# Microscopic description of collective inertia in spontaneous fission

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- Collective inertia in fission by DFT
- Fission half-life
- Outlook

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

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

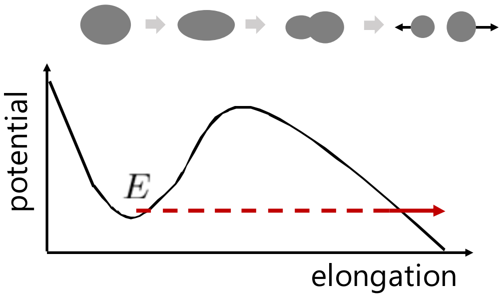
Workshop on Fission Dynamics 2026, May 11-15, 2026@Voco Hotel, Chongqing, China

# Spontaneous fission described by DFT



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

## Spontaneous fission




## WKB approximation

### Fission half-life

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

### Action

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

$s$ Collective coordinate ($Q_{20}$ etc.)

$V$ Potential

***M* Collective inertia**

# Aim of this talk



Fission observable

- Fission half-life
- Mass distribution

←

Potential energy

**Collective inertia**

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

To describe collective inertia $M$ for fission half-life based on DFT

# Collective inertia by DFT



## DFT + Cranking formula

Skyrme, Gogny, Relativistic EDFs

Low computation cost

Drawback: **ignore residual effects** (time-odd terms)

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)

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

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

## Our method: Local QRPA

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

**Include residual effects by QRPA**

**High computation cost** ➡ Finite amplitude method

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

# Local QRPA



Local QRPA for vibrational mass at each CHFB state

Hinohara et al., PRC82 (2010) 064313

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

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

$s$ : 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**

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

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

# 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 with the finite amplitude method

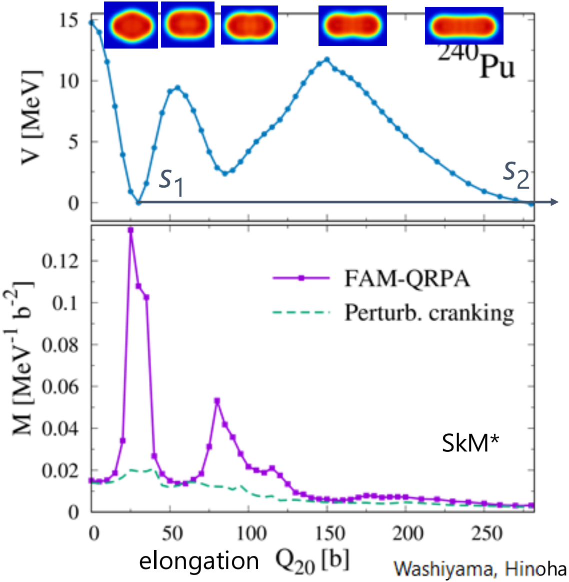
Select the most collective mode among QRPA solutions

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

Computation time: (1000 hours+500 hours) x 30--50 states, OpenMP+MPI

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

# Result: Collective inertia along fission path




QRPA inertia

- ✓ Large enhancement
- ✓ Large variation

**Action integral** $S$

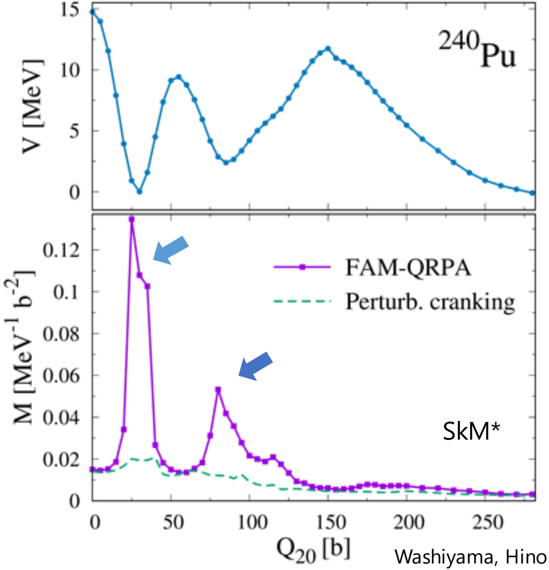
$$S = \int_{s_1}^{s_2} ds\, \sqrt{2M(s)(V(s)-E)}/\hbar$$

| | | |
|---|---|---|
| **QRPA** | $S$ = **82.0** | $5\times10^{50}$ s |
| **Cranking** | $S$ = **62.0** | $2\times10^{33}$ s |

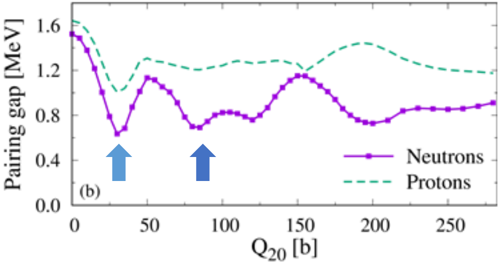
Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

60000 CPU hours
OpenMP + MPI

# Result: Collective inertia and pairing gap




## Pairing gap

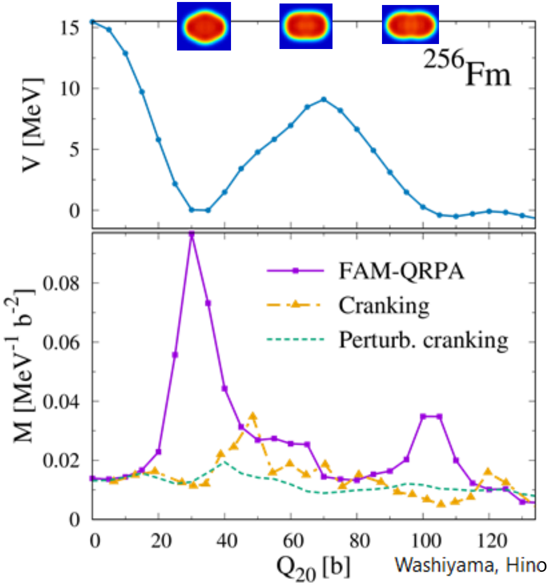



**Pair gap ⤵ ↔ Inertia**
**⤴**

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

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






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

Non-perturbative cranking formula

Baran et al., PRC84, 054321 (2011)

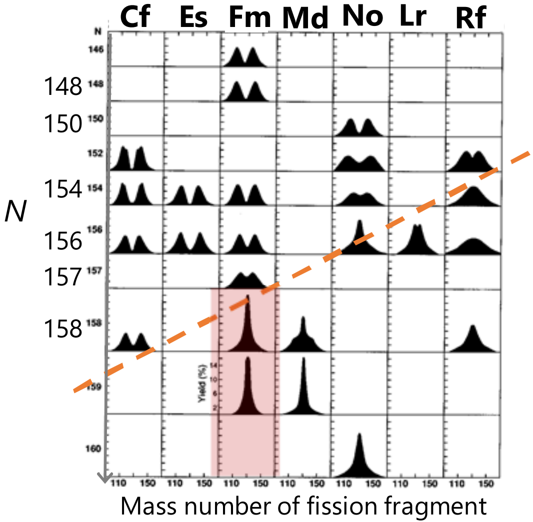
- Peak structure
- Larger inertia in QRPA

non-perturbative cranking

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

# Experimental data of fission in the actinoid region

**Mass distribution of fission fragments**



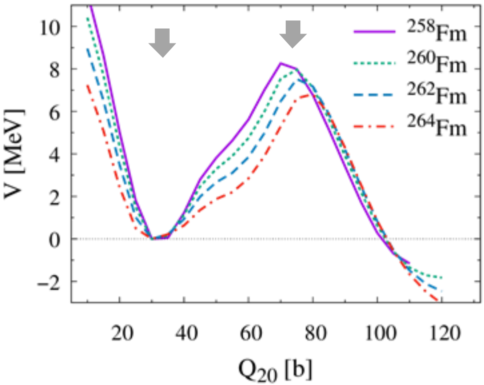

Mass symmetric fission is dominant in Fm isotopes, N ≥ 158

$Q_{30}$ = 0 may be a good approximation

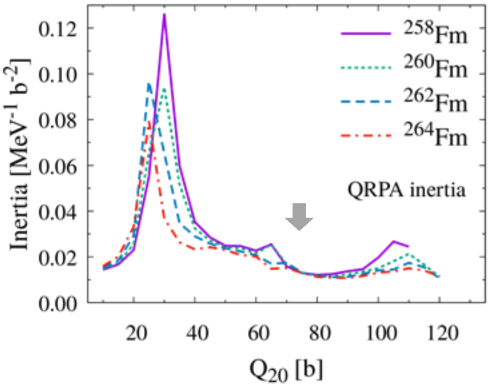
M.R. Lane et al., PRC53, 2893 (1996)

# Result: fission barrier, collective inertia in Fm isotopes

## Fission barrier




## Inertia




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

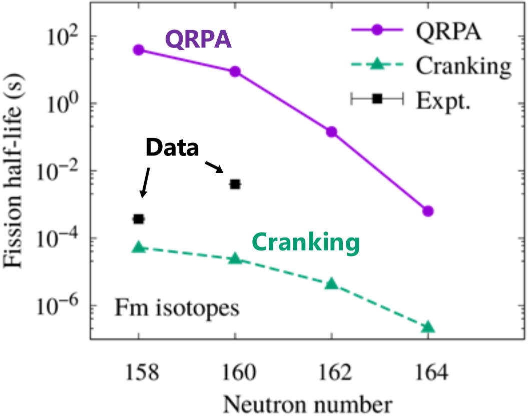
SkM* + volume pairing
25x25x35 fm$^3$, dx=1.0 fm

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

# Result: Fission half-life in Fm isotopes



## Fission 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

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

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

# Outlook



**Ground state energy**

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

When E = 0 → 0.5 MeV, half-life decreases in three orders of magnitude

**Two** (and more) **collective coordinates**

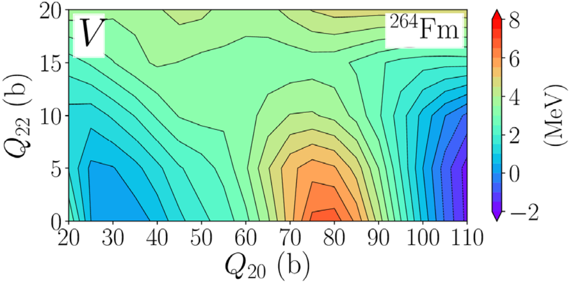
- Octupole moment, nonaxial (triaxial) quadrupole moment

# Fission barrier and collective inertia in 2D



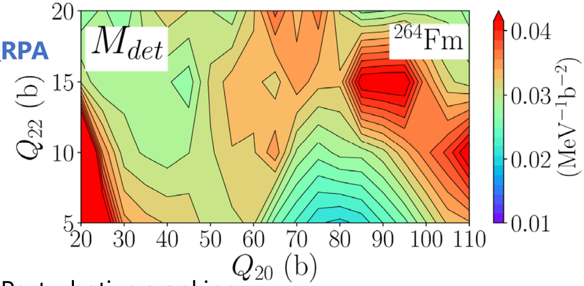
$Q_{22}$ : Triaxial shape

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

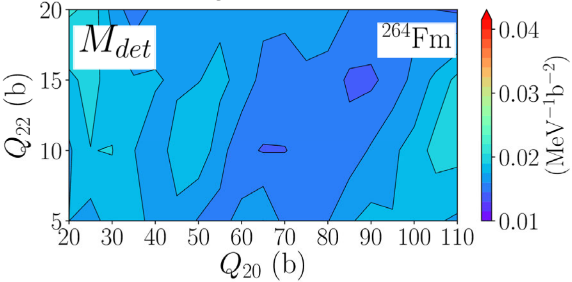



$$M_{det} := \sqrt{M_{00}M_{22} - M_{02}^2}$$

Local QRPA




Perturbative cranking



# Outlook



**Two** (and more) **collective coordinates**

- Octupole moment, nonaxial (triaxial) quadrupole moment
- **Pairing**

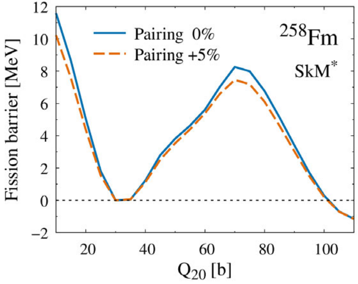
  → **Induce a large change in the inertia**

  "Pairing-induced speedup of nuclear spontaneous fission"
  J. Sadhukhan et al, PRC90, 061304 (2014)

# Pairing strength dependence

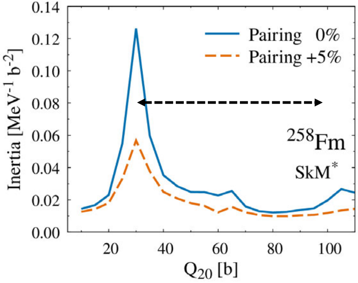


**Fission barrier**




~10% change at barrier

**Inertia**




20 – 50% change

**Action *S***

**25.6 (Pairing 0%)**

**20.6 (Pairing 5%)**

**Half-life**

$4.5 \times 10^{1}$ s **(Pairing 0%)**

$2.1 \times 10^{-3}$ s **(Pairing 5%)**

$0.37(2) \times 10^{-3}$ s (data)

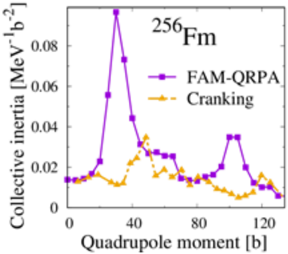
**+5% pairing**

# Summary



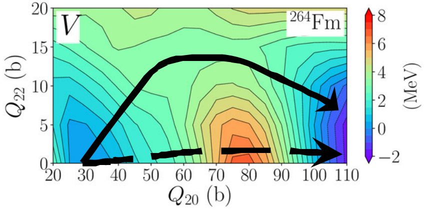
Description of collective inertia is important

- Drawbacks of the cranking formula
- Correctly including residual effects by QRPA
- Fission half-life




**Outlook**

- Octupole and triaxial quadrupole moment
- Pairing



# Relation between QRPA and collective inertia



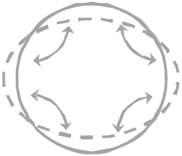
$$T = \frac{1}{2} M \left( \frac{dQ_{20}}{dt} \right)^2 \qquad Q_{\lambda\mu} = r^\lambda Y_{\lambda\mu}$$

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)

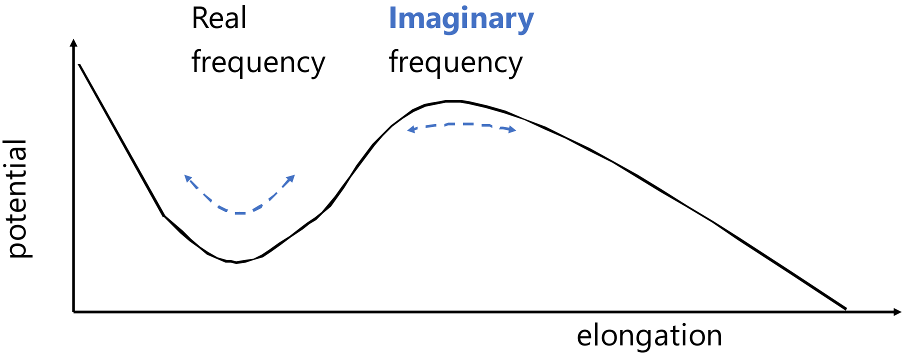
Inertia associated with collective coordinates

# Solution of Local QRPA can be imaginary



## Local QRPA = QRPA on top of constrained DFT state

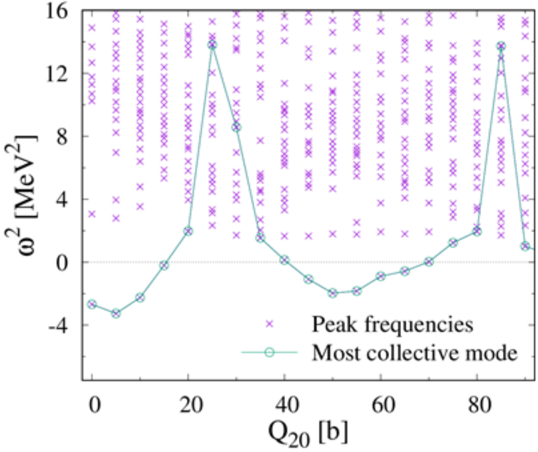
Eigen-frequency ⟷ Curvature of the potential



# LQRPA solutions and the most collective mode



$^{240}$Pu, axial states

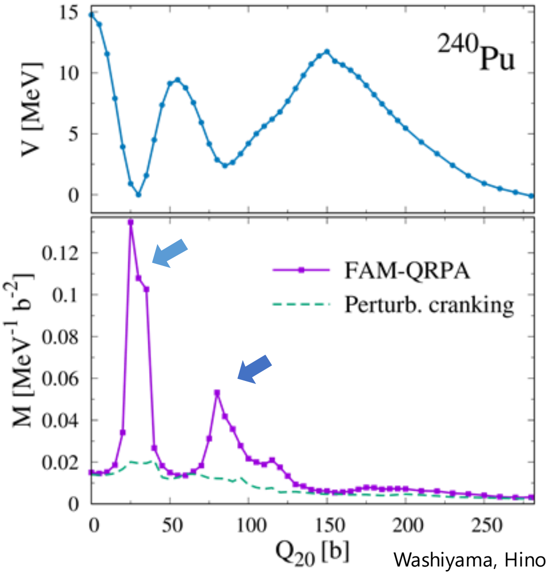



Select the most collective mode from many QRPA solutions in $\omega^2 < 16$ MeV$^2$

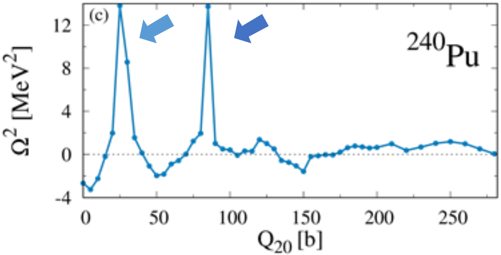
Select the smallest collective inertia $M$ = the largest strength

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

# Result: Collective inertia and eigen-frequency




**Eigen-frequency of LQRPA**




$\Omega^2$ ⤴ ⟷ **Inertia**

⤴

$\Omega$ can be imaginary near the fission barrier

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

# 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)

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

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

Note: Dynamical effects reproduce the collective inertia for translational motion

Perturbative cranking approximation

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

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

$s$ : collective variables

$\phi$ : constrained HFB states

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