Density functional theory of spontaneous fission life-times

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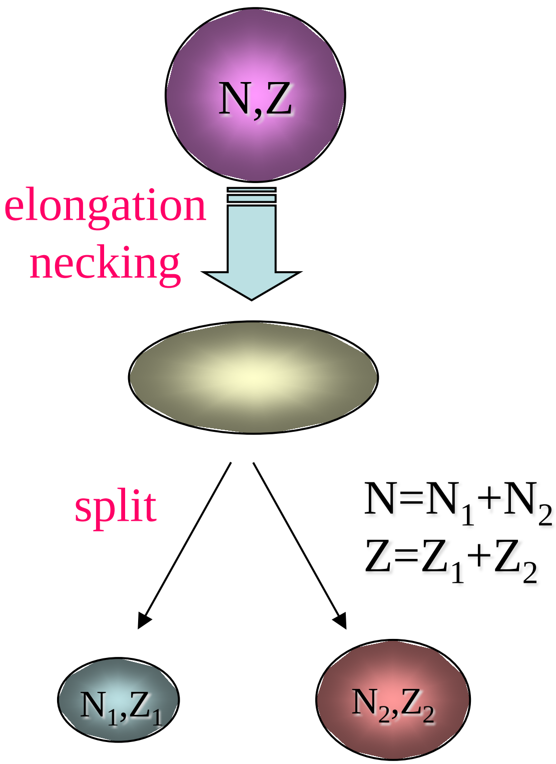
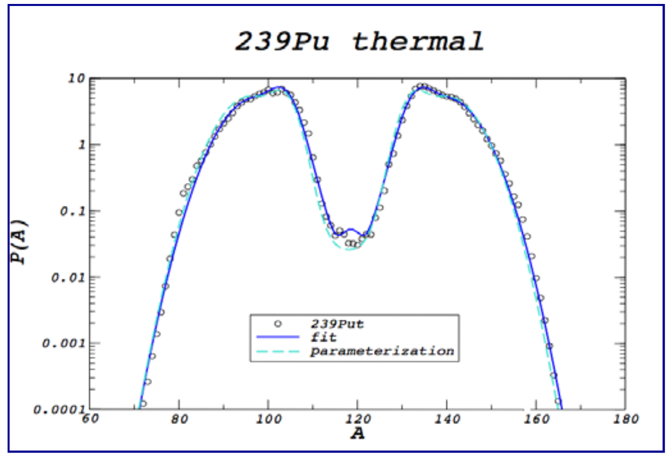
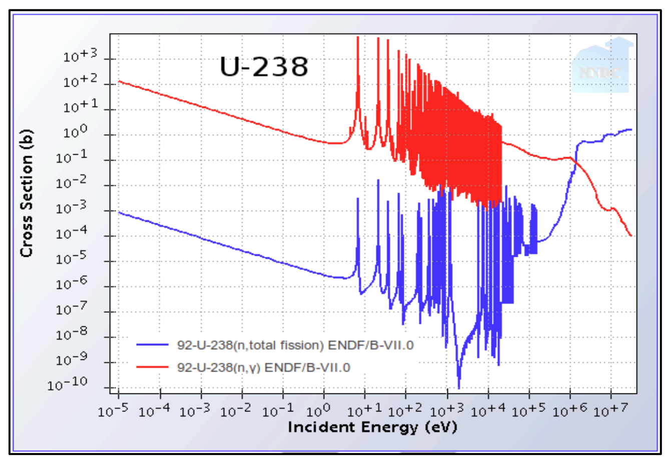
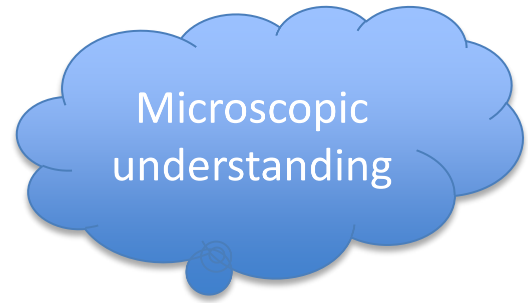
Fission

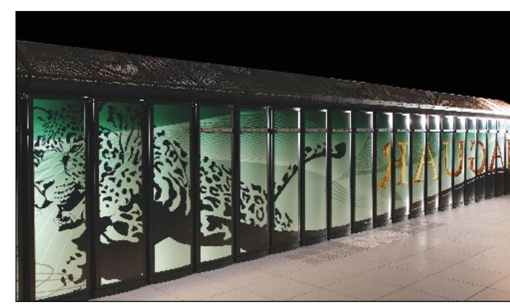




Experimental results



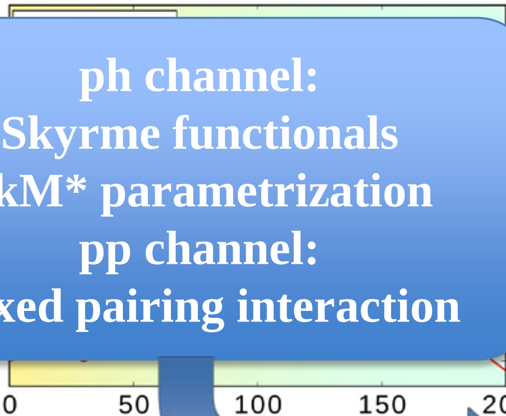




Fission: our strategy

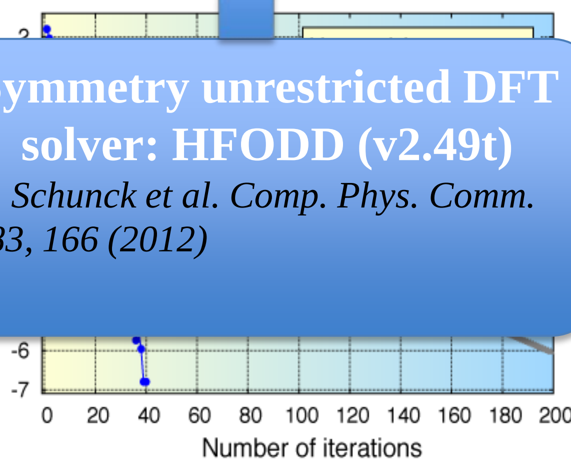
Stability of the heaviest nuclei, r-process, advanced fuel cycle

Quality Input → Large-scale Simulations on Leadership-class Computers → Dynamics



ph channel:
Skyrme functionals
SkM* parametrization
pp channel:
mixed pairing interaction

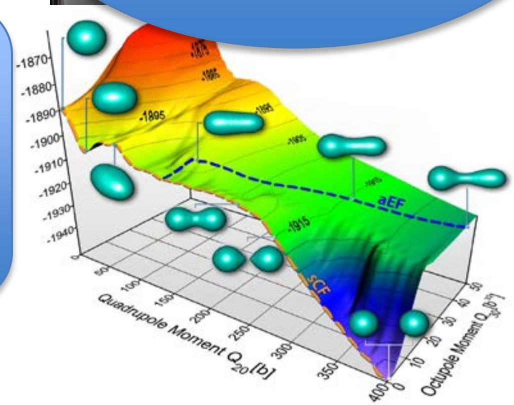
Numeric

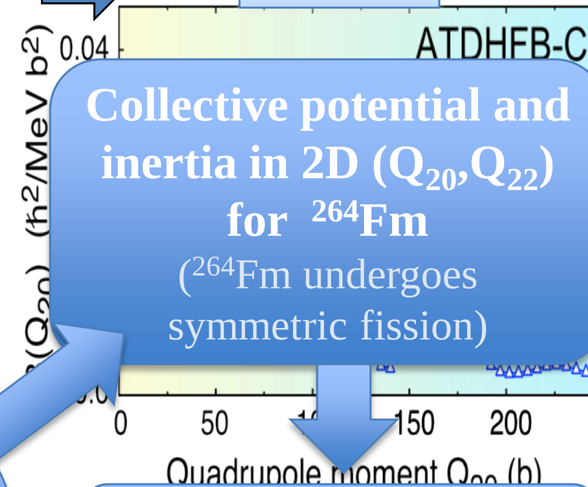


Symmetry unrestricted DFT solver: HFODD (v2.49t)

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

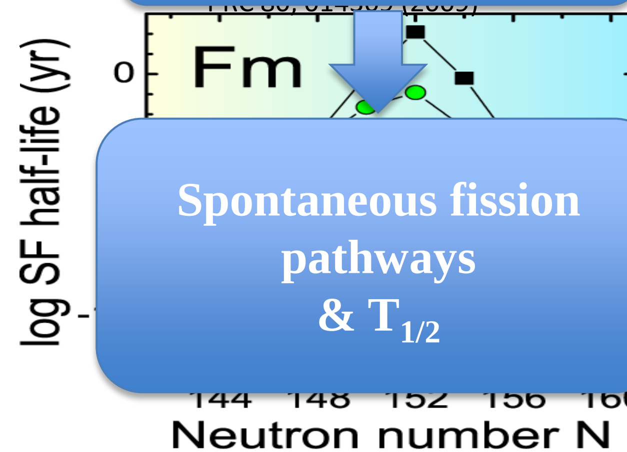
HFB for potential
ATDHFB for cranking inertia





Collective potential and inertia in 2D (Q_{20},Q_{22}) for ^{264}Fm
(^{264}Fm undergoes symmetric fission)

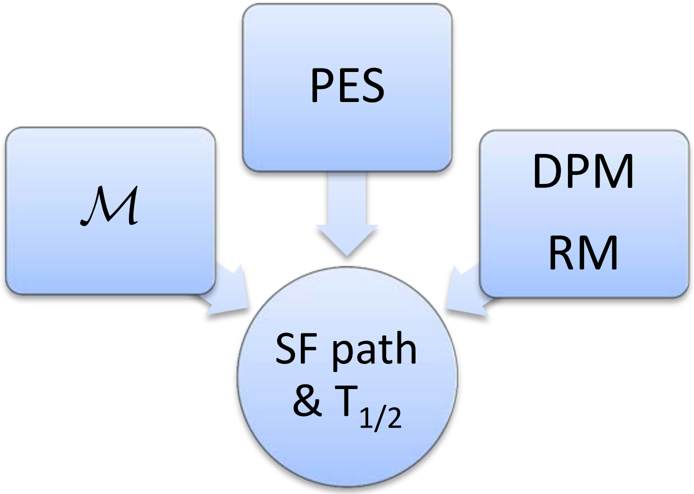
Action minimization technique



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

Plan

- ❑ Hetree-Fock-Bogoliubov (HFB) method → Potential Energy Surface (PES)
- ❑ Adiabetic Time Dependent HFB formalism → Collective Inertia ($\mathcal{M}$)
- ❑ Action minimization techniques → Dynamic Programing Method (DPM) / Ritz Method (RM)



❑ Results: Spontaneous Fission (SF) paths and Half-lives ($T_{1/2}$)

HFB formalism

P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, Berlin, 1980)

HFB equation

$$[\mathcal{W}, \mathcal{R}] = 0$$

Generalized density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

Single particle Routhian

Pairing potential

$$\mathcal{W} = \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}$$

Chemical potential

Non-linear eigenvalue equation

$$\mathcal{W}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} E$$

E → Diagonal matrix of quasiparticle energies

A, B are quasiparticle wavefunctions

Particle density $\rho = B^* B^T$ $\quad h = T + \Gamma_{ph}[\rho] + constraint(< Q >)$

Pairing density $\kappa = B^* A^T$ $\quad \Delta = \Gamma_{pp}[\kappa] = f\kappa$

Paring form factor

Calculation can be constraint at a particular value of quadrupole moment <Q>

Converged solutions Á$_0$ & º$_0$ are achieved after solving HFB equation iteratively

$$E_{tot}(Q) = Tr(T\rho_0) + Tr(\Gamma_{ph}[\rho_0]\rho_0) + Tr(\Gamma_{pp}[\kappa_0]\kappa_0) + Coulomb$$

Calculated potential energy

$\Gamma[\rho]$ → Skyrme functional with SkM* parametrization

optimized for fission barrier

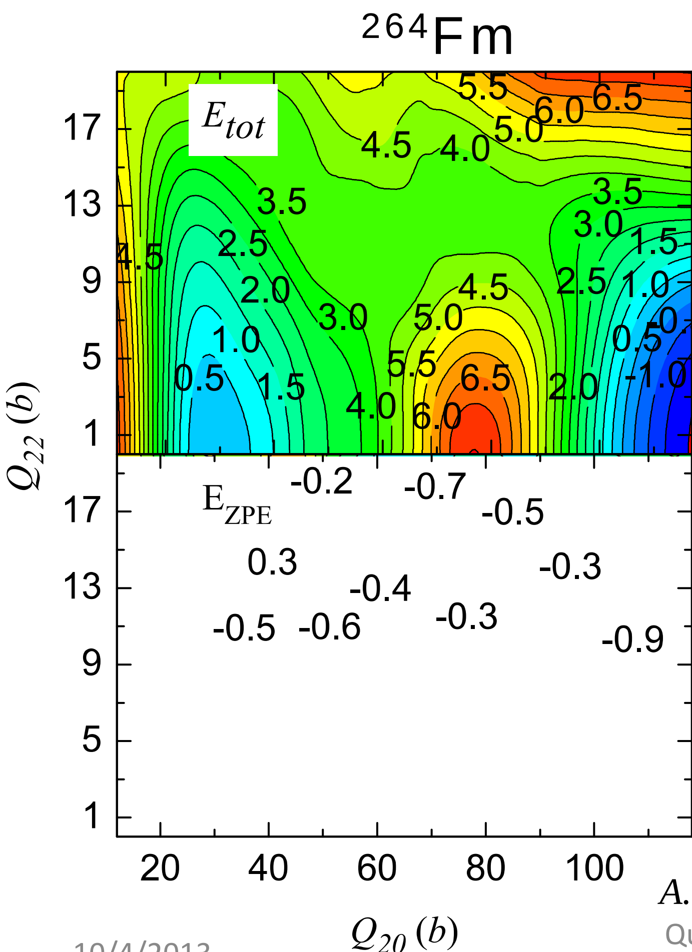
J. Bartel et al. Nucl. Phys. ***A*** *386, 79 (1982)*

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

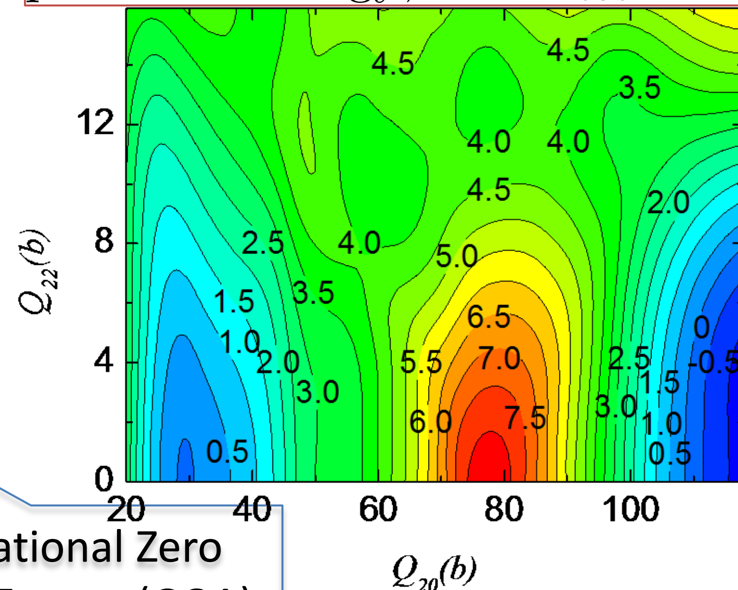
J. Dobaczewski et al. Eur. Phys. J. A, 15, ***21*** *(2002)*

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

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



potential energy, $V = E_{tot} - E_{ZPE}$



Vibrational Zero Point Energy (GOA)

A. Staszczak et al. Nucl. Phys. ***A*** *504, 589 (1989)*

ATDHFB formalism

……talk by J. Dobaczewski

Introducing dynamics :-

<u>TDHFB</u>

$$i\dot{\mathcal{R}}(t) = [\mathcal{W}, \mathcal{R}(t)]$$

Adiabatic approximation :-

M. Baranger M. Veneroni, Ann. Phys. ***114****, 123 (1978)*

$$\mathcal{R}(t) = e^{(i/\hbar)\chi(t)}\mathcal{R}_0(t)e^{-(i/\hbar)\chi(t)} \qquad \mathcal{R}_0, \chi \text{ time-even}$$

(dynamics is quasi-stationary)

Expansion in powers of collective momentum χ

time-even odd even

$$\mathcal{R} = \mathcal{R}_0 + \mathcal{R}_1 + \mathcal{R}_2 + \ldots$$

$$\mathcal{W} = \mathcal{W}_0 + \mathcal{W}_1 + \mathcal{W}_2 + \ldots$$

<u>ATDHFB</u>

$$1.\ \ i\dot{\mathcal{R}} = [\mathcal{W}_0, \mathcal{R}_1] + [\mathcal{W}_1, \mathcal{R}_0],$$

$$2.\ \ i\dot{\mathcal{R}}_1 = [\mathcal{W}_0, \mathcal{R}_0] + [\mathcal{W}_0, \mathcal{R}_2] + [\mathcal{W}_1, \mathcal{R}_1] + [\mathcal{W}_2, \mathcal{R}_0]$$

↓

J. Dobaczewski J. Skalski, Nucl. Phys. A ***369****, 123 (1981)*

Comparing with the classical expression of KE

Collective Inertia:-

$$\mathcal{M}_{ij} = \frac{i}{2\dot{q}_j} Tr\left(\frac{\partial \mathcal{R}_0}{\partial q_i}[\mathcal{R}_0, \mathcal{R}_1]\right)$$

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

$q_i s$ are collective coordinates, quadrupole moment Q for the present purpose

Calculated Inertia

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

After a few steps:-

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

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

$$-F^{i*} = \left(B^T \frac{\partial \rho_0}{\partial q_i} A + B^T \frac{\partial}{\partial} \right. \quad \ldots Z^i + Z^i E + E_1$$

A, B are quasipart… …siparticle energies

…ated to $\mathcal{W}_1$

Derivatives of densitie… using Lagrange thre… …d densities to calculate E_1)

Cranking Approxim…

$$\ldots {}^i_{\alpha\beta} F^{j*}_{\alpha\beta} \Big) \quad \ldots_\beta$$

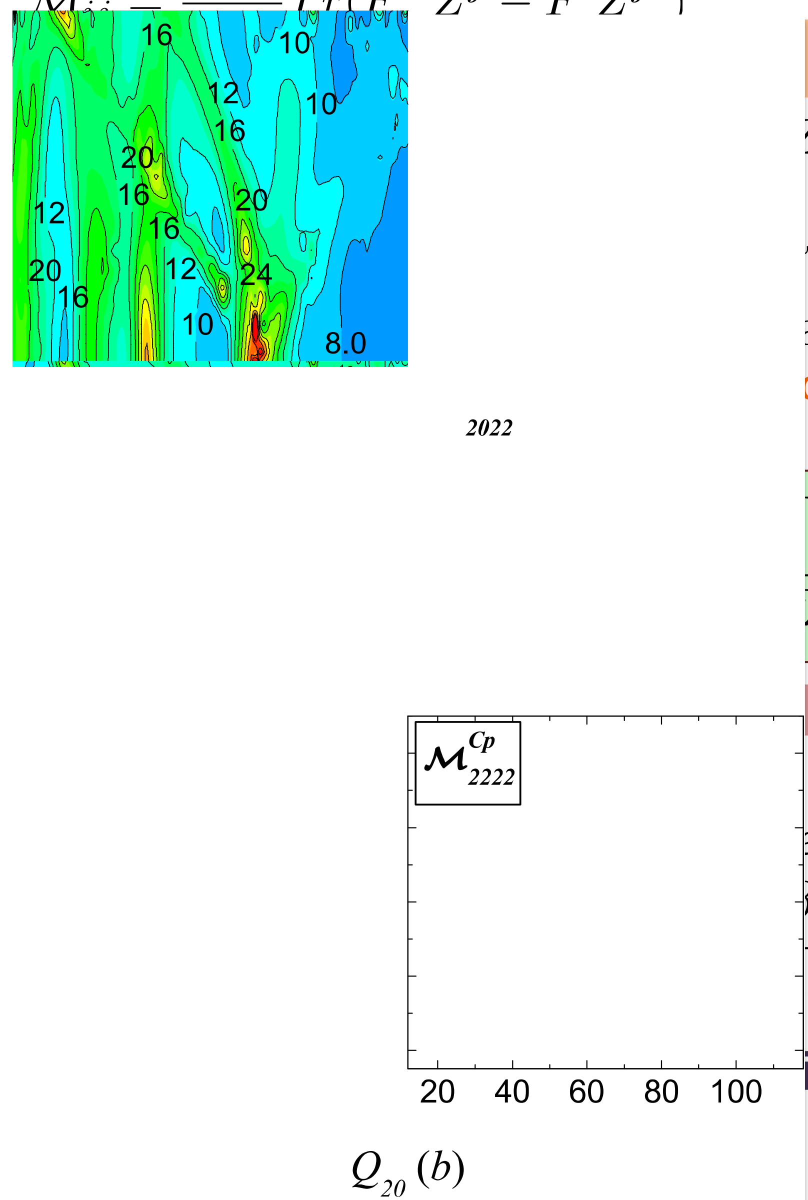
!!

more simplified way (pe… …es

Derivatives calculat…

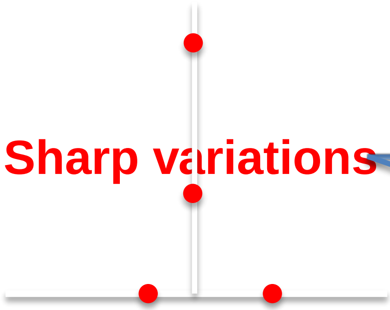
$$\mathcal{M}^{Cp} = \hbar^2 [M^{(1)}]^{-} \ldots \quad \ldots \rangle\langle\alpha\beta|\hat{Q}^\dagger_j|0\rangle \Big/ (\ldots + E_\beta)^k$$

W… …imes



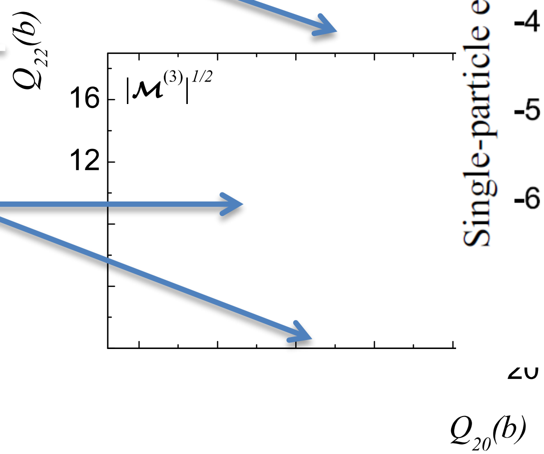
Understanding calculated Inertia

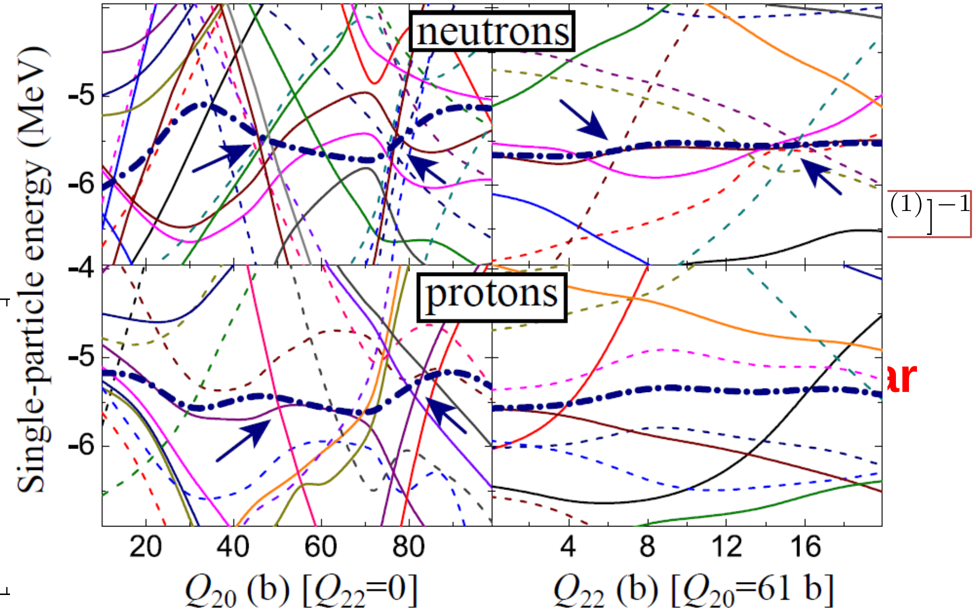
$$|\mathcal{M}|^{1/2} = (\mathcal{M}_{11}\mathcal{M}_{22} - \mathcal{M}_{12}^2)^{1/2}$$ → Invariant under rotation in 2D



Sharp variations

variations similar to $|M^C|$





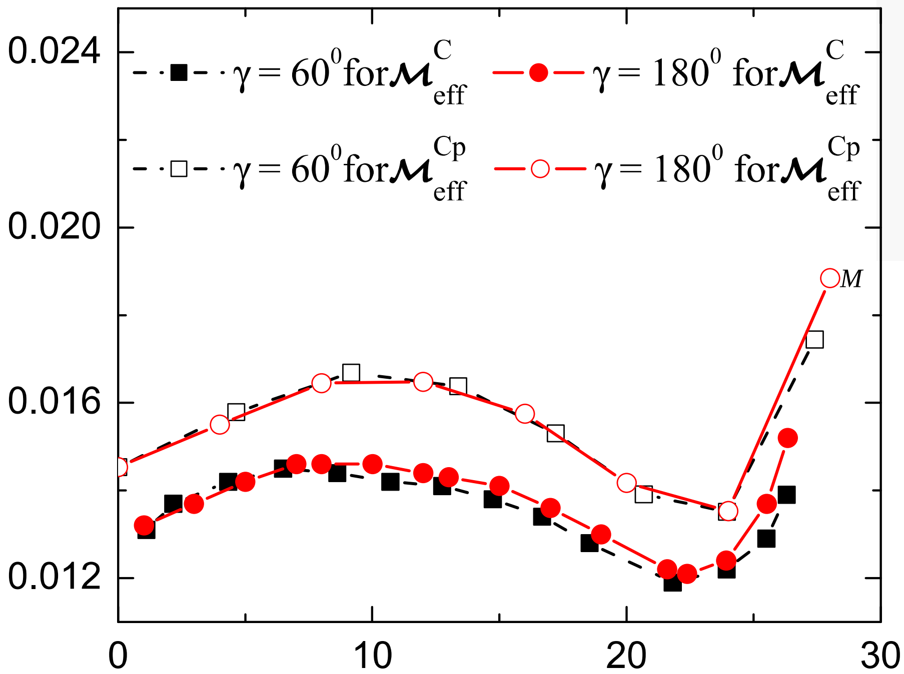
Unit = $10^{-3}\ \hbar^2/\mathrm{MeVb}^2$

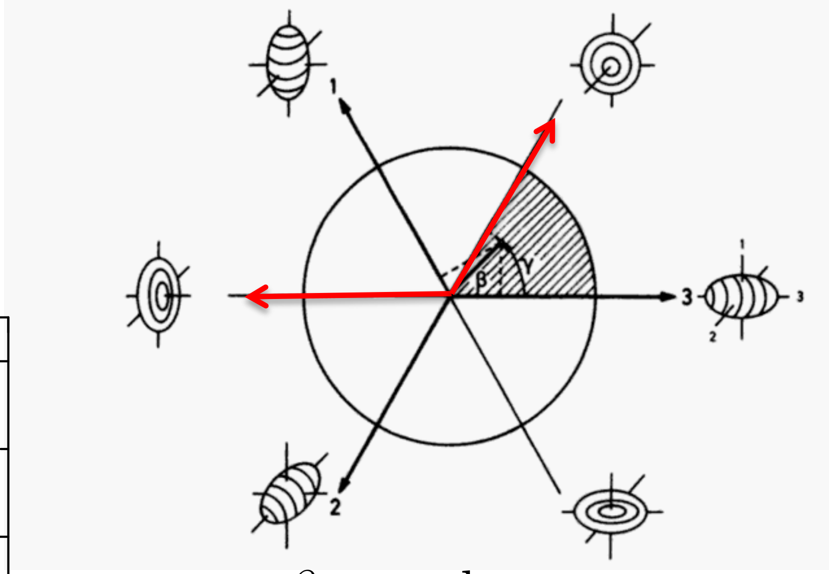
Large fluctuations of mass parameters are manifestations of crossings of single-particle levels near the Fermi energy

Numerical test

$$\mathcal{M}_{\mathrm{eff}}(s) = \sum_{ij} \mathcal{M}_{ij} \frac{dq_i}{ds}\frac{dq_j}{ds}$$

's' describes the path on 2D surface





$\beta - \gamma$ plane

Step 1:

$\mathcal{M}_{\mathrm{eft}}$ is calculated along $\gamma = 180^0$

Step 2:

Densities are rotated by Proper Eulerian angles

Step 3:

$\mathcal{M}_{\mathrm{eft}}$ is calculated along $\gamma = 60^0$

Spontaneous fission half-life

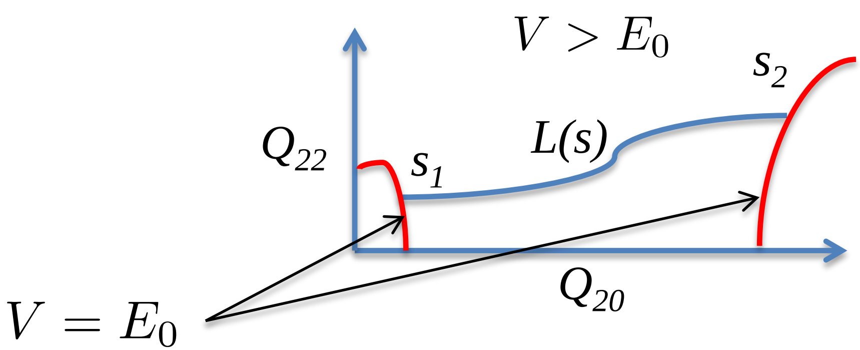
A. Baran, Phys. Lett. B ***76****, 8 (1978)*

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

n is the number of assaults on the fission barrier per unit time ≈ $10^{20.38}$ s^{-1}

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

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



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

Action minimization techniques

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

Two numerical methods → Ritz method (RM)
→ Dynamic programing method (DPM)

Ritz method (RM):-

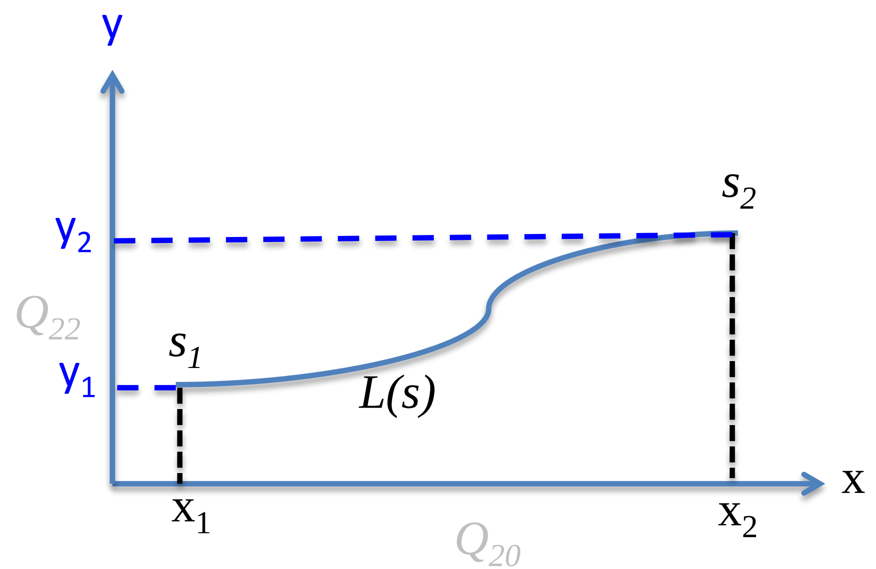
$$y(L) = \sum_k a_k \sin\left(\pi k \frac{x - x_1}{x_2 - x_1}\right) + \text{b.c.}$$

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

$$S(L) = \int_{s_1}^{s_2} \frac{1}{\hbar}\left[2\mathcal{M}_{\text{eff}}(s)\left(V_{\text{eff}}(s) - E_0\right)\right]^{1/2} ds$$

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

path is decided by varying a_i s

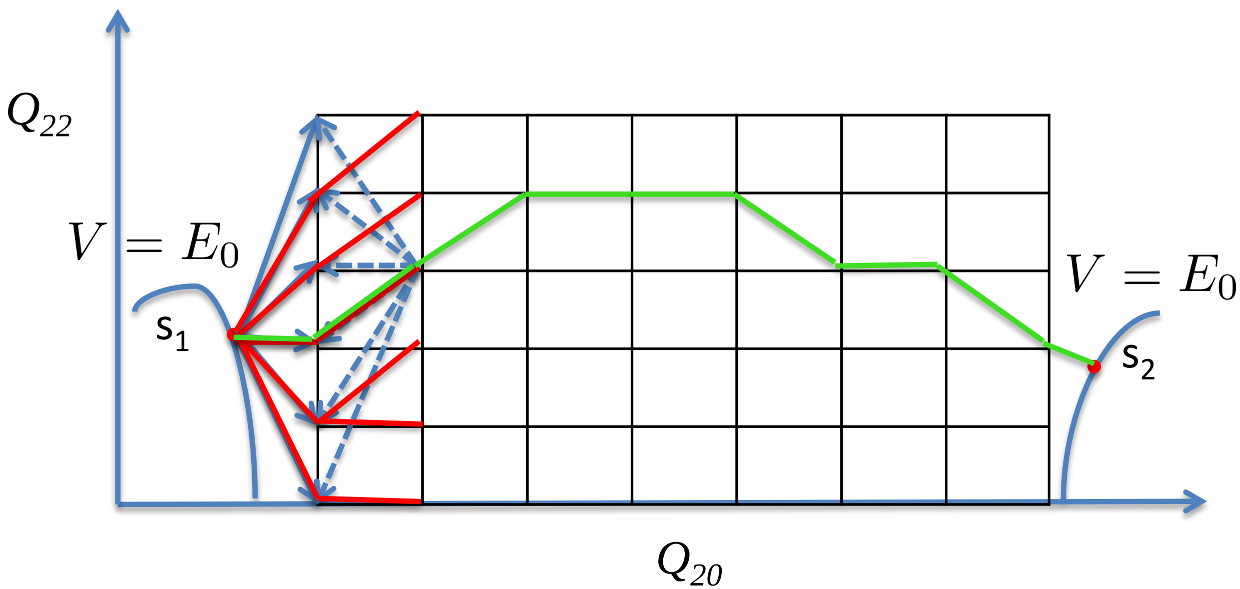


For the present calculation a_1,a_2 and a_3 are sufficient

Action minimization techniques

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

Dynamic programing method (DPM) :-



Select s_1 & s_2

Surface between s_1 & s_2 is divided into 2D mesh

S is calculated between s_1 & each point in 1^{st} column

S is calculated for each point in 2^{nd} column with all points in 1^{st} column

&

Minimum action path is retained

Repeated for all points in column 2:- minimum action paths up to column 2

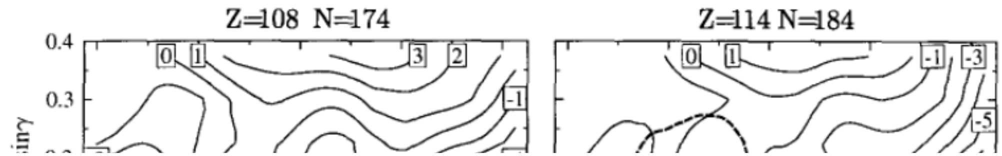
Repeated for all columns

Finally we get the minimum action path between s_1 & s_2

Results(existing)

*R. A. Gherghescu et. al. Nucl. Phys. A **651**, 237 (1999)*

242 R.A. Gherghescu et al./Nuclear Physics A 651 (1999) 237–249



Macroscopic-microscopic calculation

5. Conclusions

Non-axial quadrupole shapes seem to play a minor role in the spontaneous fission of the SHE nuclei around $^{298}114$, in spite of the fact that they can considerably lower the static fission barriers. Fission paths which exploit a non-axial saddle are rather long. The probability of the occurrence of triaxial fission trajectories is reduced by the tendency towards the minimal length of the fission path, following from the principle of the least action.

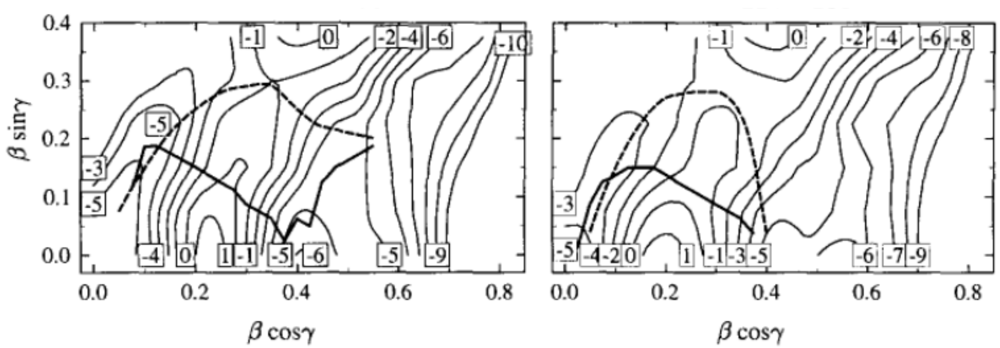
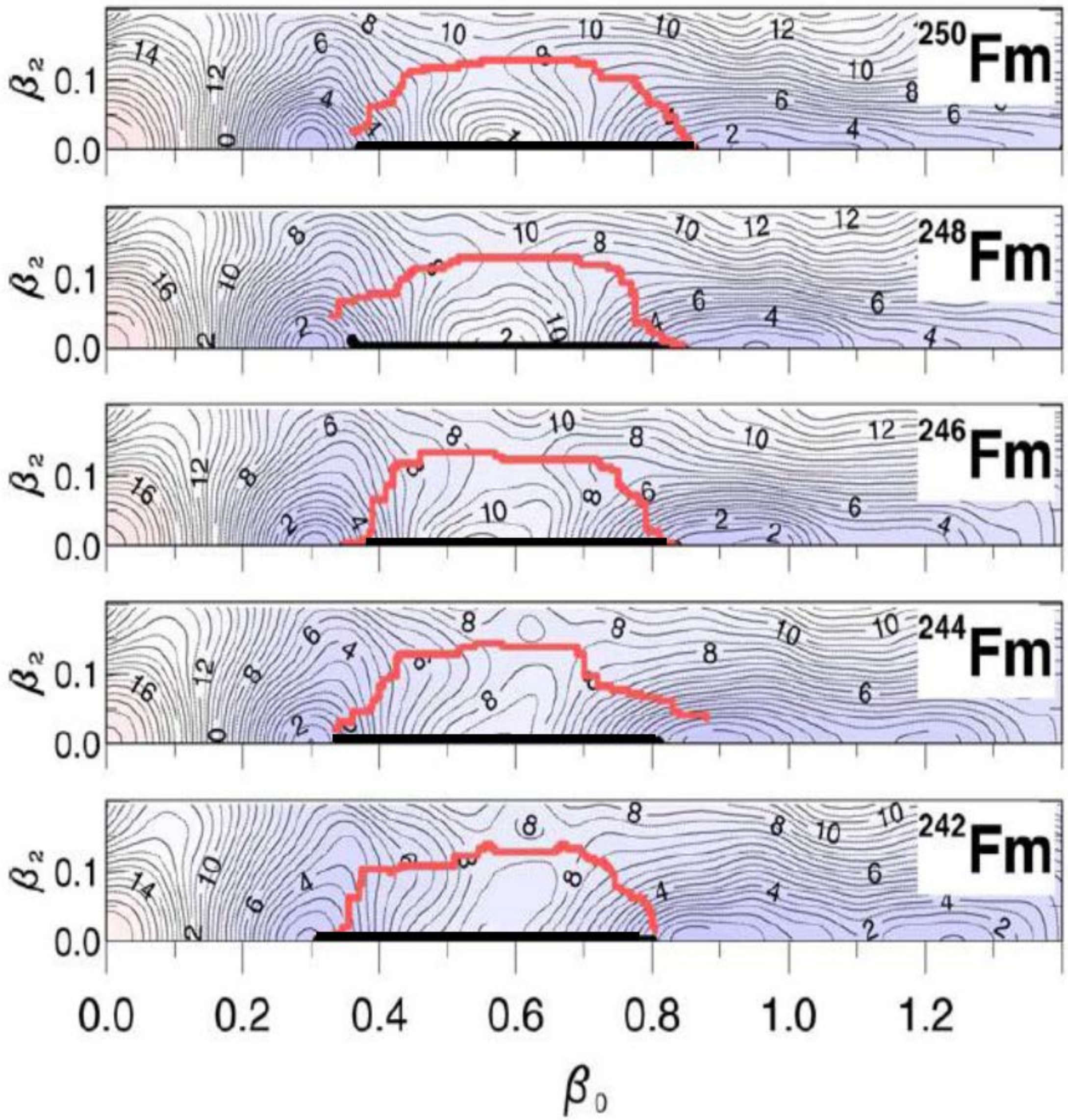


Fig. 1. The energy contour maps with drawn static (dashed) and dynamic (solid) fission trajectories for selected systems. The minimization over β_4 was performed at each (β, γ). Contour lines are 1 MeV apart. Provided contour labels help to reveal topography.

Results(existing)

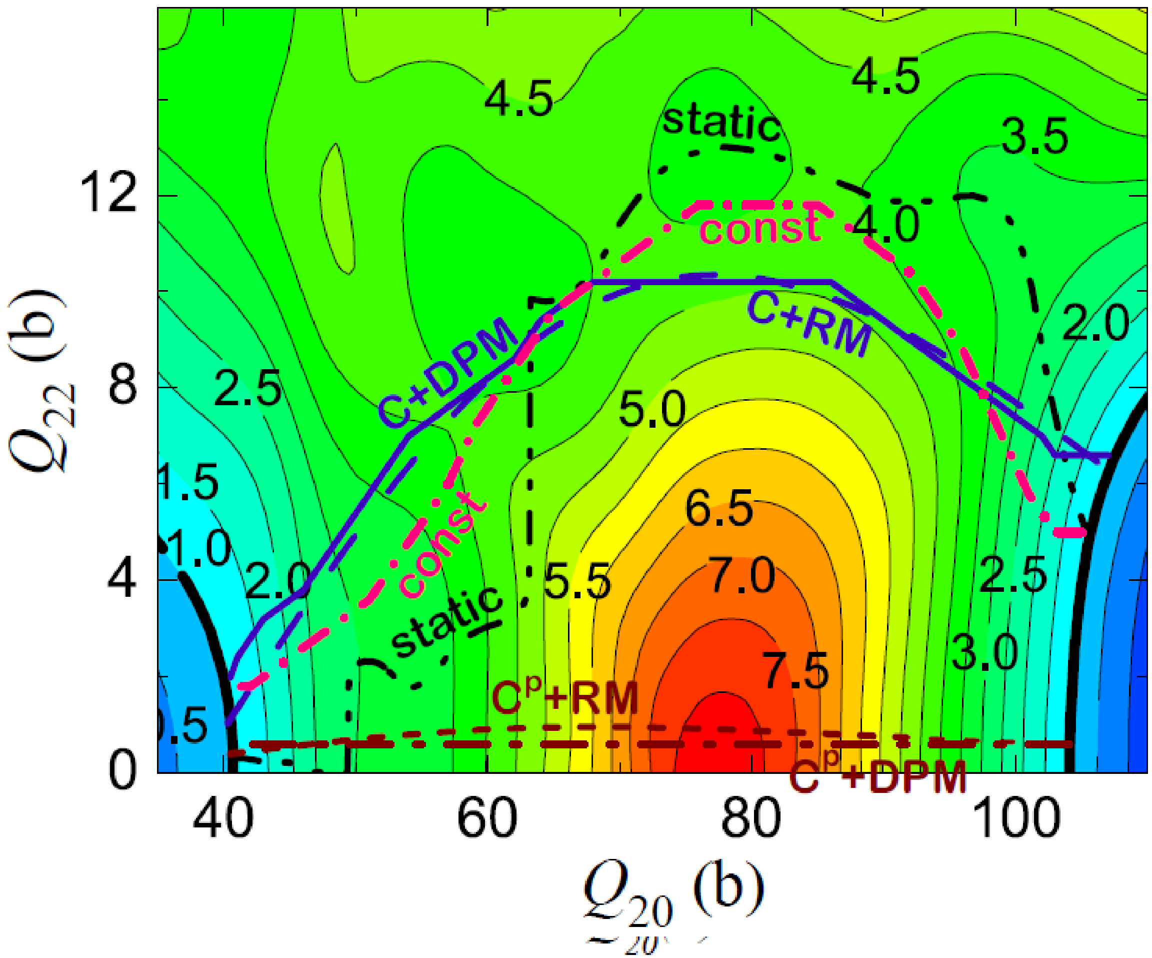
J.-P. Delaroche [a], M. Girod [a,*], H. Goutte [a], J. Libert [b] Nuclear Physics A 771 (2006) 103–168



Microscopic HFB calculation
With
Perturbative-cranking inertia

$\mathcal{M}^{Cp}$

Results(present calculation)



E_0 = 1.0 MeV

Static path (minimum potential path)

Dynamic path with cont. M
$\mathcal{M} = \mathcal{M}^{Cp}_{2020}$ at ground state
(DPM)

Dynamic path with M^C (DPM & RM)

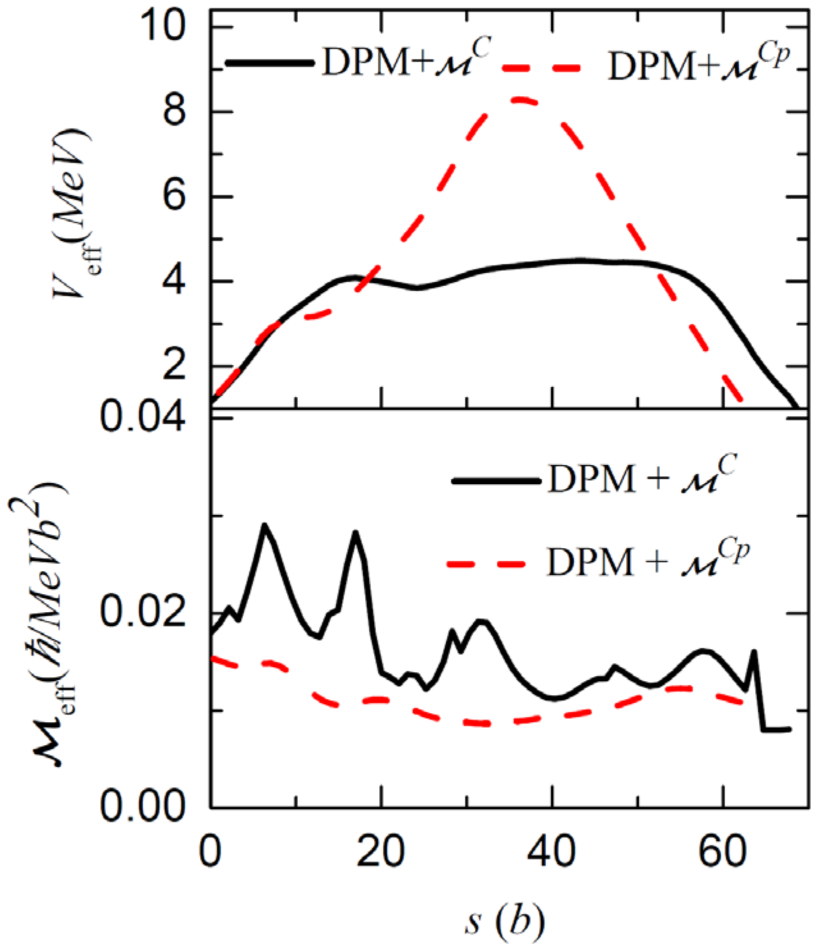
Dynamic path with M^{Cp} (DPM & RM)

Dynamical effects due to action minimization is not very prominent

With M^C :- dynamics is favoring triaxial saddle, similar to static path

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

Results(present calculation)



path	$S(L)$	$\log(T_{1/2}/\text{yr})$
Static+$\mathcal{M}^{C}$	23.4	-7.7
Static+$\mathcal{M}^{Cp}$	20.8	-10.0
DPM+$\mathcal{M}^{C}$	19.1	-11.4
RM+$\mathcal{M}^{C}$	18.9	-11.6
DPM+$\mathcal{M}^{Cp}$	16.8	-13.4
RM+$\mathcal{M}^{Cp}$	16.8	-13.4

Orders of magnitude difference in $T_{1/2}$ calculated with M^{C} and M^{Cp}

Summary & conclusion

Spontaneous fission lifetimes have been studied within a dynamic approach based on the minimization of the collective action in a two-dimensional collective space of elongation and triaxiality.

A strong dynamical effect has been predicted. Although it offsets the static reduction of the inner barrier by triaxiality when the approximate perturbative cranking inertia is used, the strong effect of triaxiality is observed with the more appropriate non-perturbative cranking inertia.

A more detailed study of dynamical effects due to triaxial and refection asymmetric degrees of freedom is in progress.

Collaborators:

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J. A. Sheikh

Thank you…