密度汎関数法による
原子核大振幅集団運動の記述に向けて

鷺山 広平、中務 孝　筑波大学計算科学研究センター

はじめに: 原子核の形の揺らぎ、四重極変形

手法：集団模型、密度汎関数法

結果：3次元Skyrme-QRPA, 慣性質量

まとめ

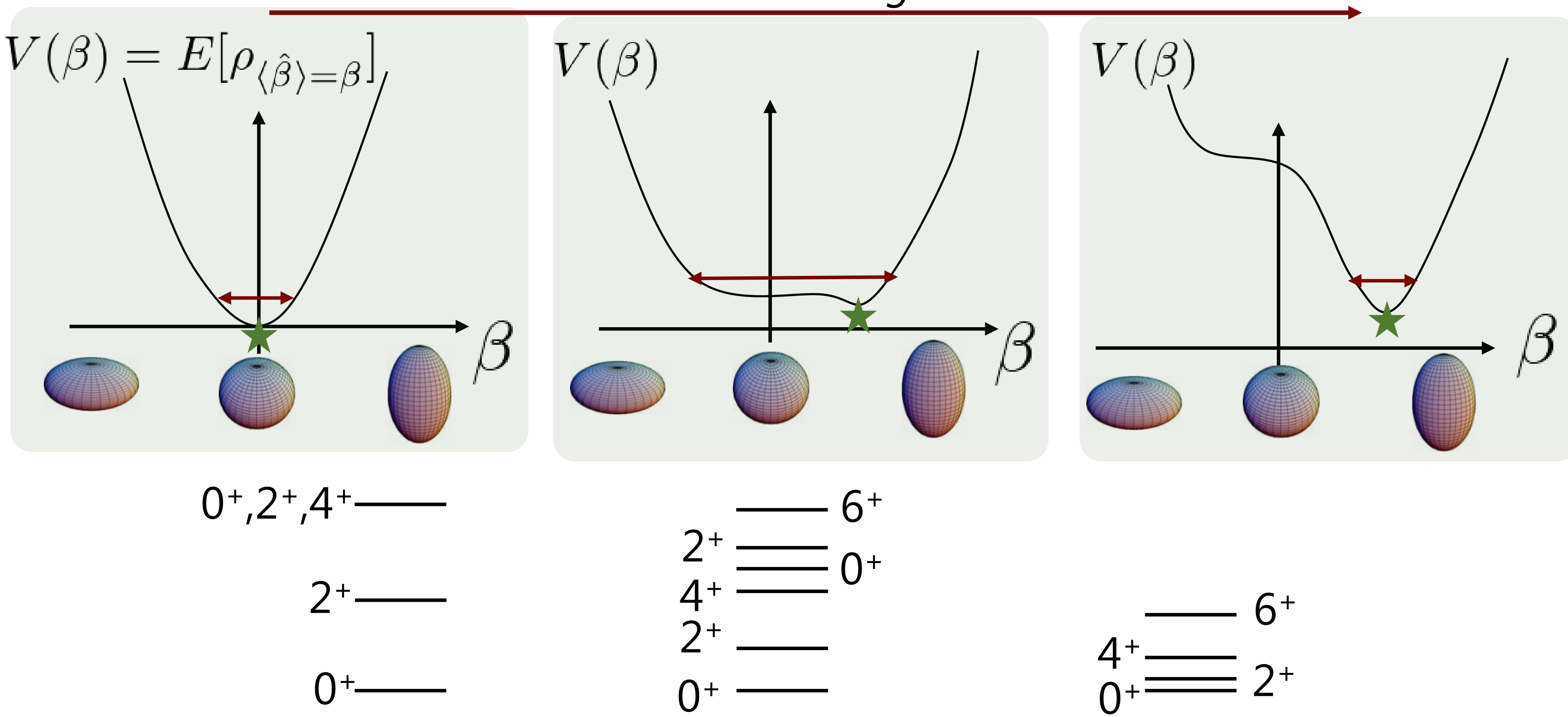
（付記）本研究は、総合科学技術・イノベーション会議が主導する 革新的研究開発推進プログラム（ImPACT）の一環として実施したものです。

はじめに：大振幅集団運動

Heyde & Wood, Rev.Mod.Phys.83(2011)1467

小振幅から大振幅へ

e.g. Neutron number

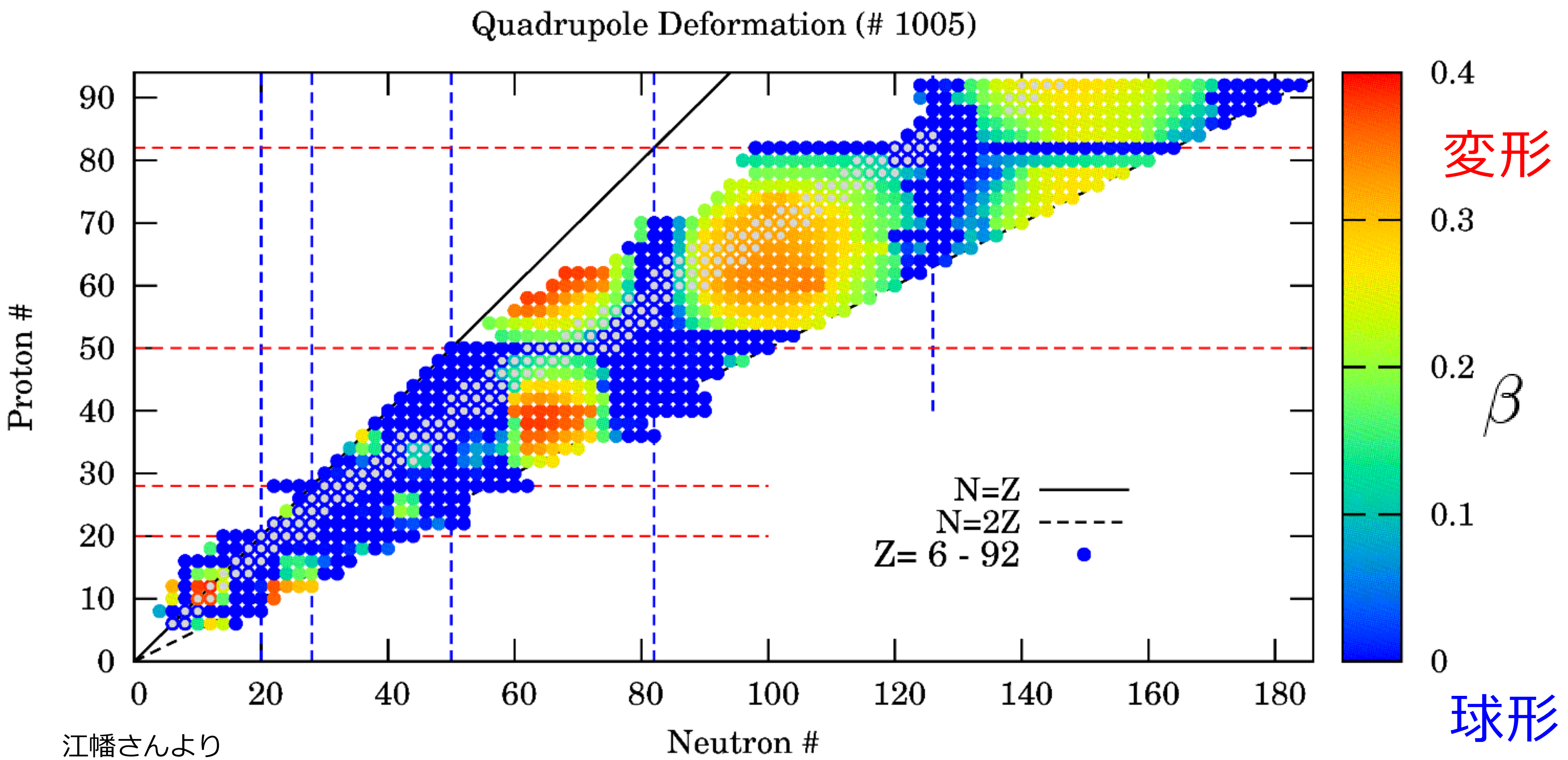


基底状態 (DFT) +
周辺の揺らぎ (RPA)

大きな形のゆらぎ

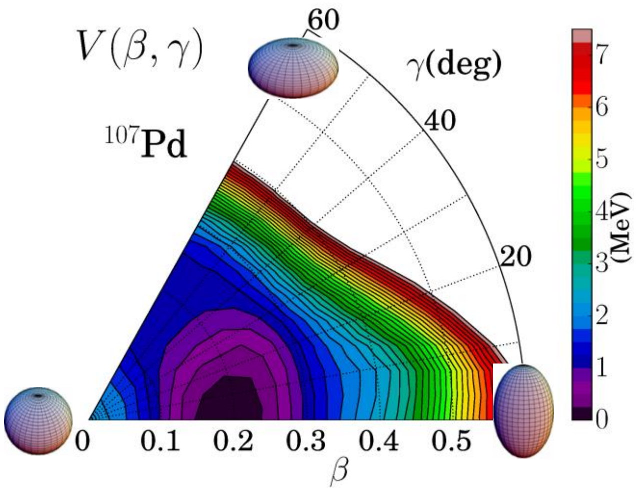
Rotational band

核図表と四重極変形度



江幡さんより

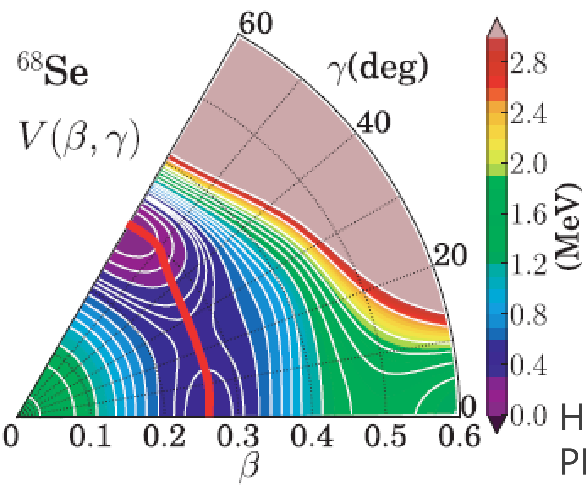
Shape fluctuation in transitional region, example:



^{107}Pd ← 長寿命核分裂生成物(LLFP)

V < 2 MeV にポテンシャル
エネルギーが広がる

➡ 形の揺らぎ



^{68}Se

2 つのエネルギー極小点

➡ 変形共存

Hinohara et al.,
PRC82 (2010) 064313

小振幅から大振幅集団運動へ

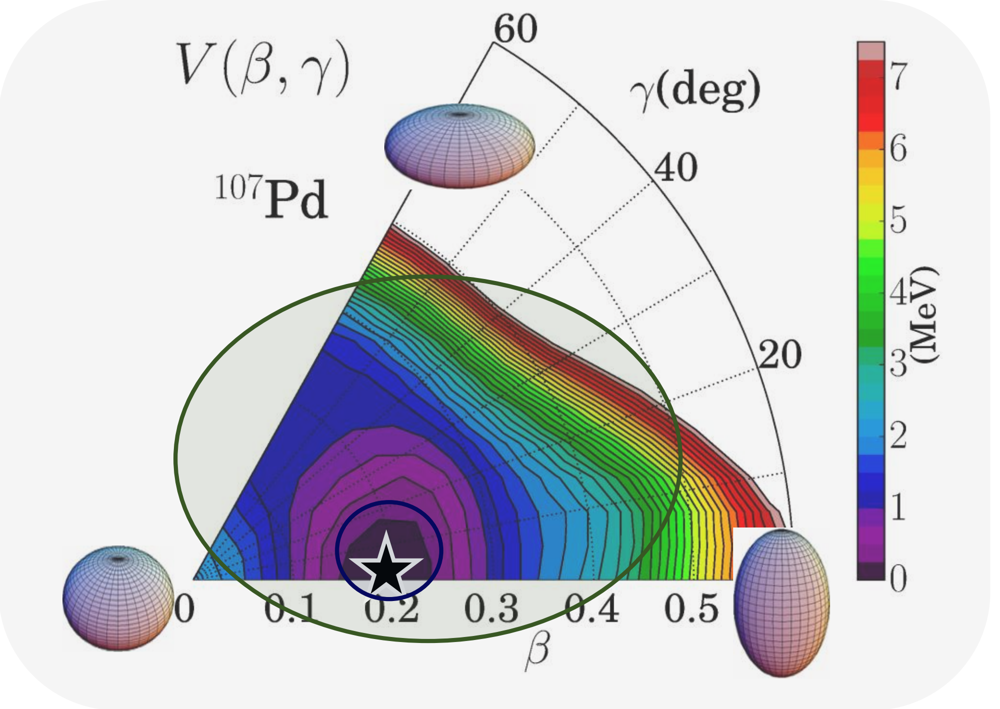
微視的な密度汎関数法による
基底状態の詳細な記述

↓

基底状態周辺の揺らぎ
Random phase approximation
(RPA)

↓

「基底状態周辺のゆらぎ」を
超えた大振幅集団運動



5D quadrupole collective (Bohr) model

HFB (potential) + Local QRPA (inertial functions) with P+Q force

Hinohara et al.,
PRC82 (2010) 064313

$$\mathcal{H} = T_{\rm vib} + T_{\rm rot} + V(\beta,\gamma)$$

$$T_{\rm vib} = \frac{1}{2} D_{\beta\beta}(\beta,\gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta,\gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2} D_{\gamma\gamma}(\beta,\gamma)\dot{\gamma}^2$$

$$T_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3} \mathcal{J}_k(\beta,\gamma)\omega_k^2$$

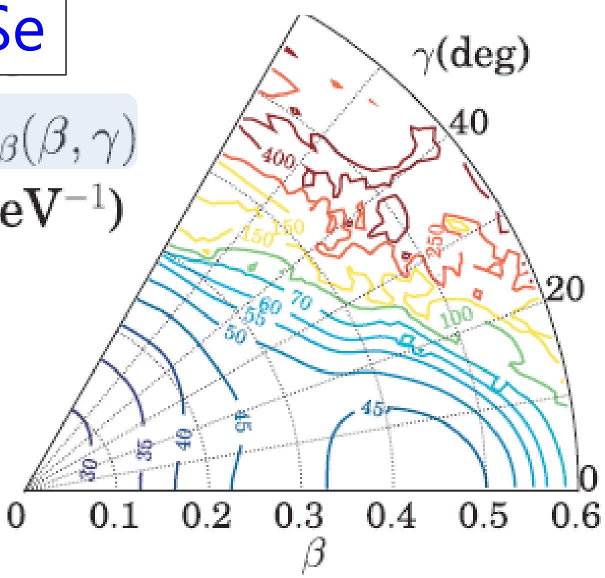
→ 量子化

↓

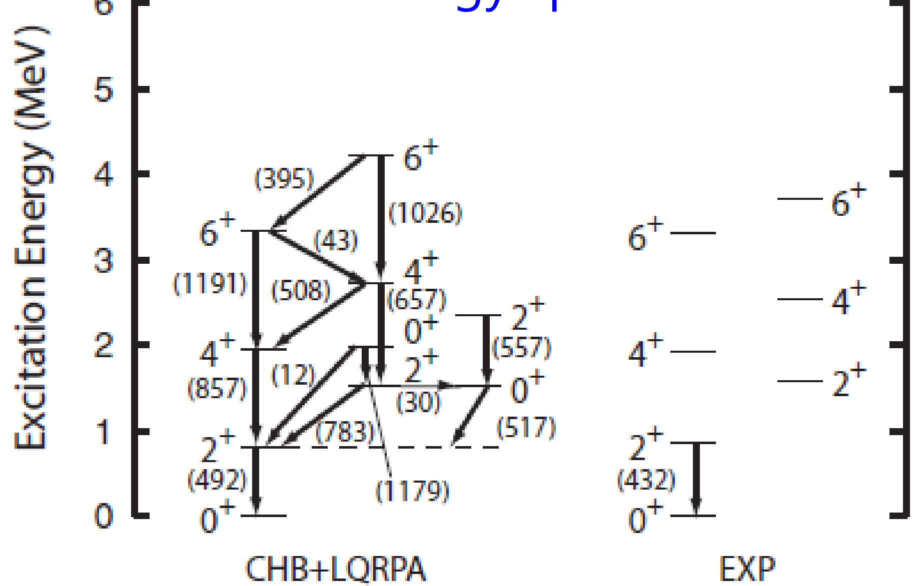
Inertial functions

^{68}Se

$D_{\beta\beta}(\beta,\gamma)$ (MeV^{-1})



Energy spectra



5D quadrupole collective (Bohr) model

HFB (potential) + Local QRPA (inertial functions) with P+Q force

$$\mathcal{H} = T_{\text{vib}} + T_{\text{rot}} + V(\beta,\gamma)$$

$$T_{\text{vib}} = \frac{1}{2}D_{\beta\beta}(\beta,\gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta,\gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2}D_{\gamma\gamma}(\beta,\gamma)\dot{\gamma}^2$$

$$T_{\text{rot}} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{J}_k(\beta,\gamma)\omega_k^2$$

→ 量子化

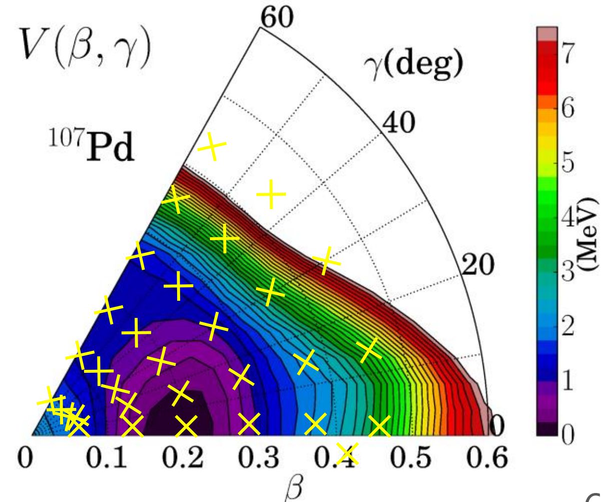
Hinohara et al.,
PRC82 (2010) 064313

本研究

P+Q force → Skyrme 型密度汎関数

$V(\beta,\gamma)$ β, γ 拘束条件付き Skyrme HFB

$D_{\mu\nu}(\beta,\gamma)$
$\mathcal{J}_k(\beta,\gamma)$ 各 β, γ 点上での Skyrme-QRPA 解



本研究の目的

5D quadrupole collective Hamiltonian の構築

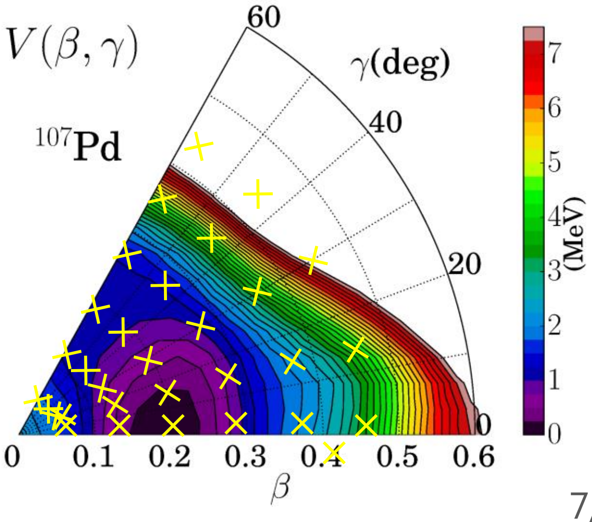
3 次元 Skyrme QRPA がないので、

- 集団質量の計算用に 3 次元 Skyrme QRPA の開発
- 有限振幅法の応用 (Finite amplitude method, FAM)

  有限振幅法：数値的に効率的な QRPA 解法

- 各 β, γ 点で Local FAM+QRPA

  ⇒ 集団質量



Finite amplitude method (FAM)

Linear response TDDFT

$$(E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) = -F^{20}_{\mu\nu}$$
$$(E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) = -F^{02}_{\mu\nu}$$

$F_{\mu\nu}$: External perturbation field

(Isoscalar quadrupole moment in this talk)

Nakatsukasa et al., PRC76 (2007) 024318
Avogadro & Nakatsukasa, PRC84(2011)014314
Stoitsov et al., PRC84 (2011) 041305
Liang et al., PRC87 (2013) 054310
Nik
Pei
Mu

QRPA matrix $\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}$	Dimension $N^2 \times N^2$
FAM matrix $\delta H_{\mu\nu}$	$N \times N$

($N \sim 10^3$ for deformed nuclei)

Finite amplitude method (FAM)

$$\delta H_{\mu\nu} = \frac{\partial H_{\mu\nu}}{\partial \mathcal{R}_{\alpha\beta}} \partial \mathcal{R}_{\alpha\beta}$$

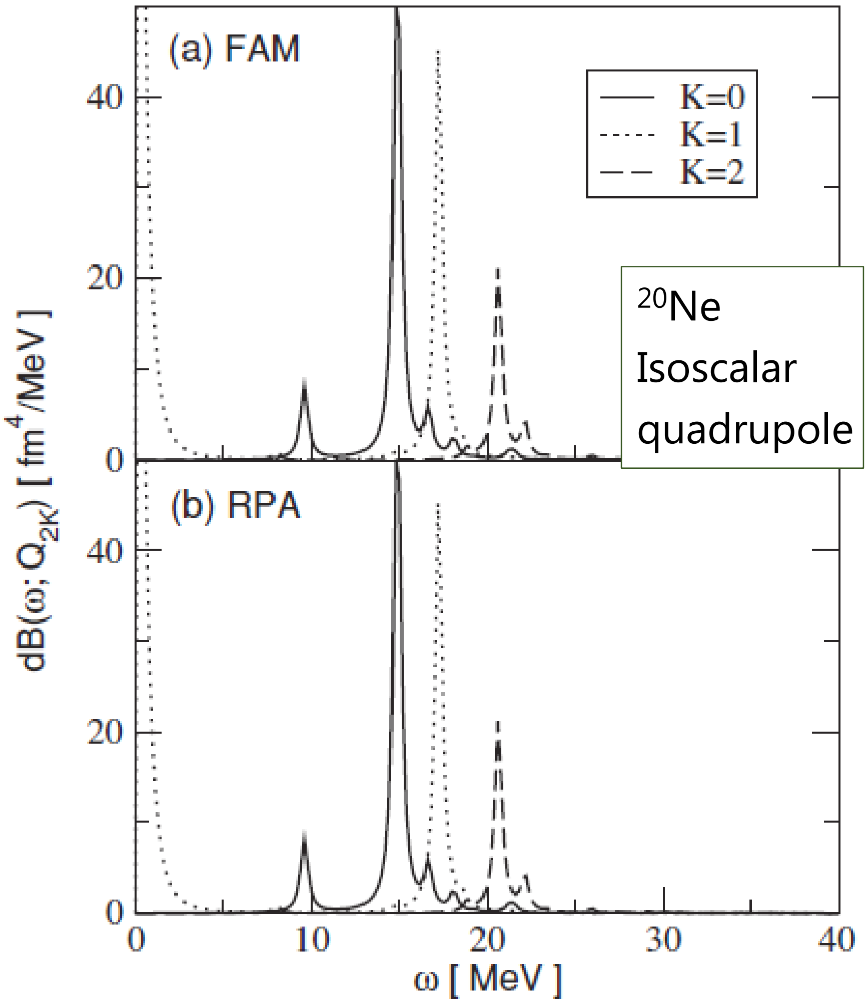
$$\Rightarrow \delta H_{\mu\nu} = \frac{1}{\eta}\{H_{\mu\nu}[\mathcal{R}_0 + \eta\delta\mathcal{R}] - H_{\mu\nu}[\mathcal{R}_0]\}$$

Residual part → finite difference form

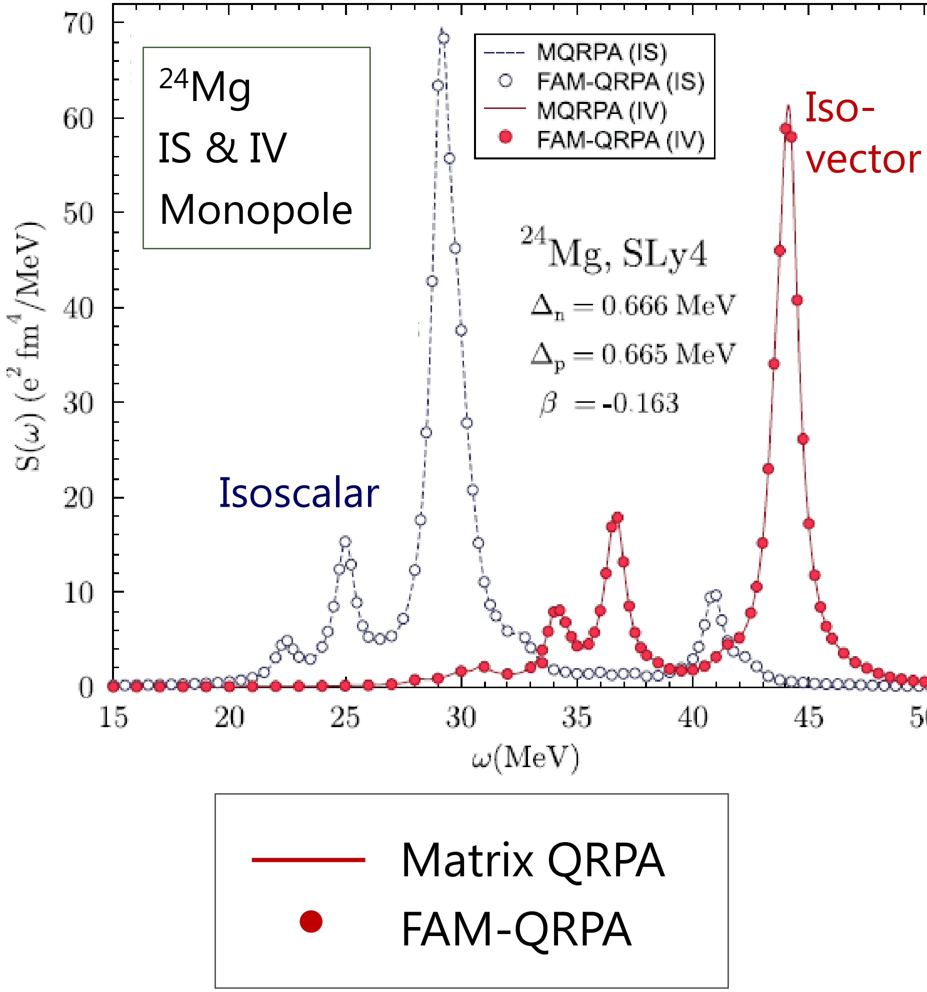
$\mathcal{R}_0$: Ground state density
$\delta\mathcal{R}$: Fluctuating density
η : Small parameter

FAM = (Q)RPA

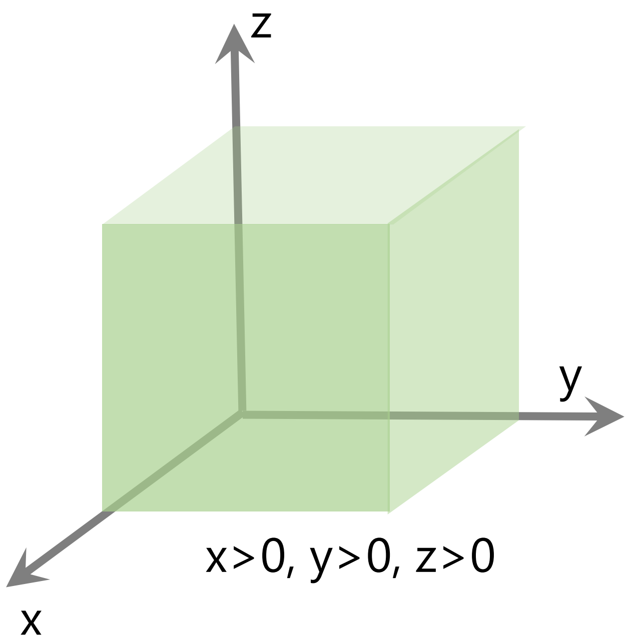
Nakatsukasa et al., PRC76 (2007)024318



Stoitsov et al., PRC84 (2011)041305



Numerical setup



- Three-dimensional Cartesian coordinate
- Parity
- Modified Broyden method for iteration
- Smearing width of γ = 0.5 MeV $\omega \to \omega + i\gamma$
- Strength function

$$S(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(\sum_{\mu<\nu} F^{20*}_{\mu\nu} X_{\mu\nu} + F^{02*}_{\mu\nu} Y_{\mu\nu}\right)$$

Hartree-Fock basis as a single-particle basis

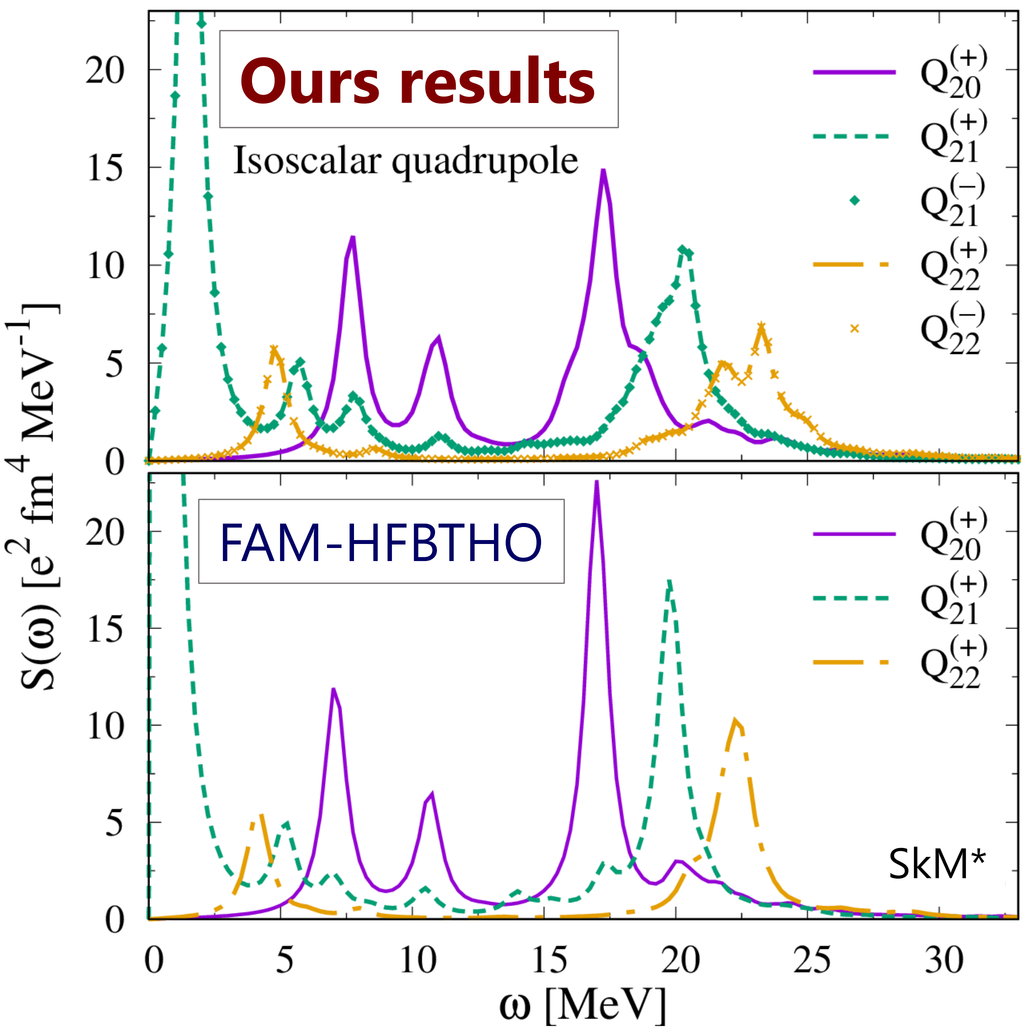
Mesh size: Δx = 0.8 fm

Δω = 0.25 MeV

Benchmark: Deformed nucleus ^{24}Mg

Isoscalar quadrupole response $Q_{2K}^{(\pm)} \propto r^2(Y_{2+K} \pm Y_{2-K})$

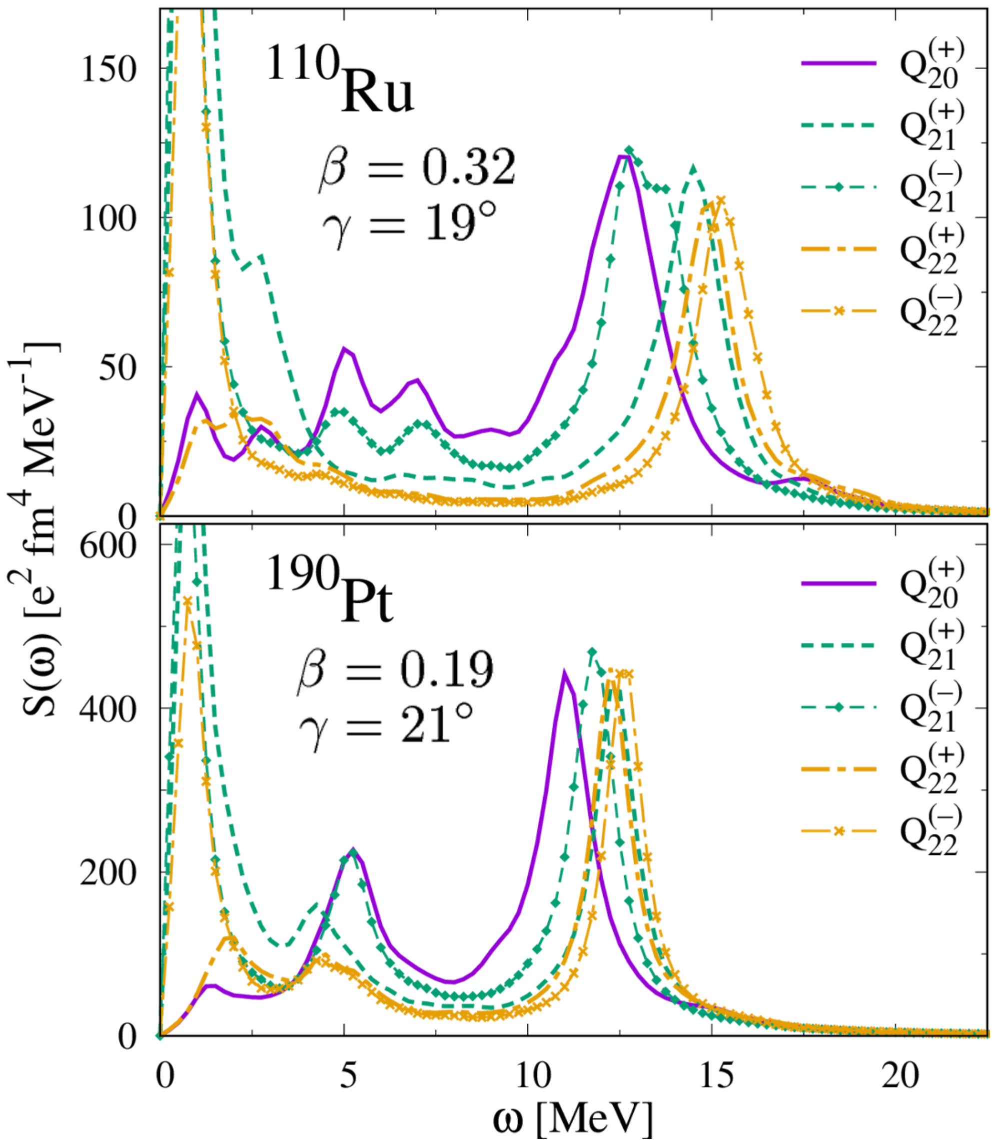
Washiyama, Nakatsukasa, PRC96, 041304(R) (2017)



- Good agreement of peak energies and shapes in each *K*
- Widths of giant resonance peaks are wider
- *K*=1 spurious mode around ω=0 due to rotation

FAM-HFBTHO: Kortelainen et al., PRC92(2015)051302

Strength of triaxial superfluid nuclei



Isoscalar quadrupole response

Five strength functions

Three spurious rotations (x, y, z)

➡ Only appear in triaxial nuclei

EWSR (ω < 50 MeV)

98.7 % (^{110}Ru)

98.6 % (^{190}Pt)

350 CPUh for 200ω

3.5 GB memory

Numerical set up

^{110}Ru: 17^3 mesh, R_{max}=14.0fm, 1120 HF states

^{190}Pt: 19^3 mesh, R_{max}=15.6fm, 1360 HF states

Moment of inertia $T_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{J}_k(\beta,\gamma)\omega_k^2$

南部Goldstone modeと質量 (Thouless-Valatin inertia)

$$S^{\rm FAM}(\hat{P}_{\rm NG},\omega) \approx \frac{M_{\rm NG}\Omega_{\rm NG}^2}{\omega^2-\Omega_{\rm NG}^2} = -M_{\rm NG} \quad (\omega=0)$$

Hinohara, PRC92(2015)034321

(e.g. Translation, rotation etc.)

$\Omega_{\rm NG}$: Energy of NG mode
$M_{\rm NG}$: Inertia of NG mode

$\Omega_{\rm NG} \neq 0$ の場合もある

Thouless-Valatin moment of inertia

$$\hat{P}_{\rm NG} = \hat{J}_z,\ M_{\rm NG} = \mathcal{J}_z^{\rm TV}$$

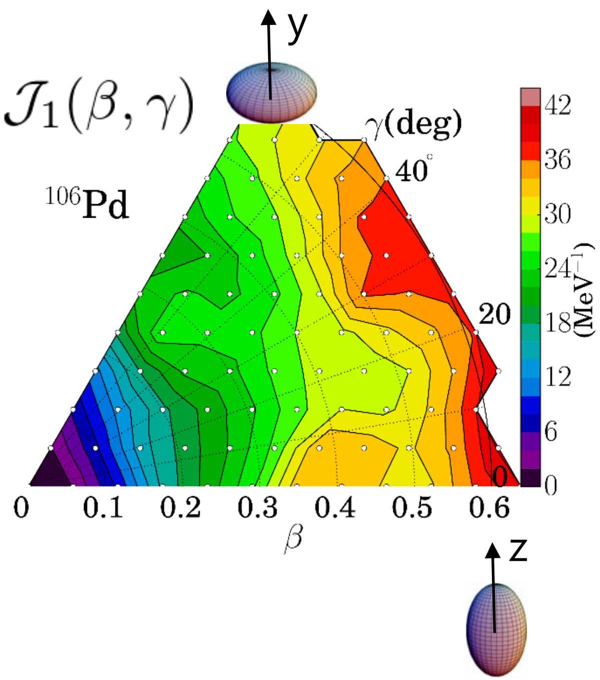
利点： ω = 0 だけ FAM 計算すればよい

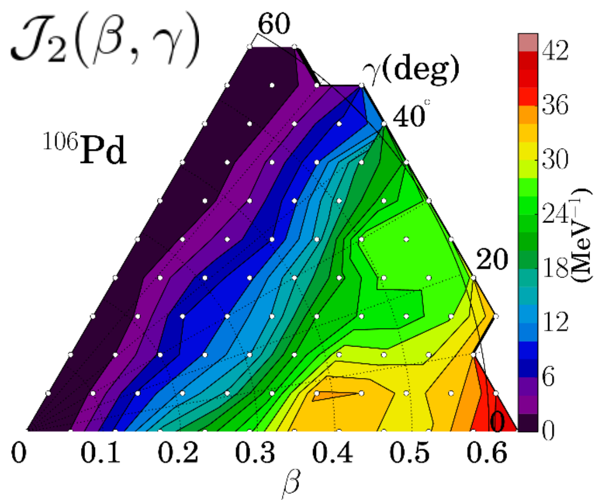
➡ 数値計算量が少ない

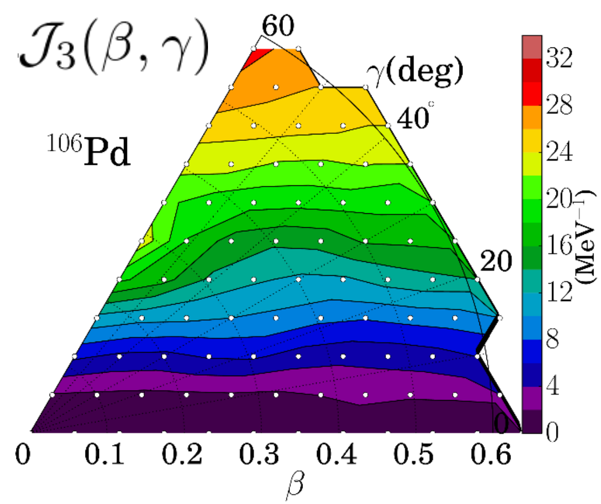
Local FAM+QRPA -- Moment of inertia

FAM を拡張、各 β–γ 点で FAM 計算による moment of inertia

$$T_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3} \mathcal{J}_k(\beta,\gamma)\omega_k^2$$

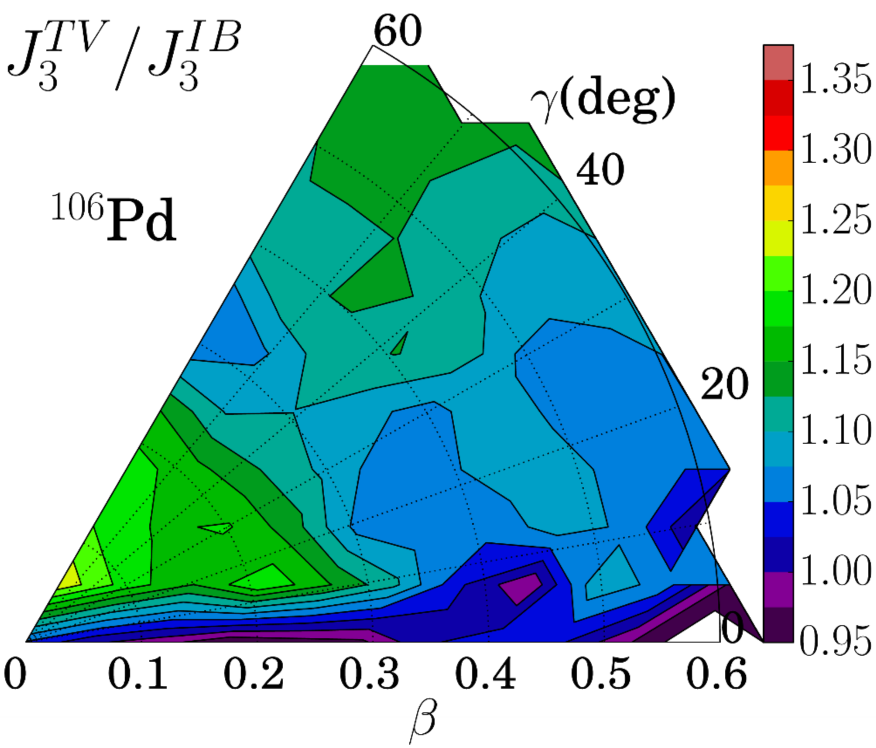






Local FAM+QRPA -- Moment of inertia

Thouless-Valatin vs. Inglis-Belyaev moment of inertia



Inglis-Belyaev moment of inertia
(residual interaction を無視した手法)

Residual interaction により moment of inertia は増加する。

先行研究の多くは J^{IB} または f x J^{IB}, f~1.2-1.4 などを使ってmoment of inertia を評価していたが、それでは不十分。β–γ 依存性が重要

Summary

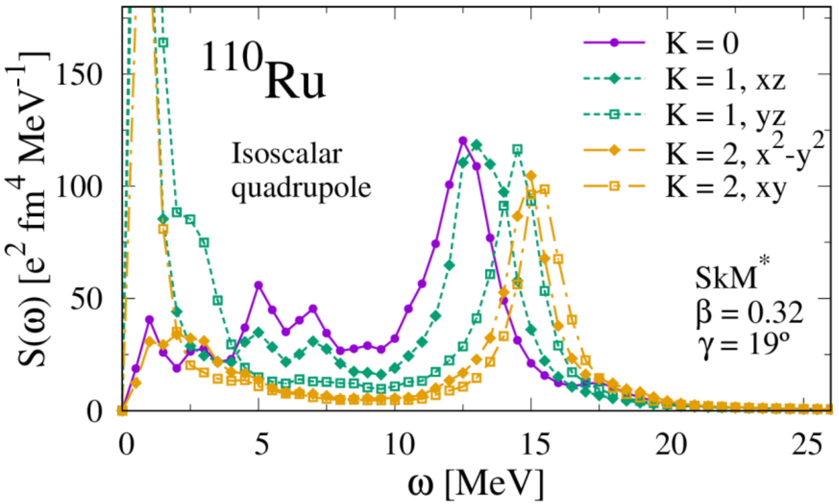
Shape fluctuation → Large amplitude collective motion

3D FAM+QRPA with Skyrme EDF is ready

Benchmark: Axial nucleus ^{24}Mg

Triaxial superfluid nucleus ^{110}Ru

Moment of inertia by Local FAM+QRPA



Future plan

Local FAM+QRPA → Mass inertial functions

5D quadrupole collective (Bohr) Hamiltonian