Microscopic description of collective inertia and fission path for spontaneous fission

Kouhei Washiyama (CCS, Univ. Tsukuba, Japan)

筑波大学
計算科学研究センター
Center for Computational Sciences

Collaborators: Takashi Nakatsukasa, Nobuo Hinohara (CCS, Univ. Tsukuba)

Spontaneous fission—subbarrier fission

Collective inertia

Density functional theory for fission

Result: Fission for one dimension

On-going: Fission for two dimensions

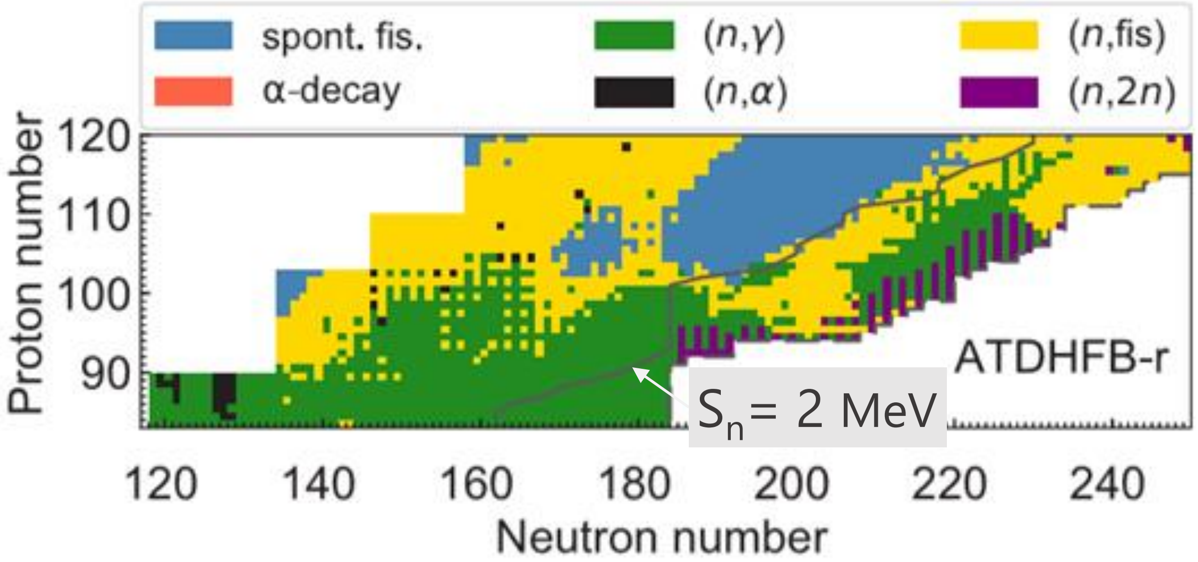
ESNT workshop: Dynamics of Nuclear Fission, Dec. 16-19, 2024@ CEA Saclay, France

Introduction: Fission and r-process

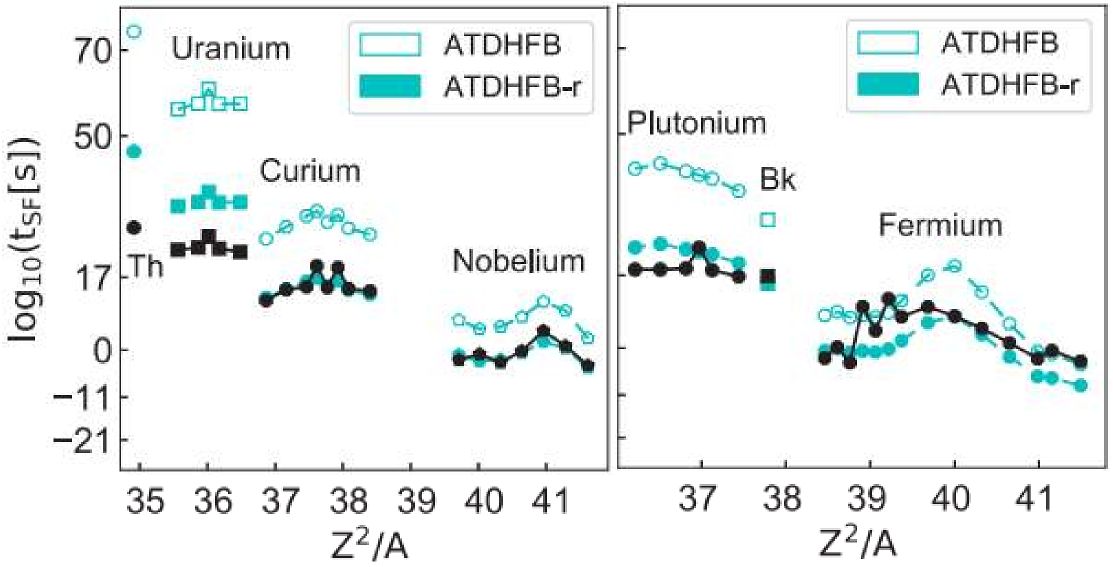
Nucleosynthesis network calculation under the r-process environment

(T= 0.9 GK, n_n= 1.0x10^{28} cm^{-3})

S.A. Giuliani, G. Martinez-Pinedo, L.M. Robledo, PRC 97, 034323 (2018)



Fission half-life



BCPM DFT

- Spontaneous fission half-life
- Neutron-induced reactions
- α decay rate

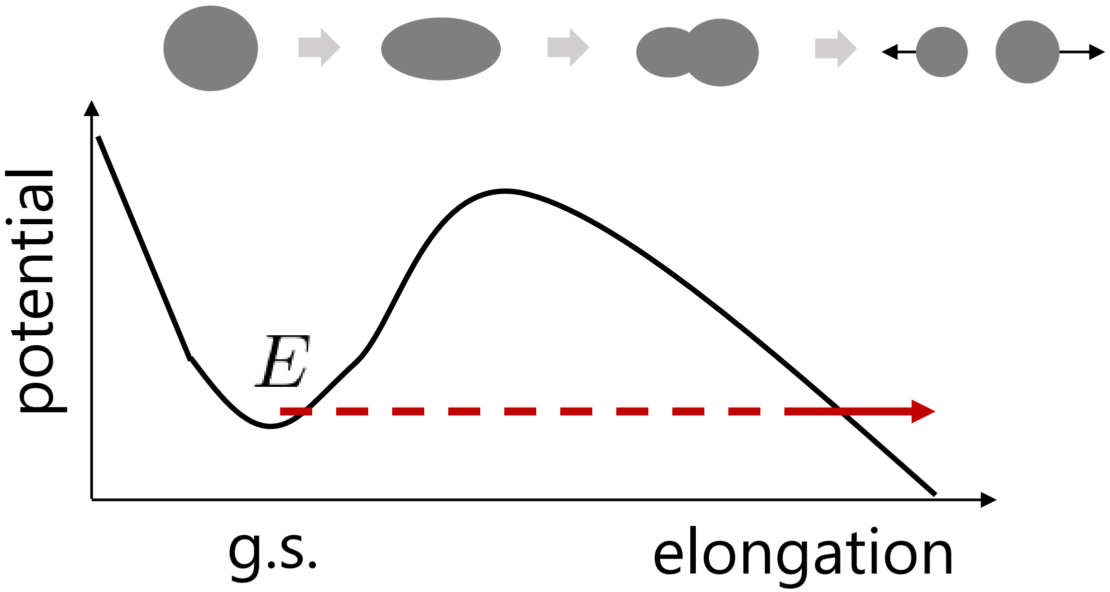
Correction to inertia

$$\mathcal{M}_r = \alpha \mathcal{M}$$

Description of spontaneous fission based on DFT

Sadhukhan et al, PRC88, 064314 (2013), etc.

Fission barrier



Spontaneous fission

➡ **Tunneling in quantum many-body system**

WKB approximation

Fission half-life

$$T_{1/2} = \ln 2/(nP) \qquad P = \frac{1}{1+\exp(2S)}$$

Action *S*

$$S = \int_{s_1}^{s_2} ds \sqrt{2M(s)(V(s)-E)}/\hbar$$

s Coordinate (Q_{20} etc.)

V Potential

M **Collective inertia**

Aim of this talk

Fission observable

- Fission half-life
- Mass distribution

←

Collective inertia

characterizes the kinetic energy

Goal: correctly evaluate collective inertia M for fission half-life

$$S = \int_{s_1}^{s_2} ds \, \sqrt{2M(s)(V(s)-E)}/\hbar$$

- To develop the method for not only collective potential (fission barrier) but also collective inertia along a fission path
- To include dynamical effects of fission on collective inertia

Nuclear density functional theory (DFT)

Bender, Heenen, Reinhard, Rev. Mod. Phys. 75 (2003) 121
Nakatsukasa, Matsuyanagi, Matsuo, Yabana, RMP88(2016) 045004

Quantum many-body system

→ non-interacting reference system in one-body potential

DFT is an exact theory

Its functional form is unknown

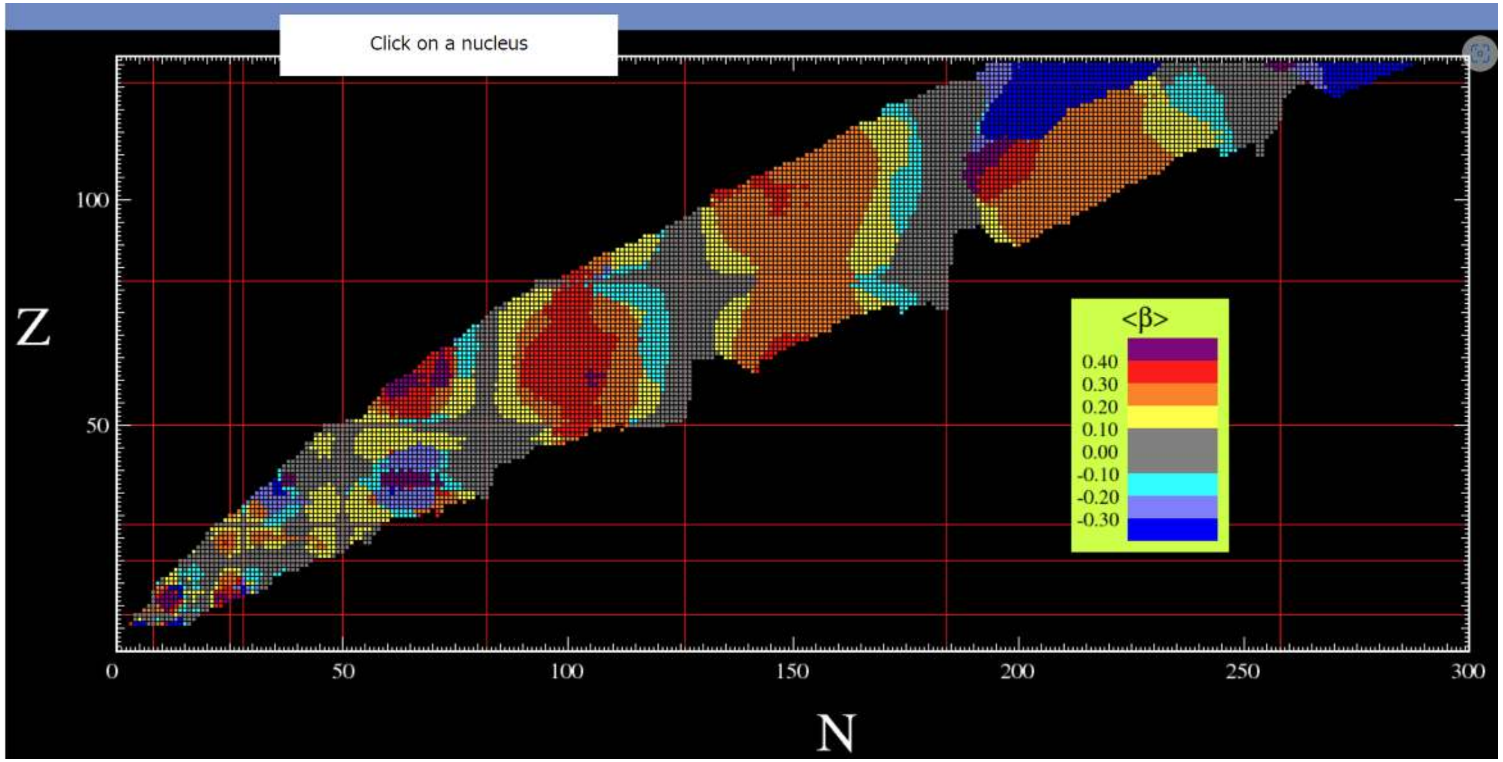
Gogny, Skyrme, Covariant, etc.

$$\mathcal{E}(\rho, \kappa, \kappa^*)$$

Good description for

- ✓ Ground state property
- ✓ Shell effect
- ✓ Deformation

https://www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire_eng.htm



Collective inertia in density functional theory (DFT)

DFT + Cranking approximation

Prochniak et al., NPA730 (2004) 59
Delaroche et al., PRC81 (2010) 014303
Baran et al., PRC84, 054321 (2011)
Sadhukhan et al, PRC88, 064314 (2013)
Giuliani and Robledo, PLB 787, 134 (2018)

Skyrme, Gogny, Relativistic EDFs

Low computation cost

Problem: Neglect dynamical effects (time-odd terms)

$$\mathcal{M}^{\rm PC} = \frac{1}{2}[M^{(1)}]^{-1}M^{(3)}[M^{(1)}]^{-1}$$

$$M_{ij}^{(n)} = \sum_{\mu<\nu}\frac{\langle\phi(s)|\hat{s}_i|\mu\nu\rangle\langle\mu\nu|\hat{s}_j^\dagger|\phi(s)\rangle}{(E_\mu+E_\nu)^n}$$

Note: Dynamical effects reproduce the collective inertia for translational motion

Perturbative cranking approximation

$$\mathcal{M}^{\rm PC} = \frac{1}{2}[M^{(1)}]^{-1}M^{(3)}[M^{(1)}]^{-1}$$

$$M_{ij}^{(n)} = \sum_{\mu<\nu}\frac{\langle\phi(s)|\hat{s}_i|\mu\nu\rangle\langle\mu\nu|\hat{s}_j^\dagger|\phi(s)\rangle}{(E_\mu+E_\nu)^n}$$

s : collective variables

ϕ : constrained HFB states

$|\mu\nu\rangle = a_\mu^\dagger a_\nu^\dagger|\phi(s)\rangle$

Collective inertia by Local QRPA

DFT + Cranking approximation

Prochniak et al., NPA730 (2004) 59
Delaroche et al., PRC81 (2010) 014303
Baran et al., PRC84, 054321 (2011)
Sadhukhan et al, PRC88, 064314 (2013)
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Our method: Local QRPA

Hinohara et al., PRC84 (2011) 061302; 85 (2012) 024323
Sato, Hinohara, NPA849 (2011) 53
Yoshida, Hinohara, PRC83 (2011) 061302

Include dynamical effects by QRPA

High computation cost ➡ Finite amplitude method

Nakatsukasa et al., PRC76, 024318(2007)
Avogadro & Nakatsukasa, PRC84, 014314(2011)

Relation between QRPA and collective inertia

$$T = \frac{1}{2} M \left(\frac{dQ_{20}}{dt} \right)^2$$

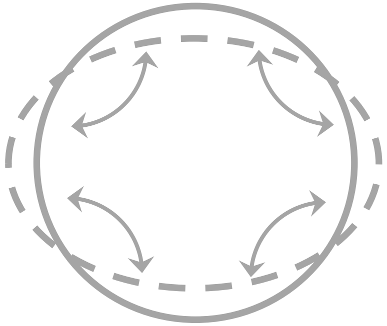
$$Q_{\lambda\mu} = r^{\lambda} Y_{\lambda\mu}$$

Collective surface vibrations

QRPA: linear response to an external field

Quadrupole
external field

$$\hat{F} = \sum_{i}^{A} r_i^2 Y_{2m}(\Omega_i)$$



Response
(strength, frequency)

Inertia associated with
collective coordinates

Local QRPA

Local QRPA for vibrational mass at each CHFB state

Hinohara et al., PRC82 (2010) 064313

$$\delta\langle\phi(s)|[\hat{H}_{\mathrm{M}}(s), \hat{Q}^i(s)] - \frac{1}{i}\hat{P}^i(s)|\phi(s)\rangle = 0$$

$$\delta\langle\phi(s)|[\hat{H}_{\mathrm{M}}(s), \frac{1}{i}\hat{P}^i(s)] - C_i(s)\hat{Q}^i(s)|\phi(s)\rangle = 0$$

s : deformation parameters

=

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} Q^i \\ -Q^{i*} \end{pmatrix} = \frac{1}{i}\begin{pmatrix} P^i \\ -P^{i*} \end{pmatrix}$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} P^i \\ -P^{i*} \end{pmatrix} = iC_i\begin{pmatrix} Q^i \\ -Q^{i*} \end{pmatrix}$$

at deformation *s*

- Low-lying collective modes

  Eigen-frequency $\hat{Q}^i,\ \hat{P}^i,\ C_i = \Omega_i^2$

- $M(s)$ **Collective inertia for quadrupole vibration**

$$\frac{\partial s_m}{\partial q^i} = \langle\phi(s)|[\hat{s}_m, \frac{1}{i}\hat{P}_i]|\phi(s)\rangle$$

$$M(s) = \frac{\partial q^1}{\partial s_1}\frac{\partial q^1}{\partial s_1} \qquad s_1 = r^2 Y_{20}$$

Finite amplitude method (FAM)

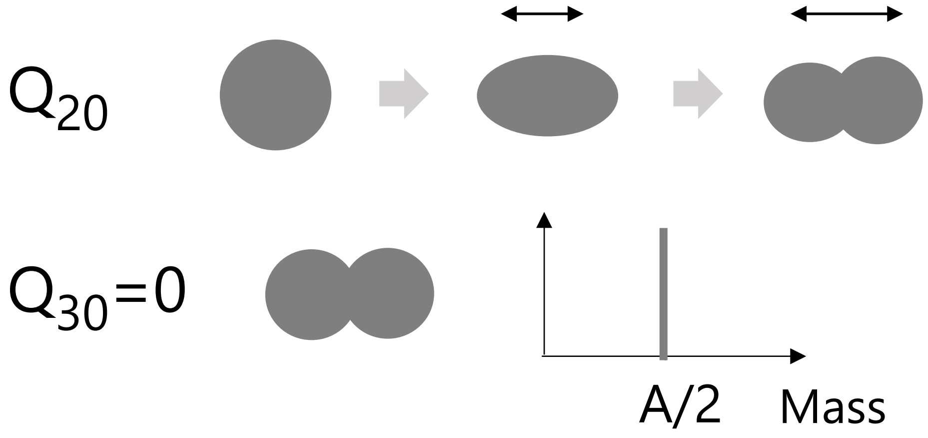
Nakatsukasa et al., PRC76 (2007) 024318
Avogadro & Nakatsukasa, PRC84, 014314

- ✓ Small computational cost
- ✓ equivalent to QRPA response

Calculation set-up

Constrained HFB along the fission path

- Constrained on Q_{20}
- Fix $Q_{30}=0$
- → symmetric fission path only
  - Box: 26 fm x 26 fm x 39 fm
  - Volume pairing, SkM* EDF
  - $E_{QP} \approx 60$ MeV



Local QRPA on constrained HFB states

- Select the most collective mode among QRPA solutions
  - Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

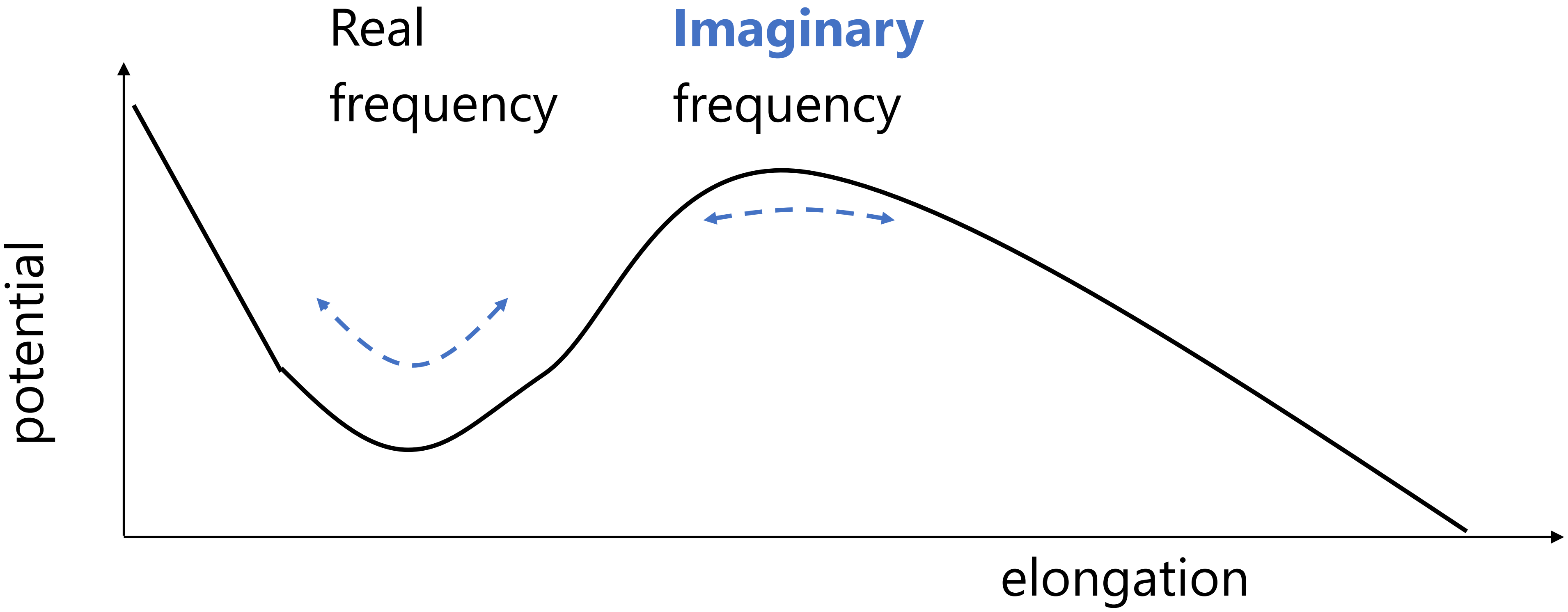
Computation time: (1000 hours+500 hours) x 50 states

This research used computational resources of OFP & Wisteria/BDEC-01 Odyssey (Univ. Tokyo), provided by the Multidisciplinary Cooperative Research Program in CCS, Univ. Tsukuba.

Solution of Local QRPA can be imaginary

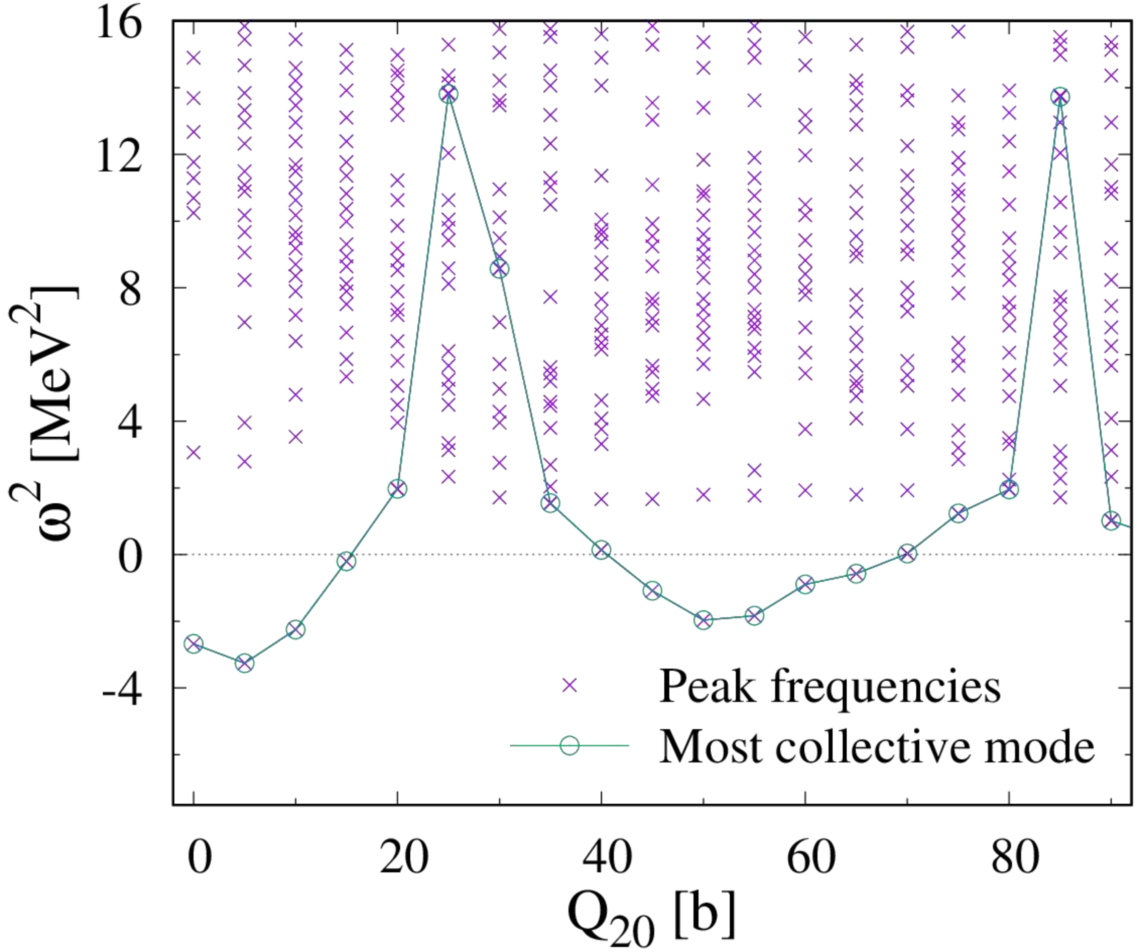
Local QRPA = QRPA on top of constrained DFT state

Eigen-frequency ⟷ Curvature of the potential



LQRPA solutions and the most collective mode

^{240}Pu, axial states

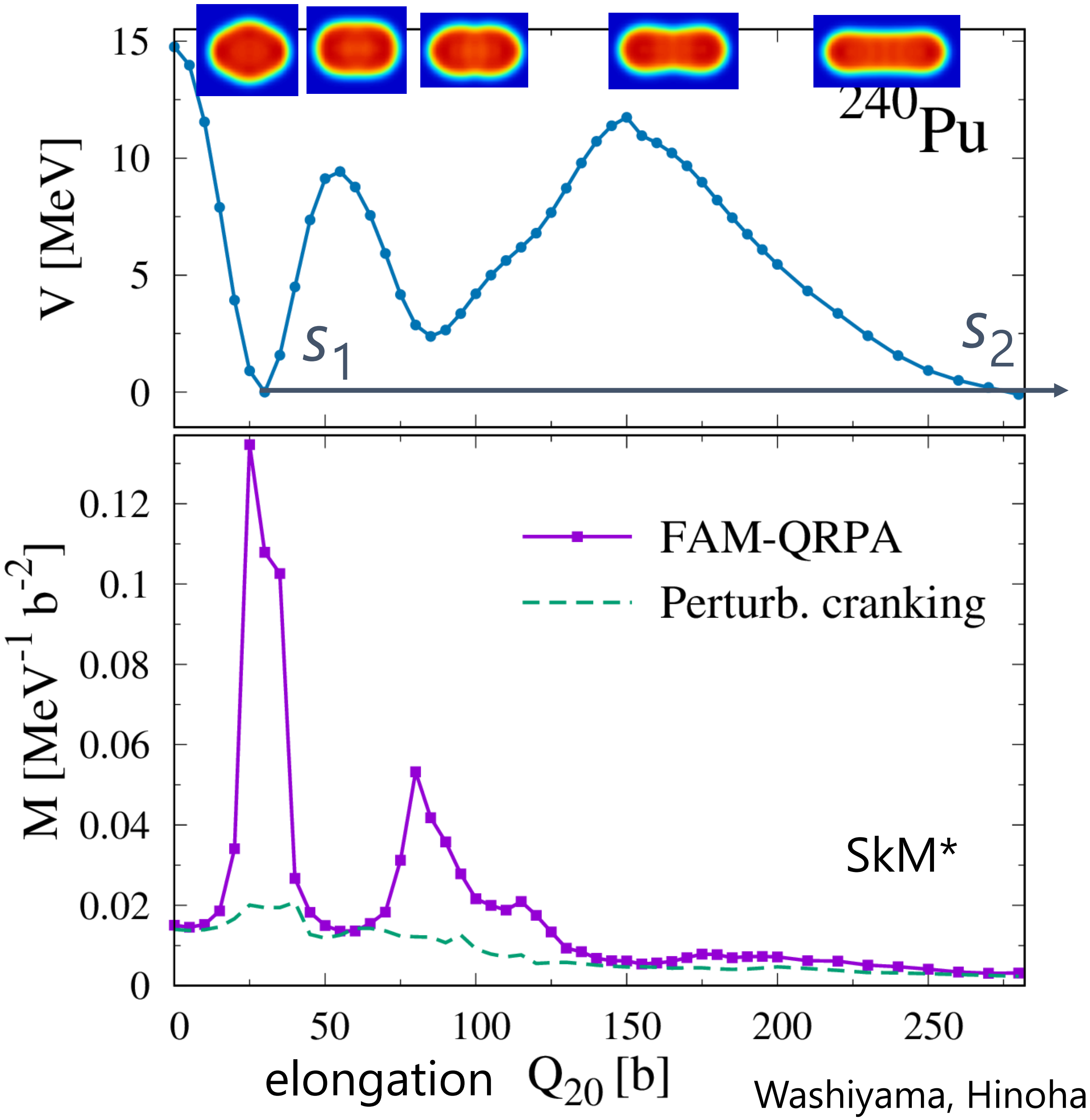


Select the most collective mode from many QRPA solutions in $\omega^2 < 16$ MeV^2

Select the smallest collective inertia M = the largest strength

Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Result: Collective inertia along fission path



- ✓ Mass symmetric fission
  - ➡ Too high second barrier
- ✓ Large change in M by QRPA
- ✓ Smooth in cranking M

Action integral S

$$S = \int_{s_1}^{s_2} ds \sqrt{2M(s)(V(s)-E)}/\hbar$$

QRPA S = **82.0**

Cranking S = **62.0**

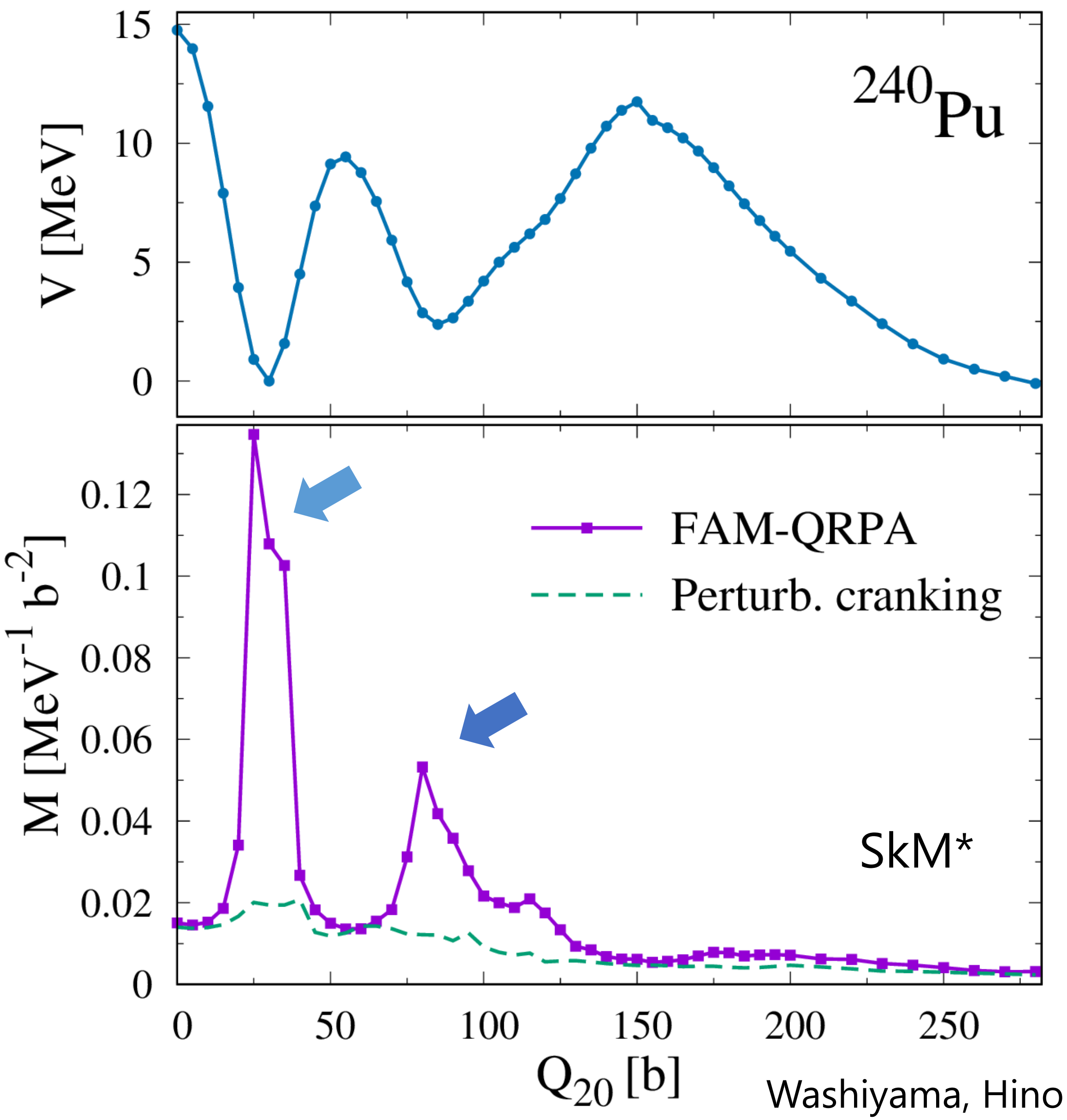
M

60000 CPU hours

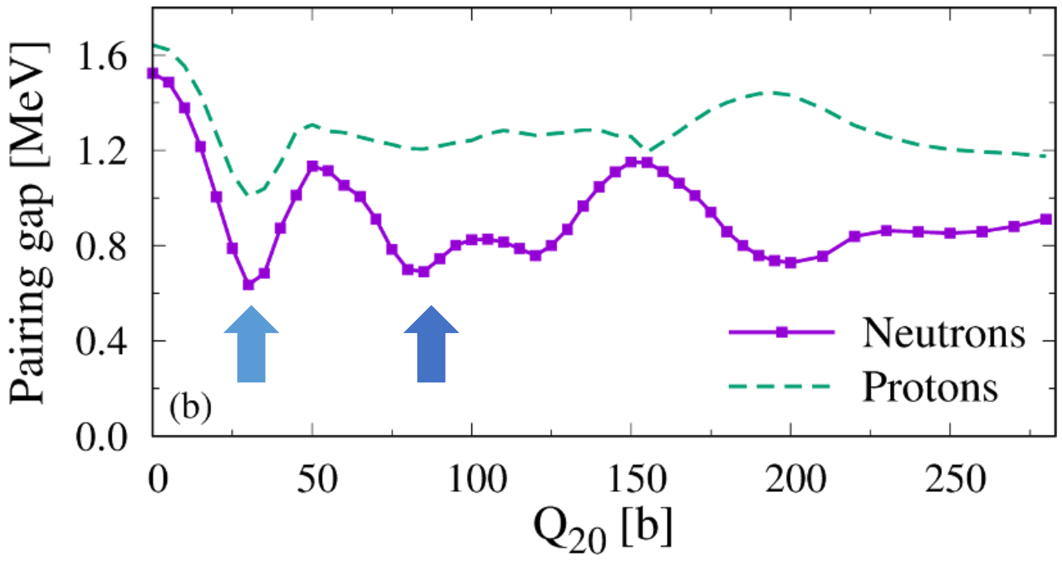
OpenMP + MPI

Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Result: Collective inertia and pairing gap



Pairing gap



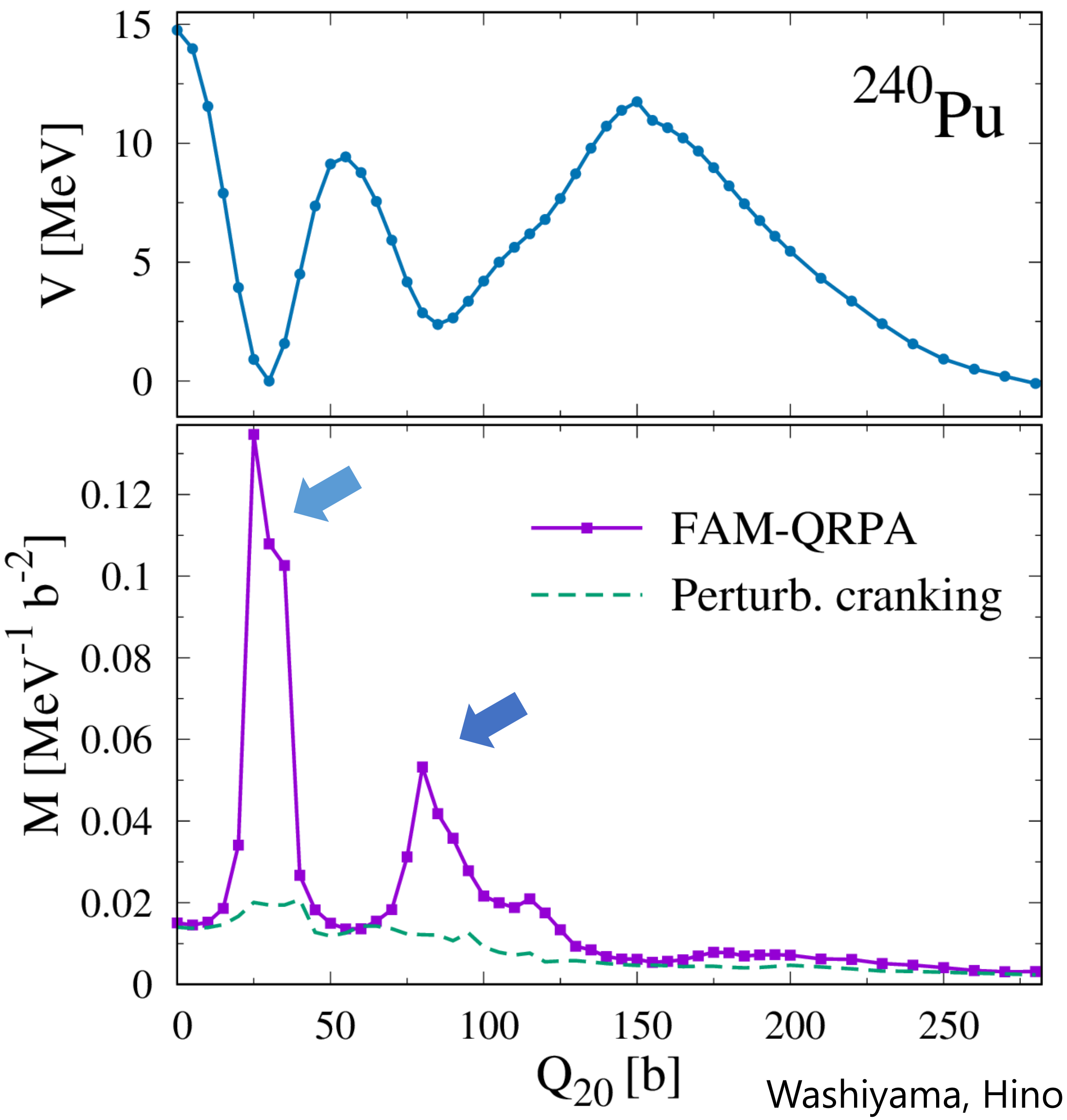
Pair gap ↘ ⟺ Inertia ↗

$$\mathcal{M} \propto \Delta^{-2}$$

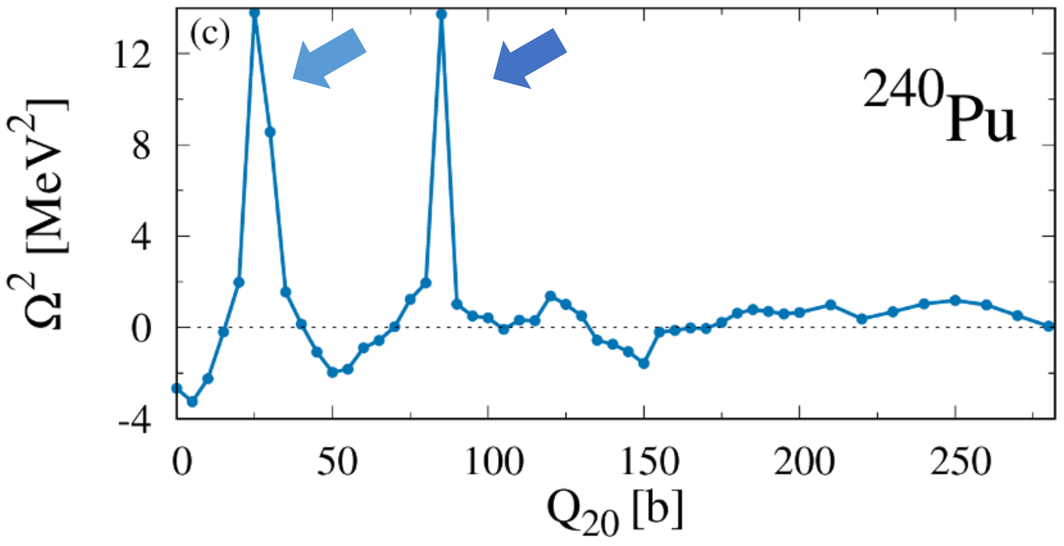
Inertia pairing gap

Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Result: Collective inertia and eigen-frequency



Eigen-frequency of LQRPA

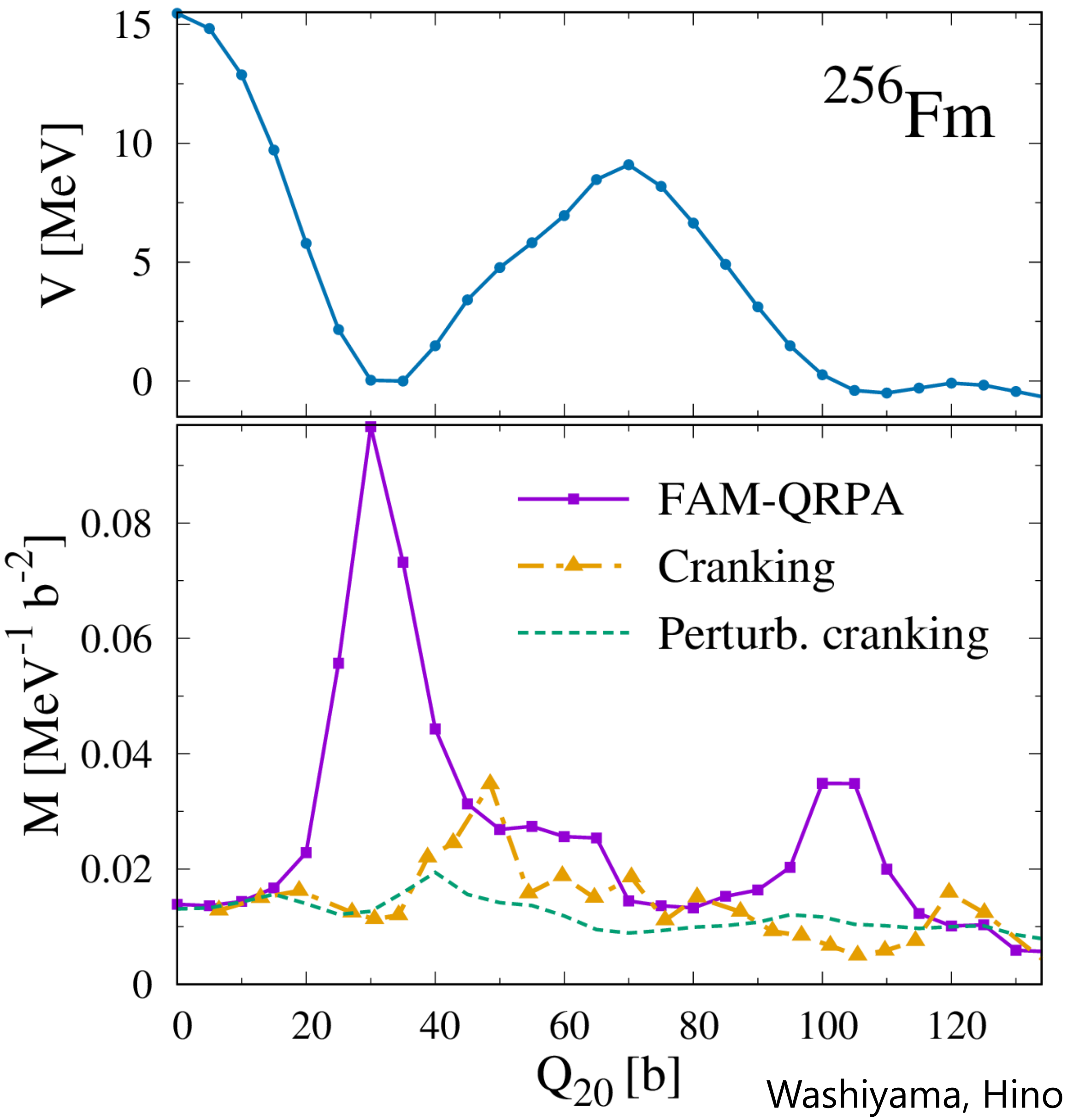


Ω^2 ↗ ⇔ **Inertia** ↗

Ω can be imaginary near the fission barrier

Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Result: Comparison to previous work: ^{256}Fm case



Non-perturbative cranking approximation

Baran et al., PRC84, 054321 (2011)

- Peak structure
- Larger inertia in QRPA

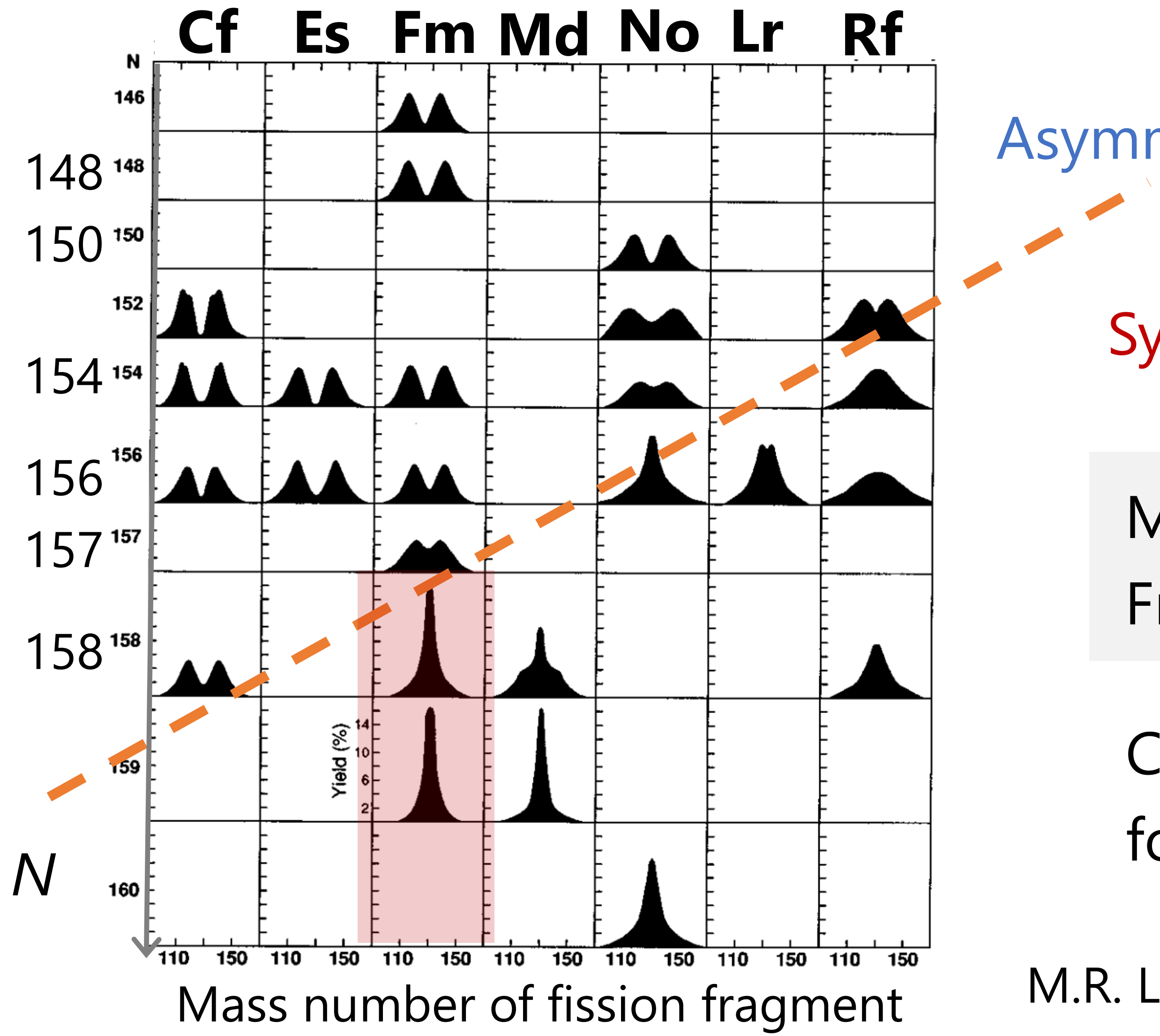
non-perturbative cranking

$$\frac{F^i}{\dot{s}_i} = U^\dagger \frac{\partial \rho}{\partial s_i} V^* + U^\dagger \frac{\partial \kappa}{\partial s_i} U^* - V^\dagger \frac{\partial \rho^*}{\partial s_i} U^* - V^\dagger \frac{\partial \kappa^*}{\partial s_i} V^*,$$

Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Experimental data of fission in the actinoid region

Mass distribution of fission fragments



Asymmetric fission

Symmetric fission

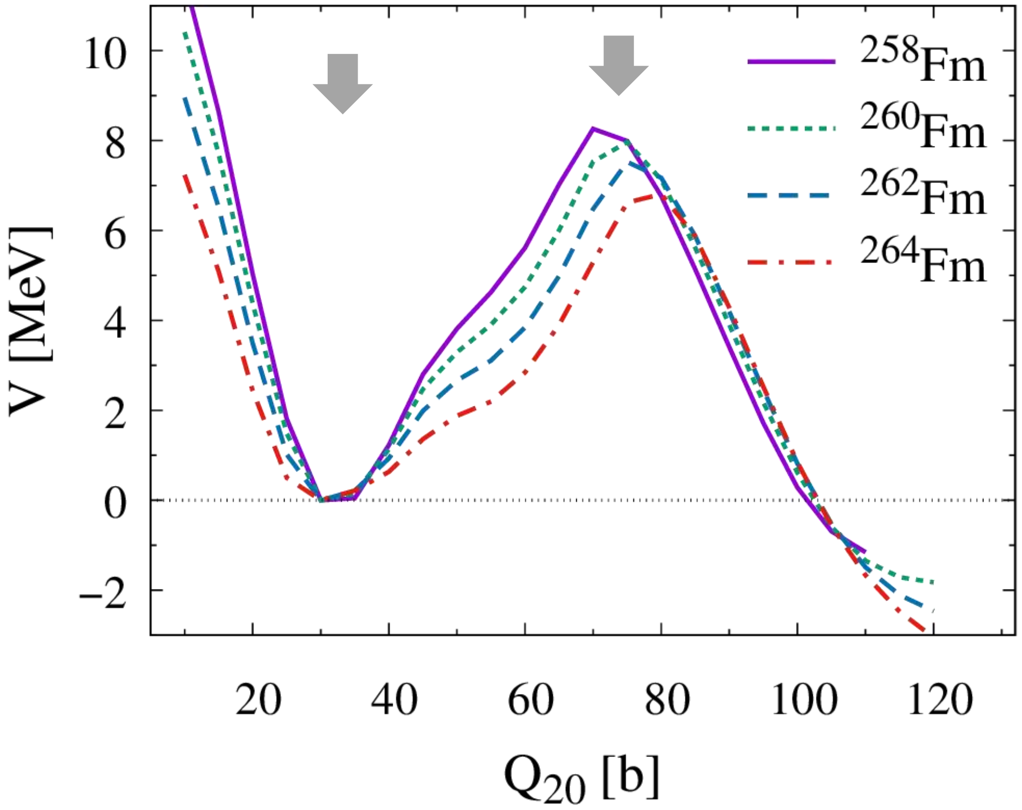
Mass symmetric fission in Fm isotopes with N ≥ 158

Calculation without Q_{30} may be sufficient for fission half-life

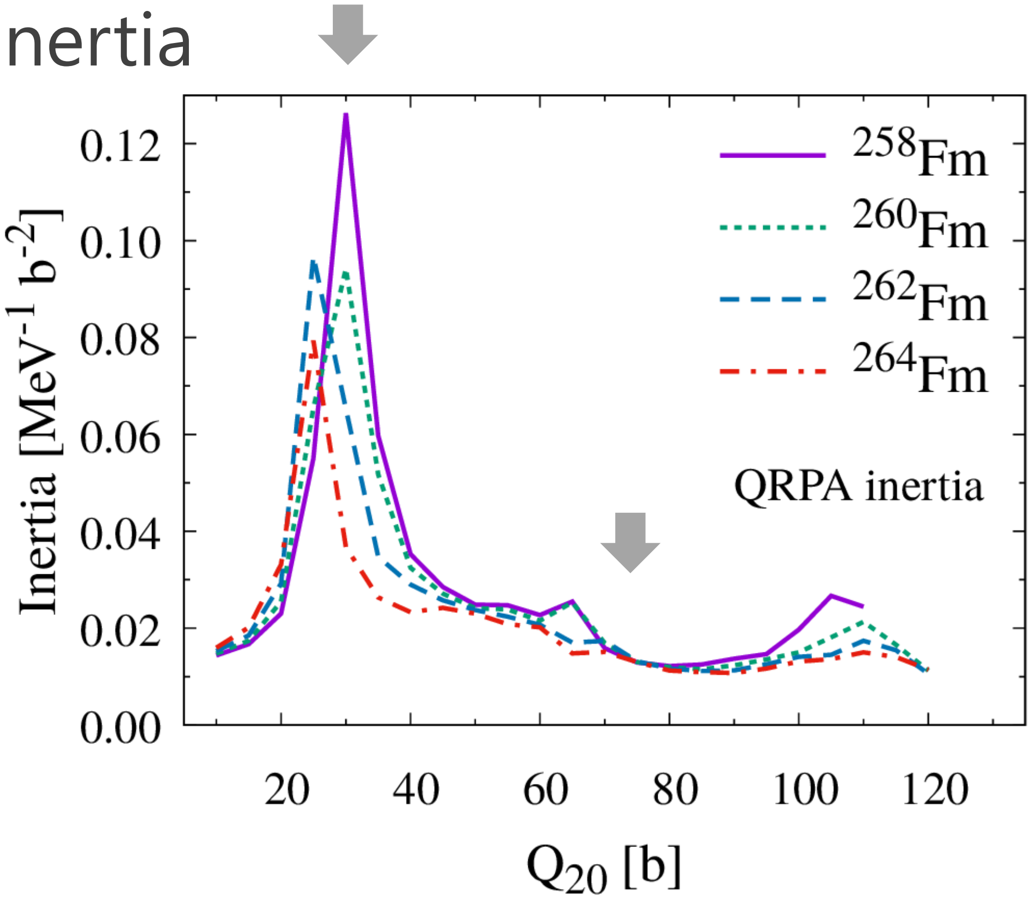
M.R. Lane et al., PRC53, 2893 (1996)

Result: fission barrier, collective inertia in Fm

Fission barrier



Inertia



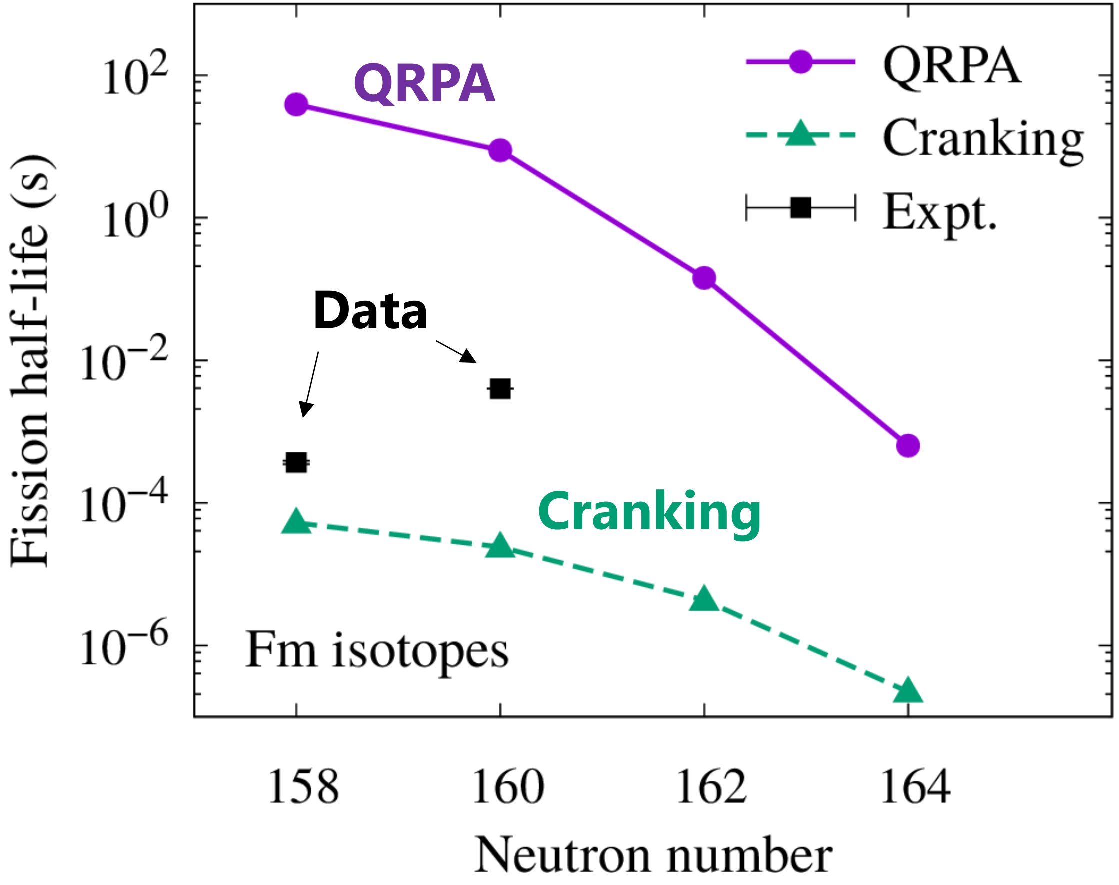
- Ground state Q~ 30 b (β~0.26)
- 258Fm > 260Fm > 262Fm > 264Fm

SkM* + volume pairing
25x25x35 fm^3, dx=1.0 fm

Washiyama, EPJ Web of Conf. 306, 01026 (2024)

Result: Fission half-life in Fm isotopes

Isotope dependence of half-life



$$T_{1/2} = \ln 2/(nP)$$

$$n = 10^{20.38}\ \mathrm{s}^{-1} \qquad P = \frac{1}{1+\exp(2S)}$$

A. Baran, Phys. Lett. B 76, 8 (1978)
Sadhukhan et al, PRC88, 064314 (2013), etc.

Larger *V* & *M* → longer half-life

Difference in inertia → Half-life

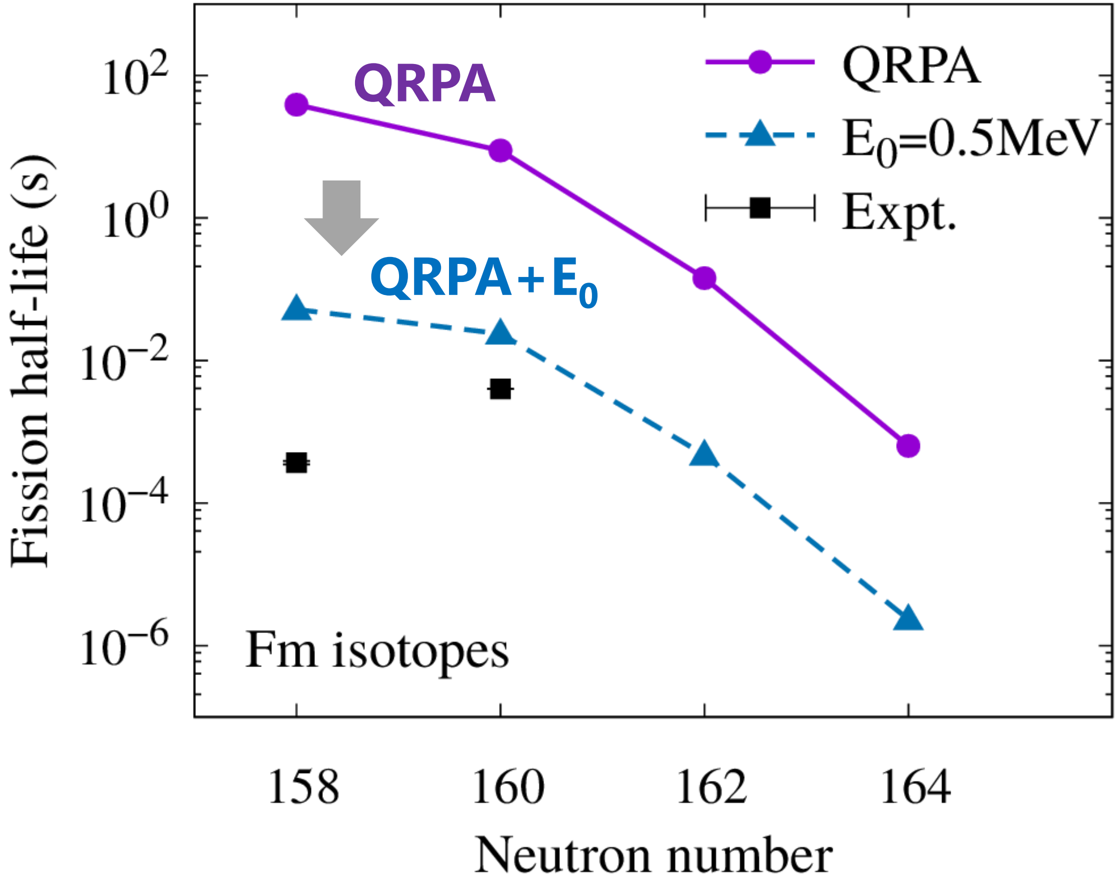
Overestimation
- Triaxial shape
- Zero-point correction

Data from N. E. Holden and D. C. Hoffman, Pure Appl. Chem. 72, 1525 (2000)

Washiyama, EPJ Web of Conf. 306, 01026 (2024)

Result: Fission half-life in Fm isotopes

Zero-point correction, E_0



$$S = \int_{s_1}^{s_2} ds \, \sqrt{2M(s)(V(s) - E)}/\hbar$$

$$E \to E + E_0$$

Zero-point correction E_0 = 0.5 MeV

→ Decrease half-life

Fission half-life is sensitive to fission barrier, collective inertia, and zero-point correction energy

Data from N. E. Holden and D. C. Hoffman, Pure Appl. Chem. 72, 1525 (2000)

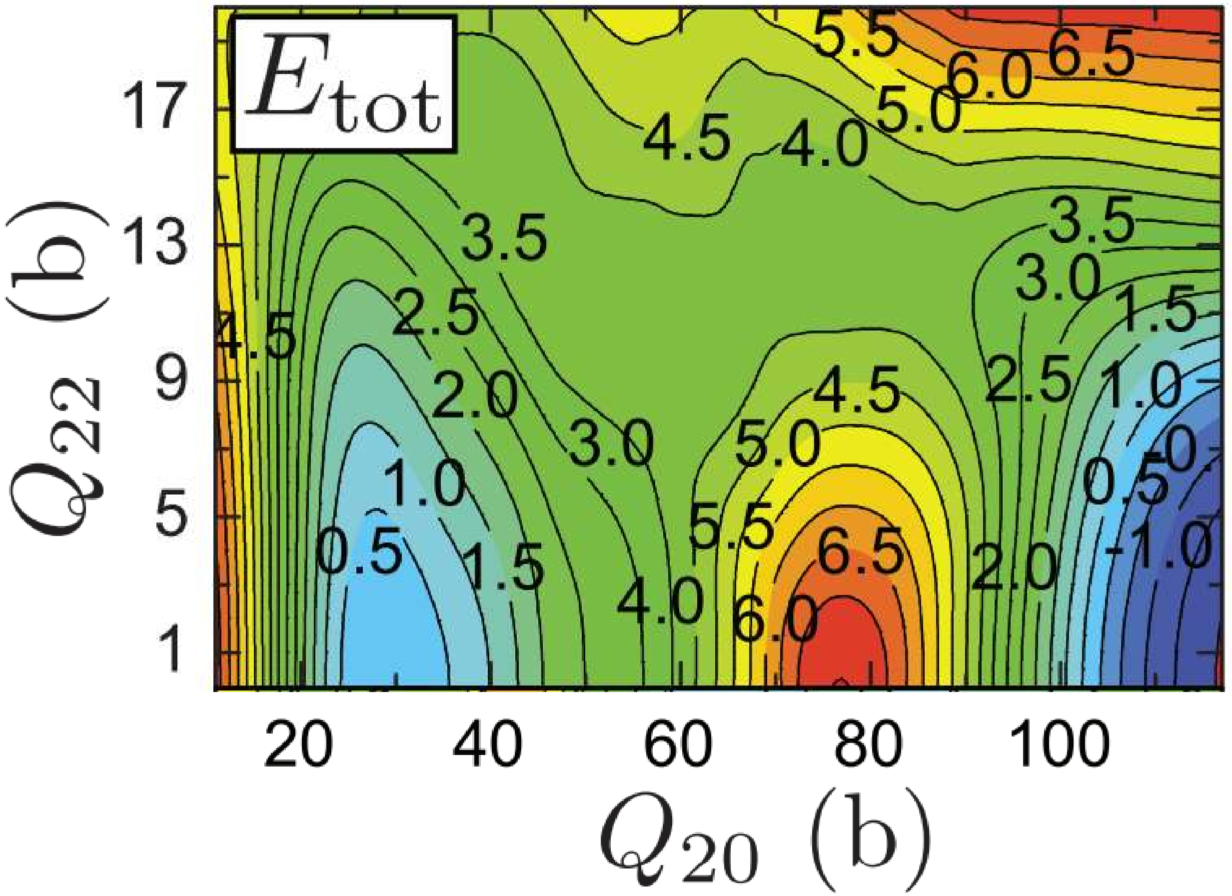
On going work,

Spontaneous fission in two-dimensional collective space —Determination of the fission path and fission half-life

Fission in multi-dimensional collective space

Description of SF in ^{264}Fm

Sadhukhan et al, PRC88, 064314 (2013)



Fission path = Minimizing the action

$$S = \int_{s_1}^{s_2} ds \sqrt{2M(s)(V(s) - E)}/\hbar$$

Multi-dimensional case

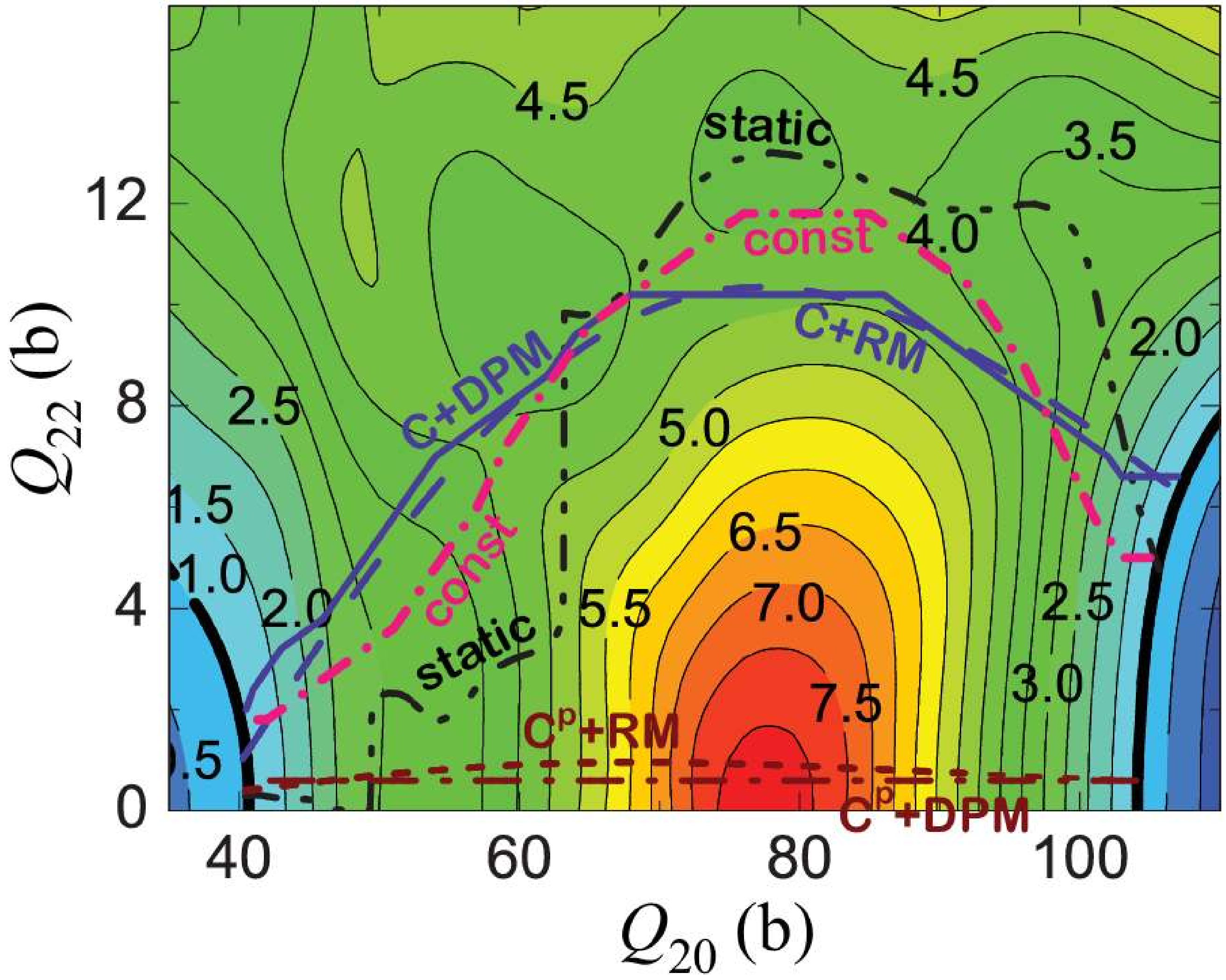
$$\mathcal{M}_{\text{eff}}(s) = \sum_{ij} \mathcal{M}_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds}$$

Inertia tensor

Fission in multi-dimensional collective space

Description of SF in ^{264}Fm

Sadhukhan et al, PRC88, 064314 (2013)



Fission path = Minimizing the action

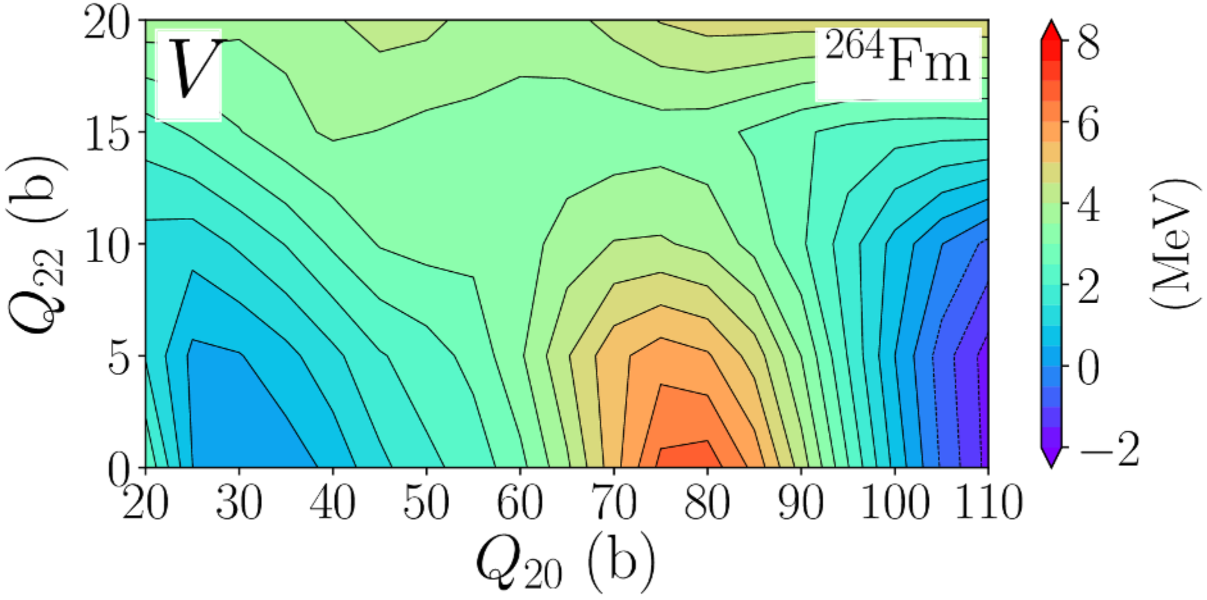
$$S = \int_{s_1}^{s_2} ds\ \sqrt{2M(s)(V(s)-E)}/\hbar$$

Spontaneous fission path strongly depends on the choice of collective inertia

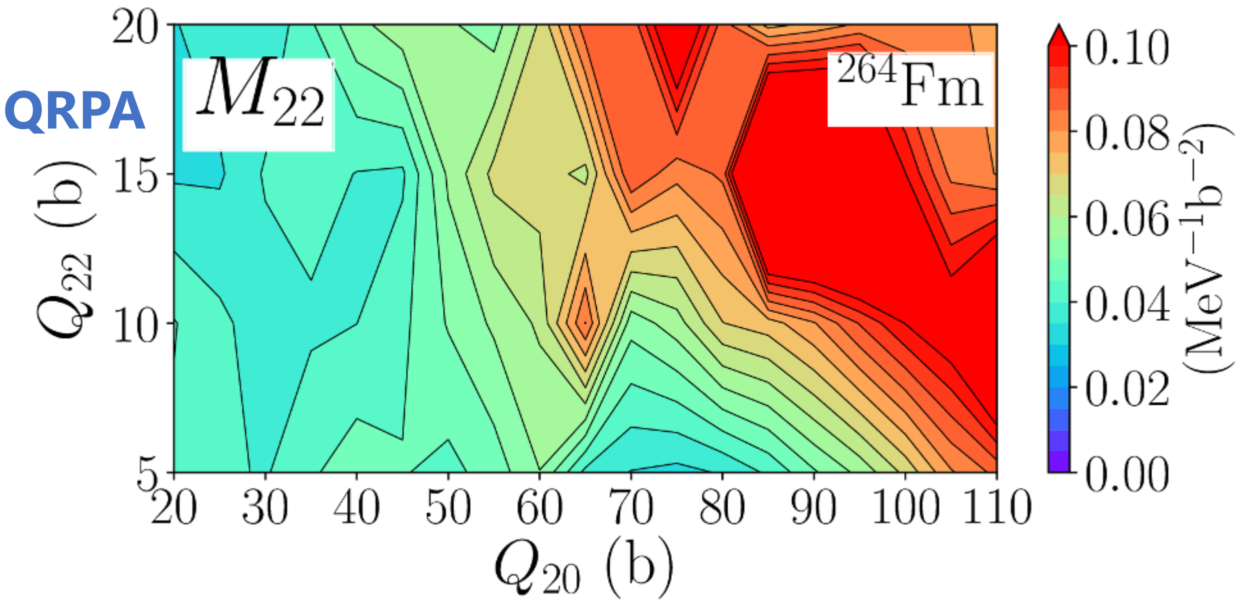
Result: Fission barrier and collective inertia

Q_{22} : Triaxial shape

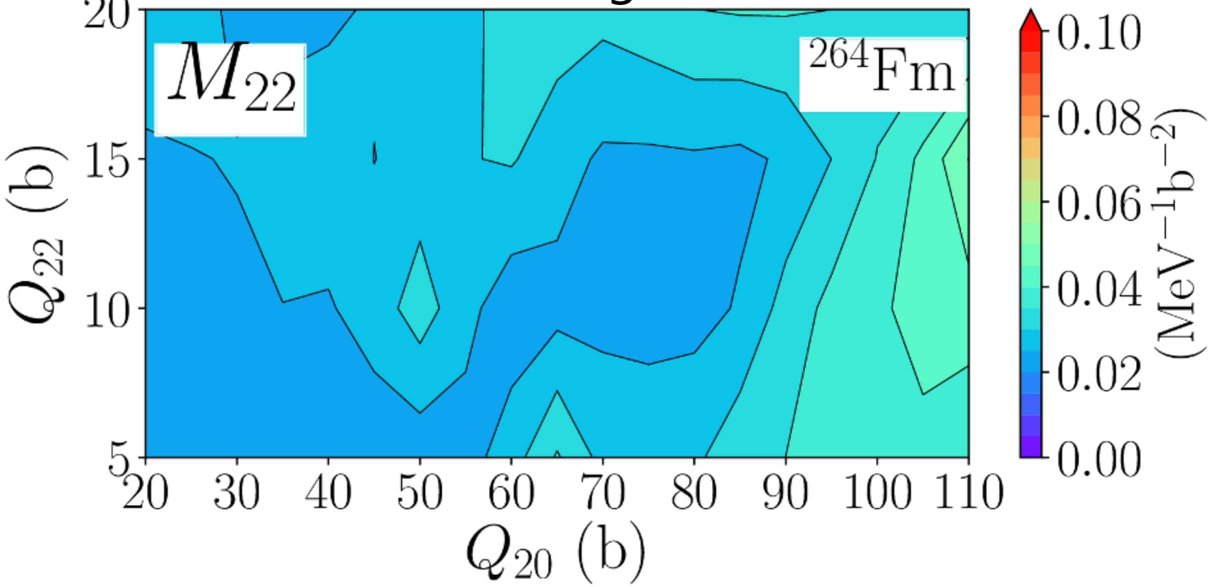
$$Q_{22} \propto r^2 (Y_{22} + Y_{2-2})$$



Local QRPA



Perturbative cranking

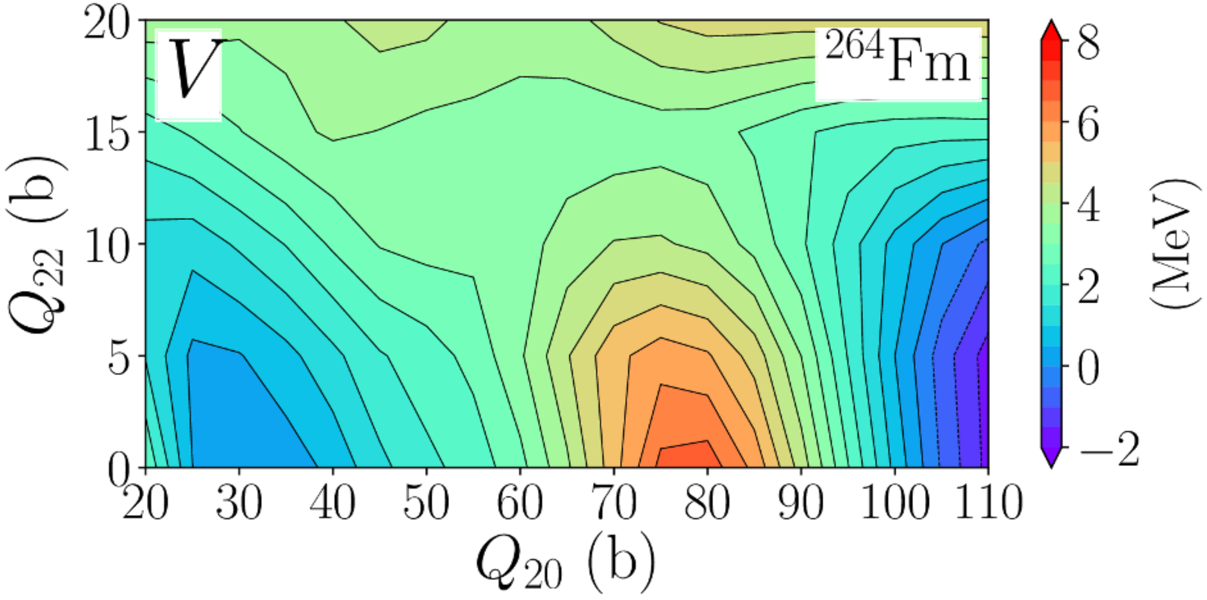


$$M_{22} = M_{Q_{22}Q_{22}}$$

Result: Fission barrier and collective inertia

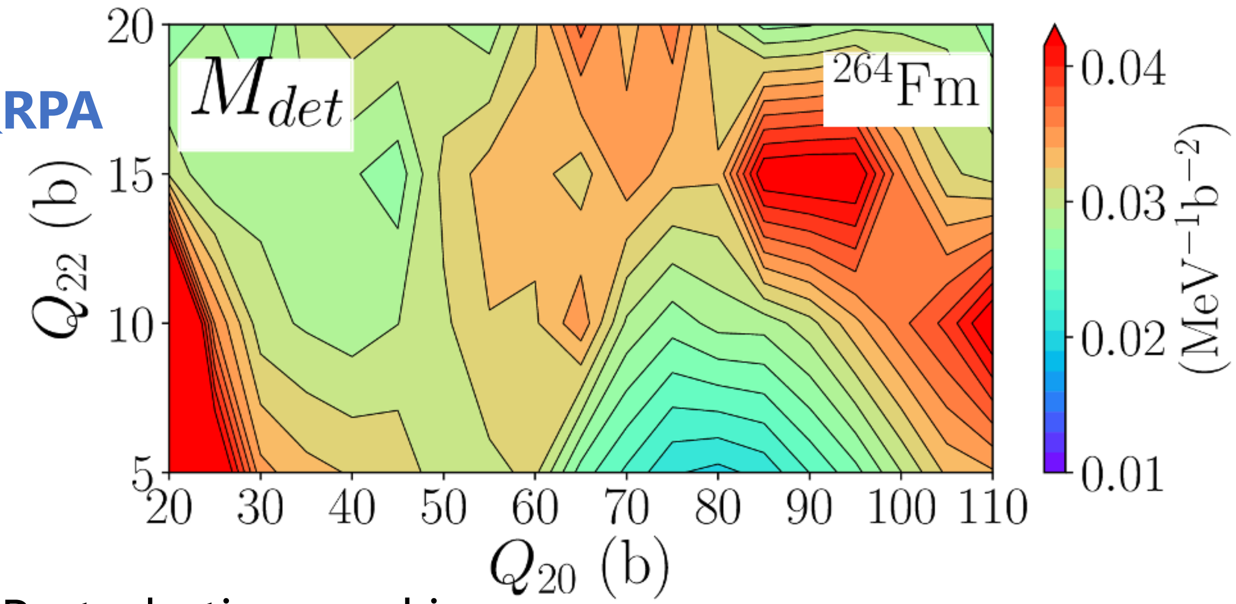
Q_{22} : Triaxial shape

$$Q_{22} \propto r^2(Y_{22} + Y_{2-2})$$

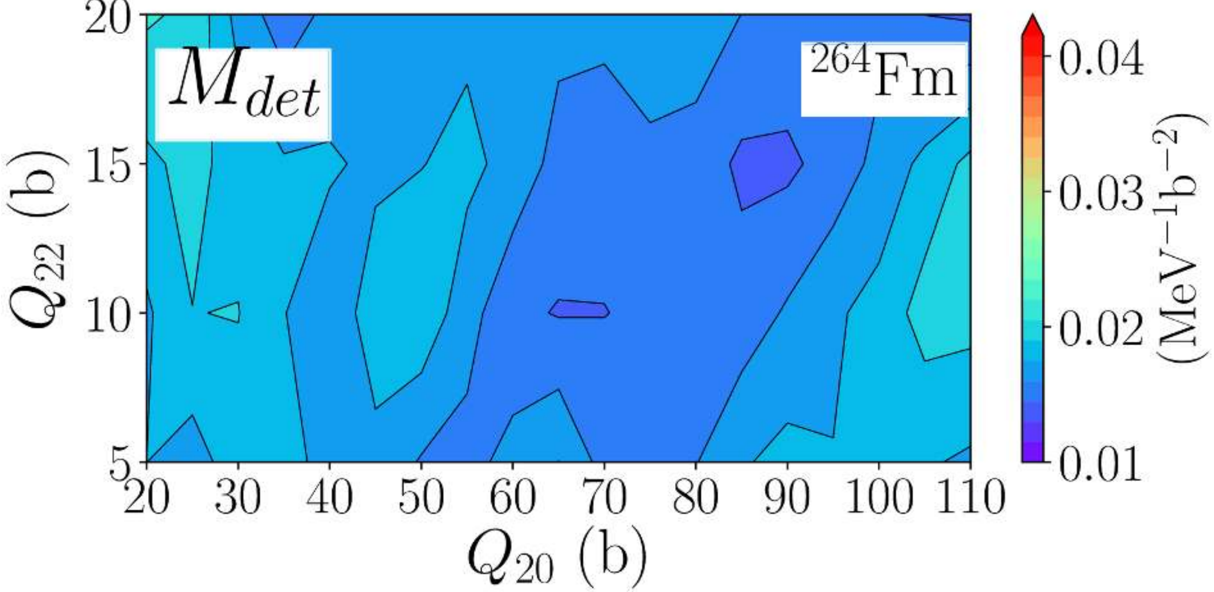


$$M_{det} := \sqrt{M_{00}M_{22} - M_{02}^2}$$

Local QRPA



Perturbative cranking



Summary

Spontaneous fission by DFT

Description of collective inertia by DFT + Local QRPA

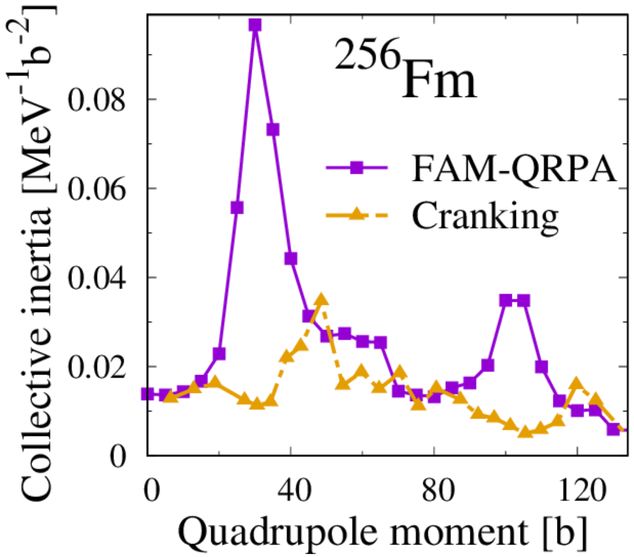
- Correct description on dynamical residual effects
- Pronounced peaks at g.s. and fission isomer
- $M_{\mathrm{QRPA}} > M_{\mathrm{cranking}}$

Fission half-life in Fm isotopes

- Strong dependence of choice of inertia
- Zero-point correction

On-going works

- Fission paths in multidimensional space



Half-life