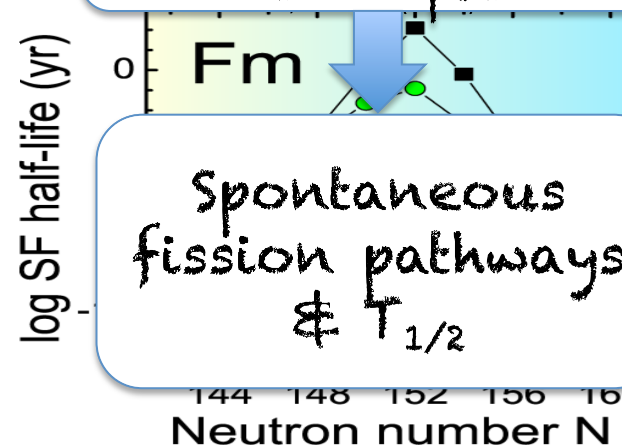


Collective potential and inertia



Action minimization technique

Spontaneous fission pathways & $T_{1/2}$



Calculated potential energy

$\Gamma[\rho]$ → Skyrme functional with SkM* parametrization
*J. Bartel et al. Nucl. Phys. **A** 386, 79 (1982)*

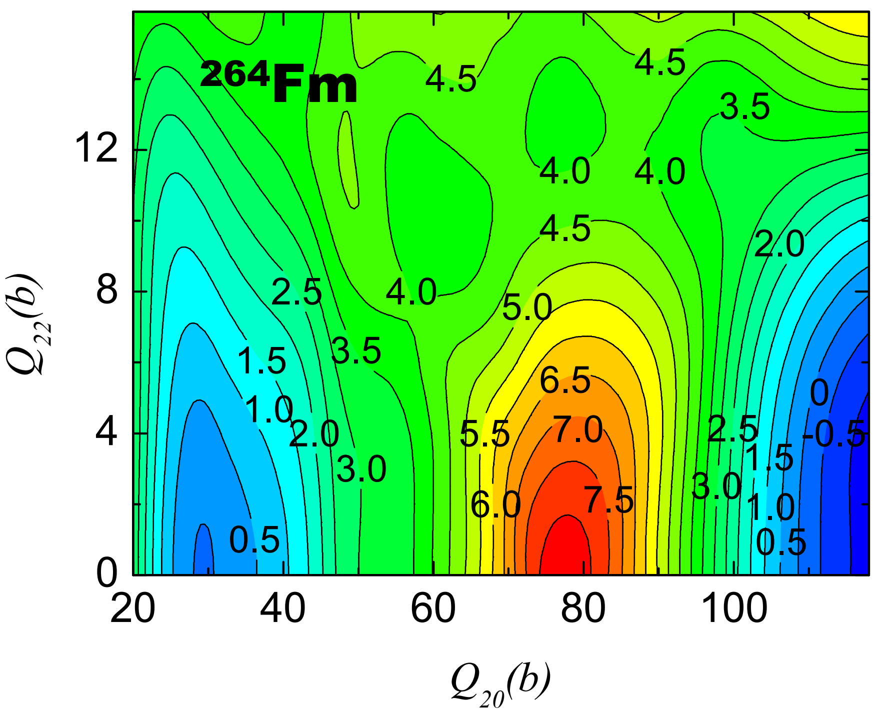
optimized for fission study

$$f(r) = V_0^{(n,p)}\left[1 - \frac{1}{2}\frac{\rho(r)}{\rho_c}\right] \qquad \rho_c = 0.16fm^{-1} \qquad \begin{aligned} V_0^n &= -268.9MeV\,fm^3 \\ V_0^p &= -332.5MeV\,fm^3 \end{aligned}$$

J. Dobaczewski et al. Comp. Phys. Comm., 158, 158 (2004)

Adjusted to reproduce the
'n' & 'p' pairing gaps of ^{252}Fm

*A. Staszczak et al. Phys. Rev. C **87**, 024320 (2013)*



Calculated with two constraints
Q_{20} (elongation) and Q_{22} (triaxiality)

Calculation of inertia

*A. Baran et al. Phys. Rev. **C** 84, 054321 (2011)*

ATDHFB Inertia:-

$$\mathcal{M}_{ij} = \frac{\sqrt{-1}}{\ \ } Tr\left(F^{i*}Z^j - F^i Z^{j*}\right)$$

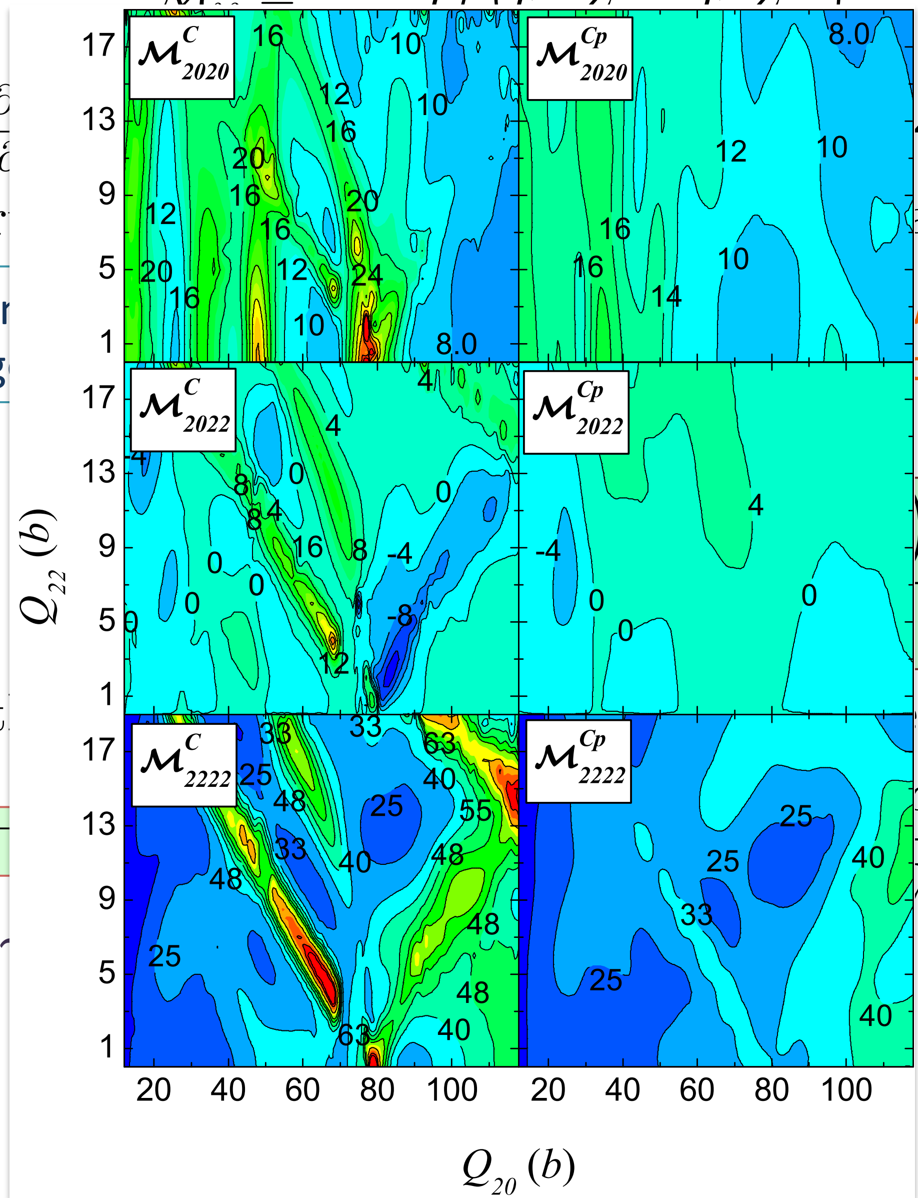
Unit = $10^{-3}\ \hbar^2/\mathrm{MeVb}^2$

$$-F^{i*} = \left(B^T \frac{\partial \rho_0}{\partial q_i} A + B^T \frac{\partial}{\partial} \right. \quad Z^i + Z^i E + \cancel{E}_1$$

A, B are quasipar … asiparticle energies

Derivatives of static de… using Lagrang…

…w time-odd densities … calculate E_1



ρ_0, κ_0 required at t… …rturbative approximation)

$$\mathcal{M}^{C\mathrm{p}} = \hbar^2 [M^{(1)}]^{-} \quad \ldots \alpha\beta\rangle\langle\alpha\beta|\hat{Q}_j^\dagger|0\rangle \over \ldots E_\alpha + E_\beta)^k$$

Action minimization techniques

A. Baran et al. Nucl. Phys. A ***361****, 83 (1981)*

Two numerical methods

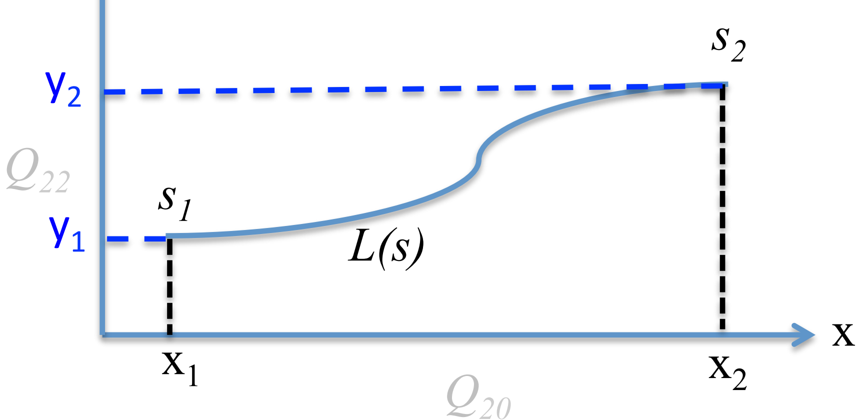
Ritz method (RM):-

$$y(L) = \sum_k a_k \sin\left(\pi k \frac{x - x_1}{x_2 - x_1}\right) + \text{b.c.}$$

b.c. decided by $s_1(x_1, y_1)$ and $s_2(x_2, y_2)$

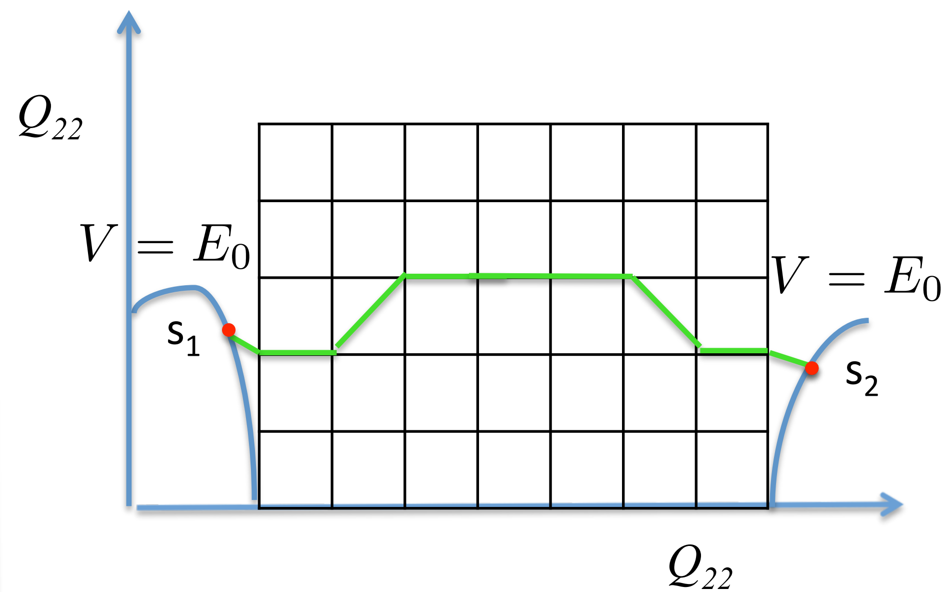
$$S(L) \rightarrow S(a_1, a_2, \ldots a_n)$$

path is decided by varying a_i s



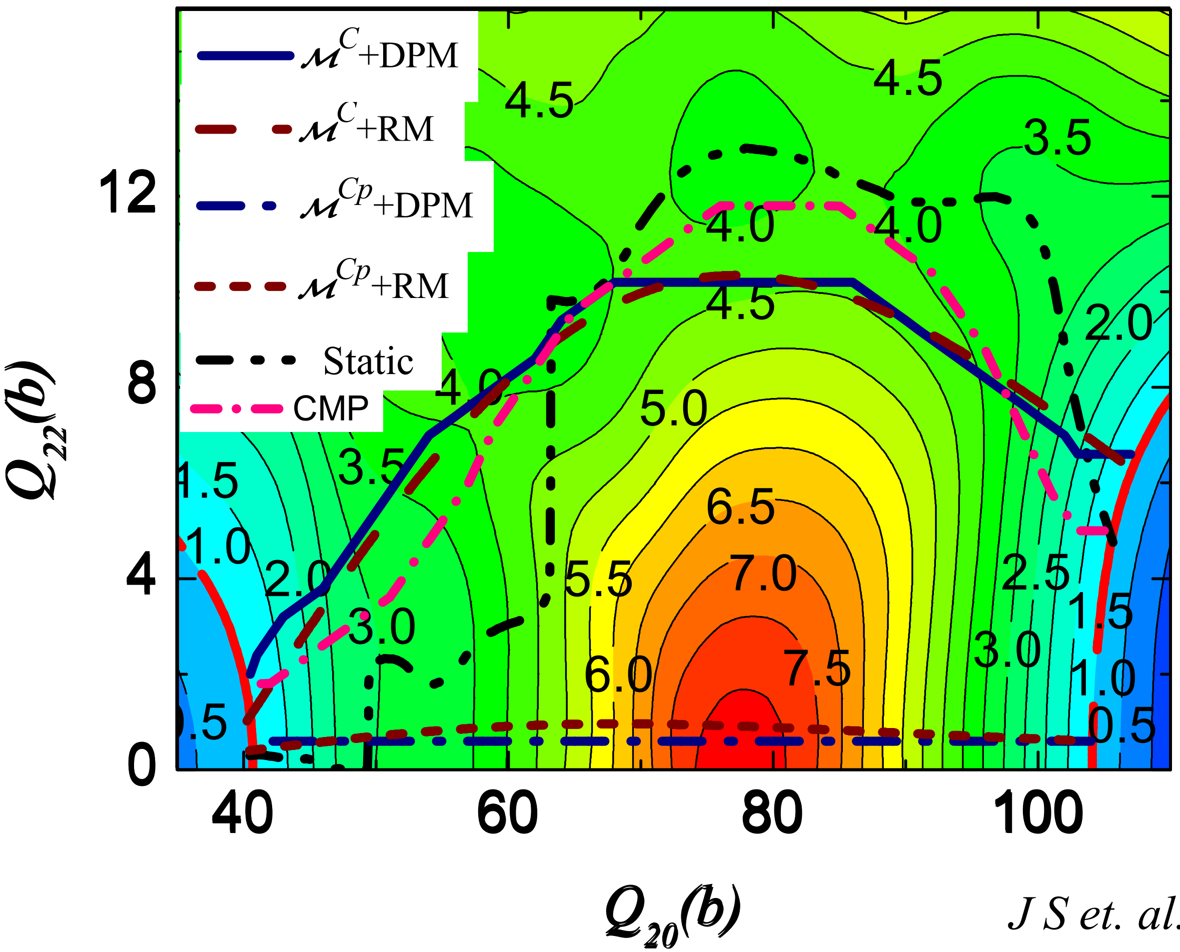
a_1,a_2 and a_3 are sufficient

Dynamic programing method (DPM) :-



Trajectory becomes smooth enough as the grid size is reduced

How Inertia impacts the results



$E_0 = 1.0$ MeV

Static path (minimum potential path)

Dynamic path with cont. $\mathcal{M}$

$\mathcal{M} = \mathcal{M}^{Cp}_{2020}$ at ground state

(DPM)

Dynamic path with $\mathcal{M}^{Cp}$ (DPM & RM)

Dynamic path with $\mathcal{M}^{C}$ (DPM & RM)

J S et. al. , Phys Rev C 88, 064314 (2013)

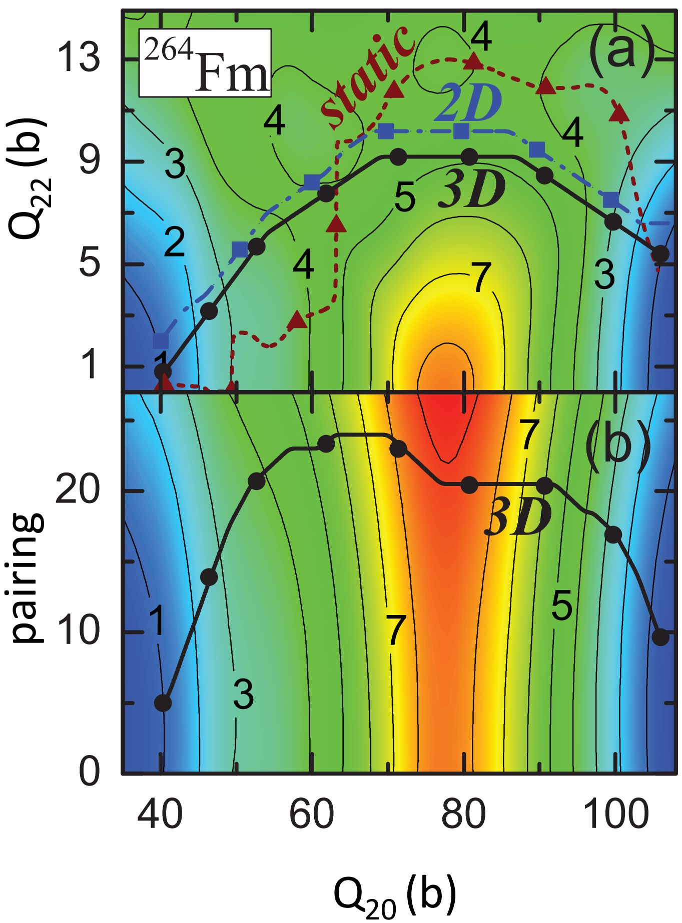
Dynamical effects due to action minimization is not very prominent

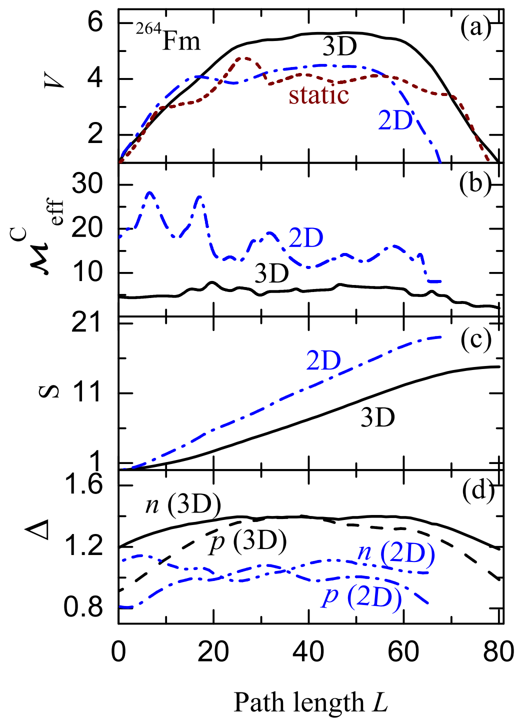
With $\mathcal{M}^{Cp}$:- Strong dynamical effects, triaxiality becomes unimportant

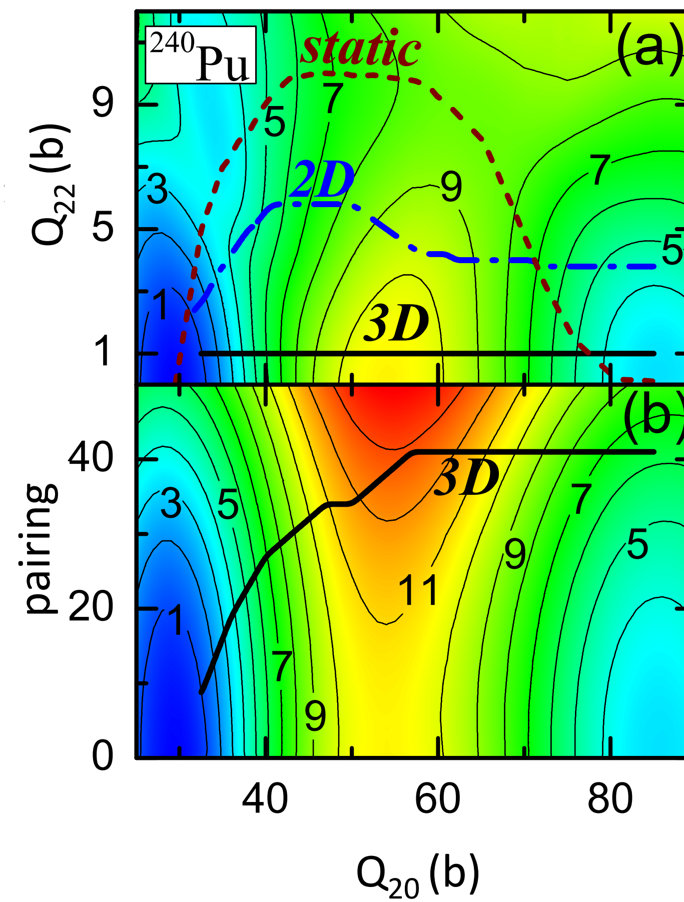
With $\mathcal{M}^{C}$:- dynamics is favoring triaxial saddle, similar to static path

Importance of pairing degree of freedom

$$\hat{H}' = \hat{H}_{HFB} - \sum_{\mu=0,2} \lambda_\mu \hat{Q}_{2\mu} - \sum_{\tau=n,p} \left(\lambda_\tau \hat{N}_\tau - \boxed{\lambda_{2\tau} \Delta \hat{N}_\tau^2} \right)$$





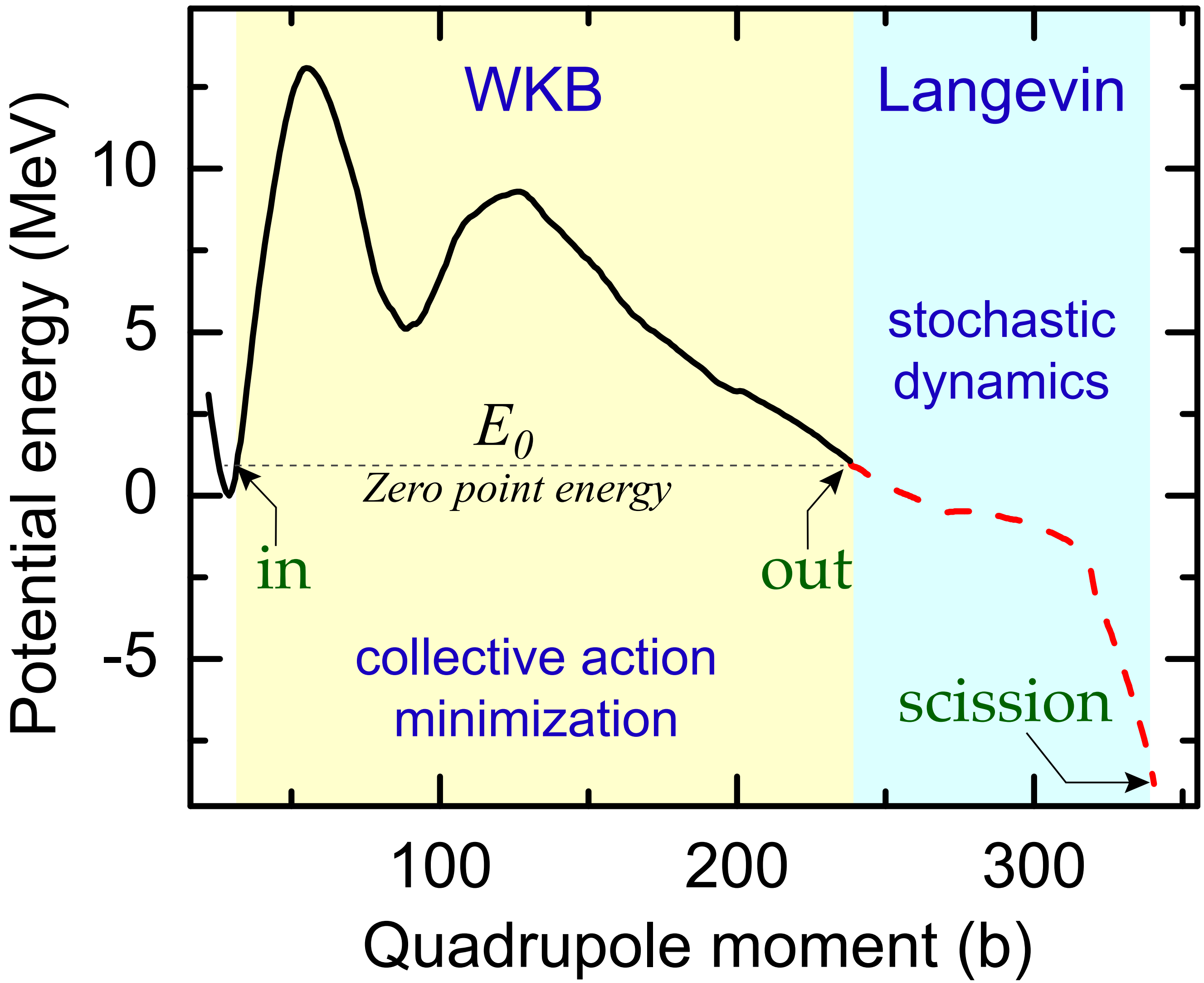


$T_{1/2}(3D)/T_{1/2}(2D) \sim 10^{-4}$

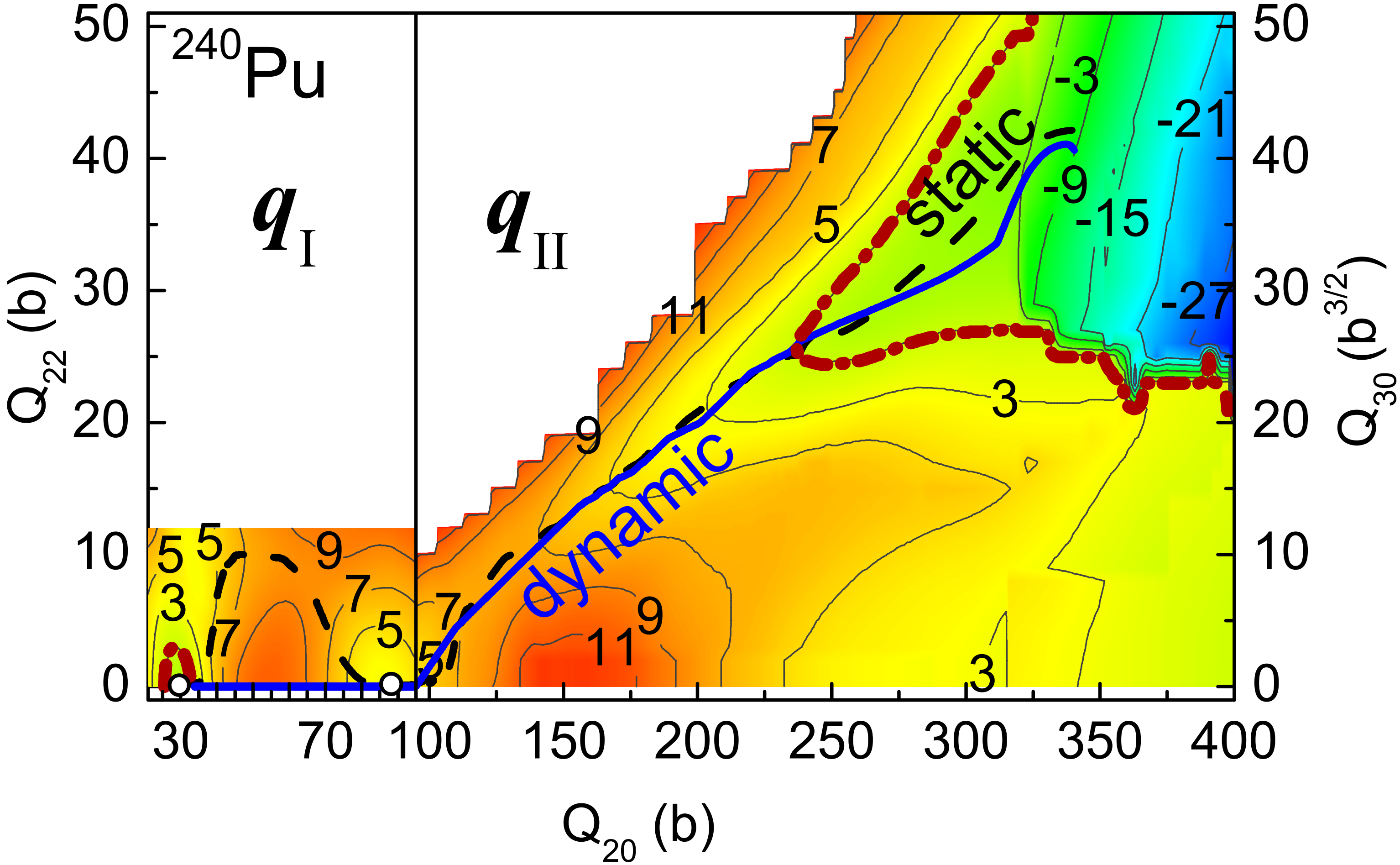
J Sadhukhan et. al. Phys. Rev. C 90, 061304(R) (2014)

Spontaneous fission yields distribution

Fission fragment mass distribution: Our strategy

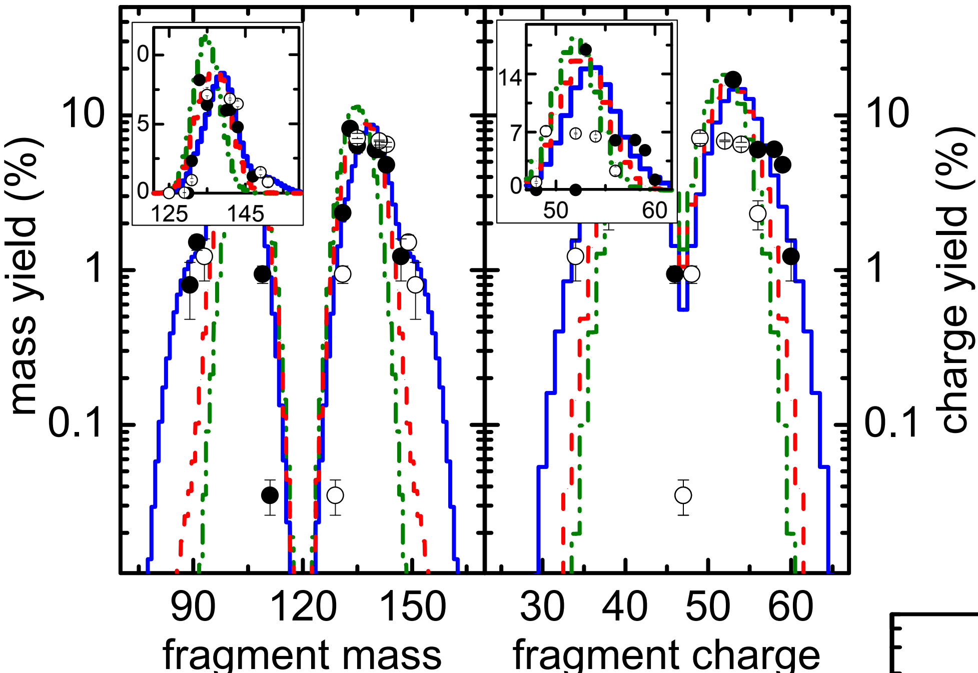


Spontaneous fission path of ^{240}Pu



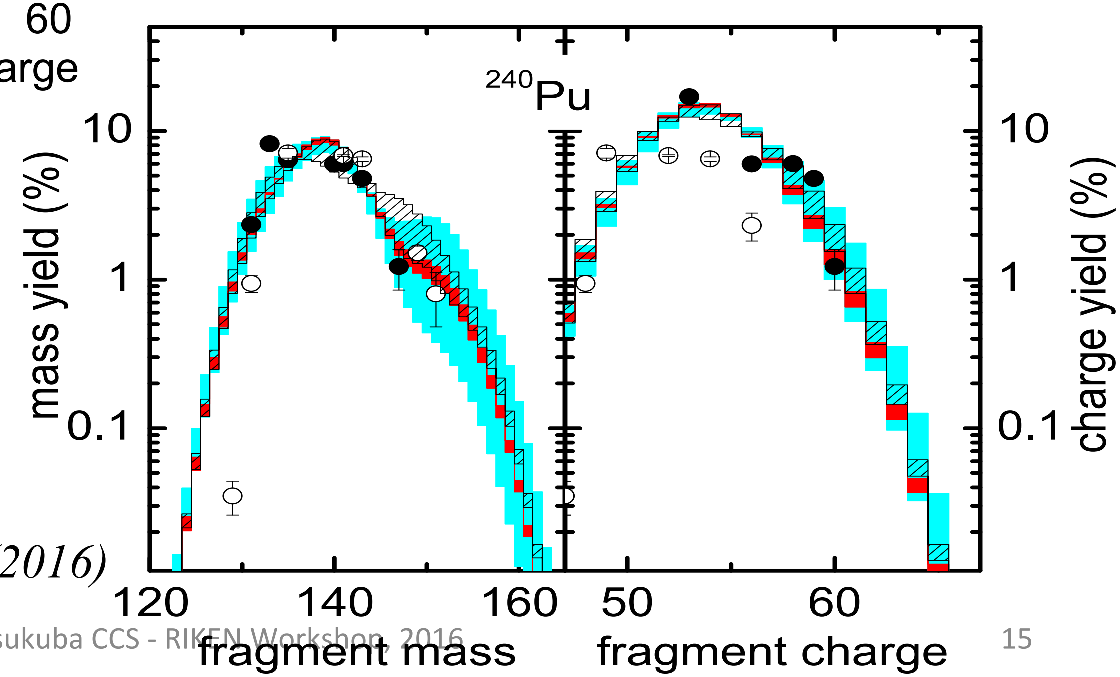
J S, W Nazarewicz, N Schunck. Phys. Rev. C 93, 011304(R) (2016)

Spontaneous fission mass & charge distributions of ^{240}Pu



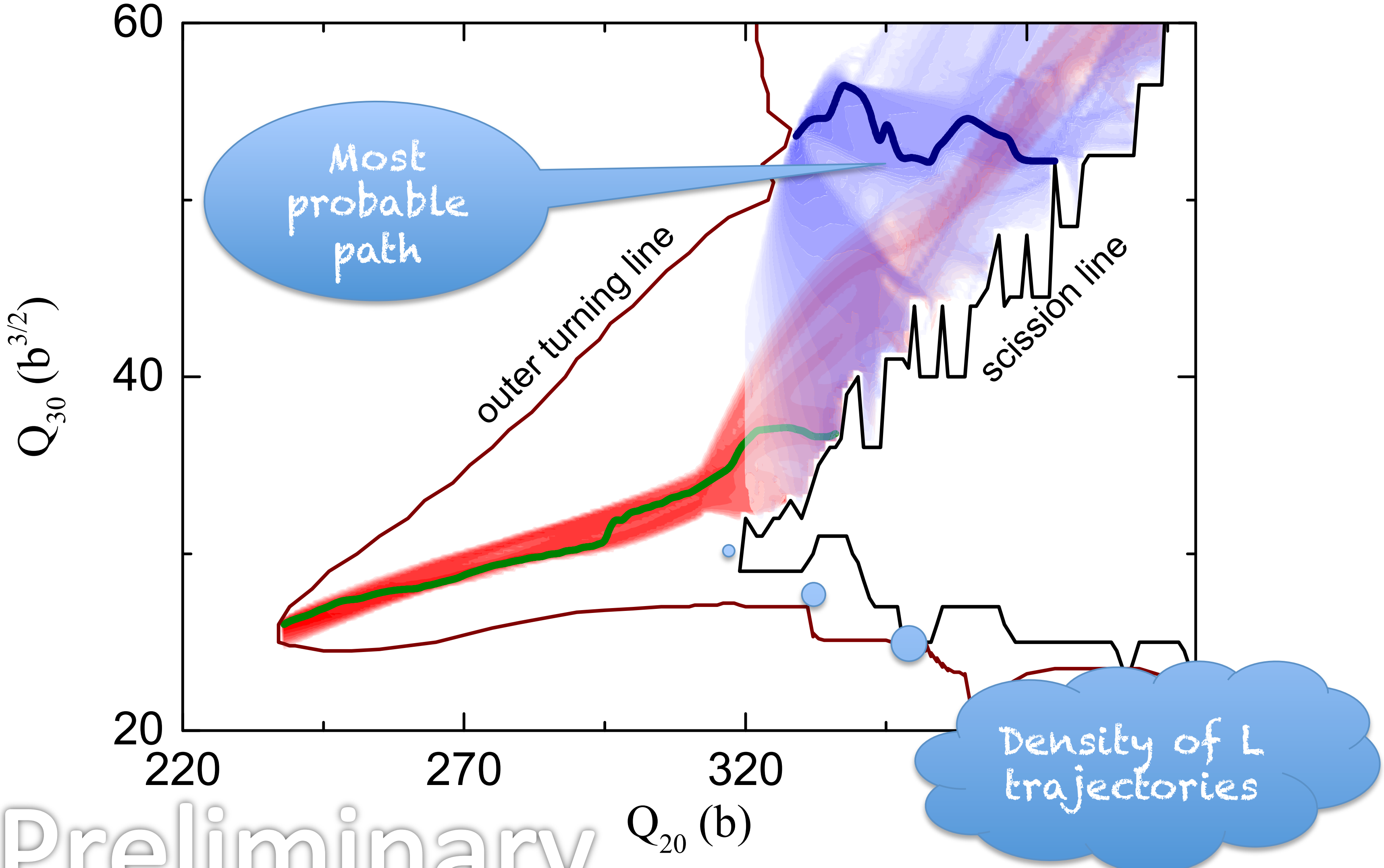
Mass & charge distributions for spontaneous fission of ^{240}Pu

Uncertainties in mass & charge distributions related to variation in the parameters of the model



J S et. al. Phys. Rev. C 93, 011304(R) (2016)

Partial contribution from different outer-turning points



Preliminary

Nucleon localization function: predicting fragment properties

P.-G. Reinhard et. al. Phys. Rev. C 83, 034312 (2011)

C. L. Zhang et. al. arXiv:1607.00422v1 [nucl-th] 1 Jul 2016

The spatial localization measure was originally introduced in atomic and molecular physics to characterize chemical bonds in electronic systems.

$$R_{q\sigma}(\vec{r},\delta) \approx \frac{1}{3}\left(\tau_{q\sigma} - \frac{1}{4}\frac{|\vec{\nabla}\rho_{q\sigma}|^2}{\rho_{q\sigma}} - \frac{\vec{j}^{\,2}_{q\sigma}}{\rho_{q\sigma}}\right)\delta^2 + \mathcal{O}(\delta^3)$$

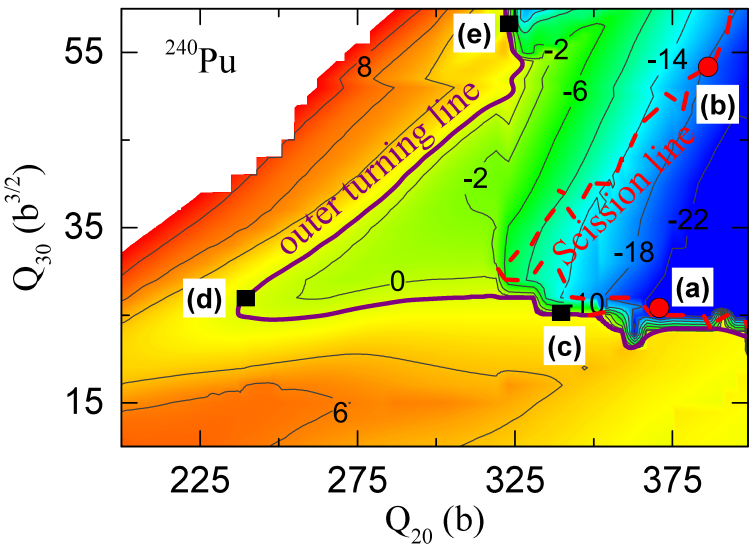
$$\mathcal{C}_{q\sigma}(\vec{r}) = \left[1 + \left(\frac{\tau_{q\sigma}\rho_{q\sigma} - \frac{1}{4}|\vec{\nabla}\rho_{q\sigma}|^2 - \vec{j}^{\,2}_{q\sigma}}{\rho_{q\sigma}\tau^{\mathrm{TF}}_{q\sigma}}\right)^2\right]^{-1}.$$

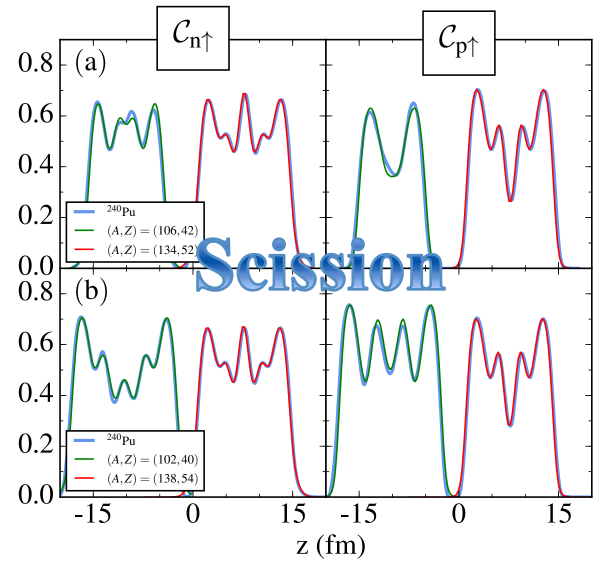
$$\rho_{q\sigma}(\vec{r}) = \sum_{\alpha\in q} v_\alpha^2|\psi_\alpha(\vec{r}\sigma)|^2 \qquad \tau_{q\sigma}(\vec{r}) = \sum_{\alpha\in q} v_\alpha^2|\vec{\nabla}\psi_\alpha(\vec{r}\sigma)|^2 \qquad \vec{j}_{q\sigma}(\vec{r}) = \sum_{\alpha\in q} v_\alpha^2 \mathrm{Im}[\psi^*_\alpha(\vec{r}\sigma)\vec{\nabla}\psi_\alpha(\vec{r}\sigma)],$$

$$\vec{\nabla}\rho_{q\sigma}(\vec{r}) = 2\sum_{\alpha\in q} v_\alpha^2 \mathrm{Re}[\psi^*_\alpha(\vec{r}\sigma)\vec{\nabla}\psi_\alpha(\vec{r}\sigma)]$$

NLF successfully describes the cluster structures in light and heavy nuclei

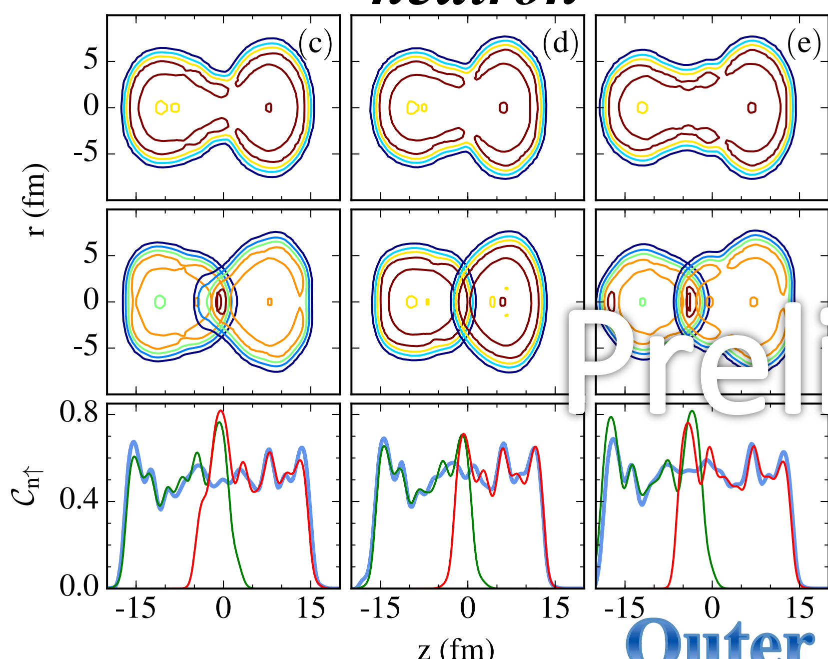
NLFs



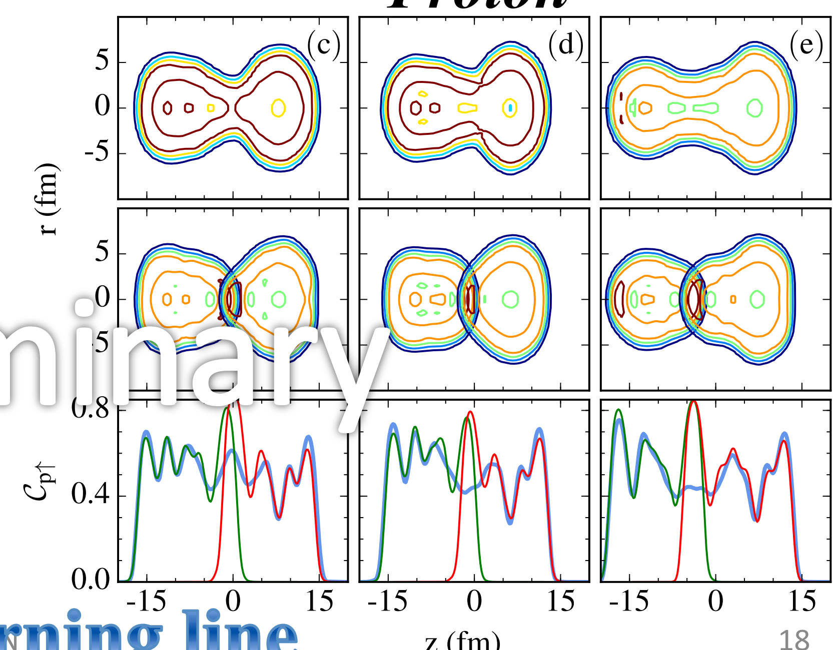


Scission

neutron



Proton



Preliminary

Outer turning line

Summary

- ❑ *Importance of non-perturbative inertia is established*
- ❑ *Importance of nuclear pairing as a dynamical coordinate is studied*
- ❑ *A hybrid (WKB+Langevin) framework is described in the contest of SF yield distributions*

Future works:

- ❑ *Implementation of latest energy density functionals to study fission*
- ❑ *Development of Finite Temperature formalism*

Collaborators: ***Witek Nazarewicz (MSU), Andrzej Baran (Lublin), Jacek Dobaczewski (York), Katarzyna Mazurek (Krakow), Nicolas Schunck (LLNL), Javid Sheikh (India), Zachary Matheson (MSU), Chunli Zhang (MSU)***

Thank You……………