Large-amplitude collective dynamics with collective Hamiltonian derived from nuclear DFT + local QRPA

Kouhei Washiyama

(Center for Computational Sciences, University of Tsukuba)

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

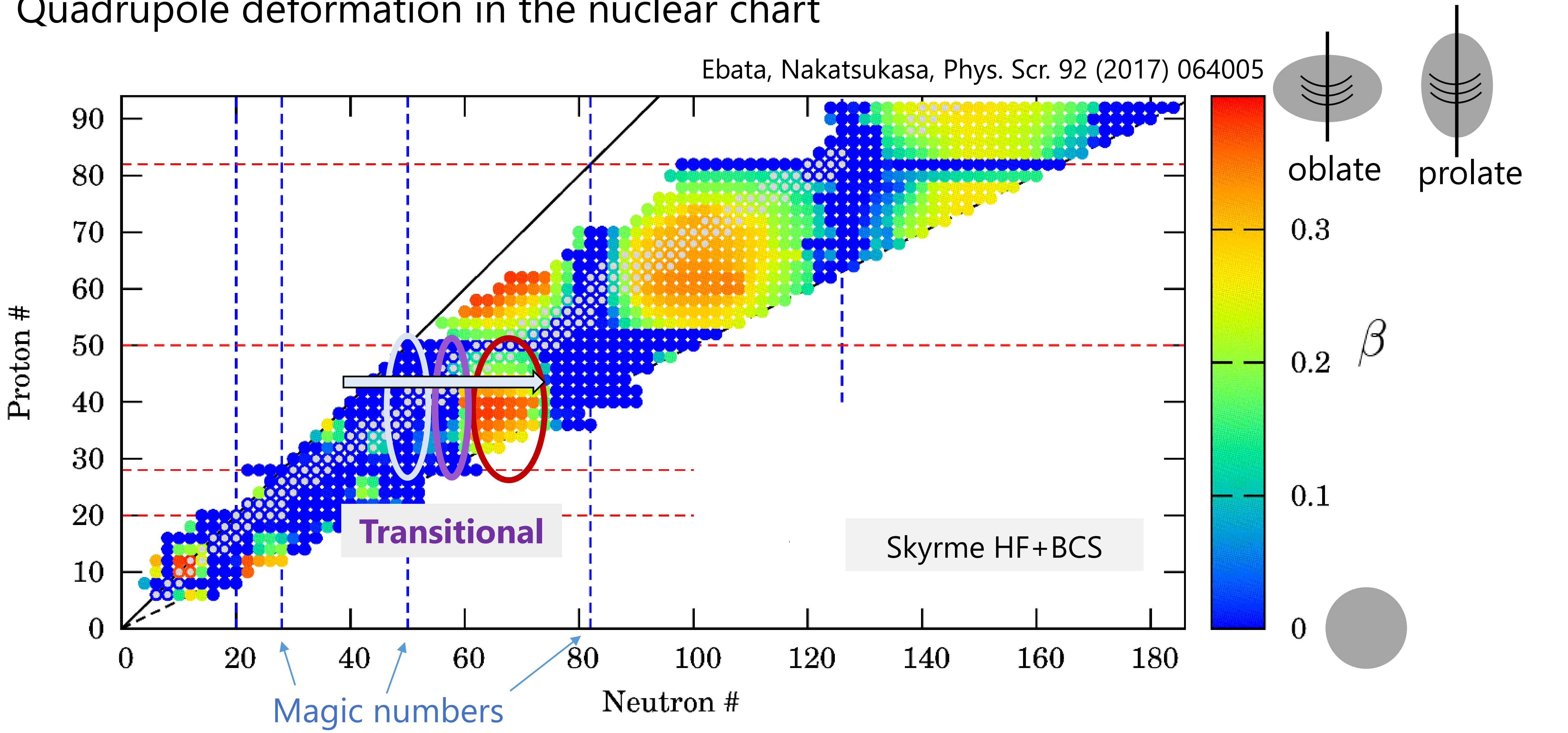
1. Introduction: Shape of nuclei
2. Method: Evaluation of collective inertia by local QRPA
3. Result: Comparison of collective inertia, low-lying spectra

Fundamentals in density functional theory (DFT2022), 2022/12/12 at YITP, Kyoto Univ.

Introduction: Shape of atomic nuclei

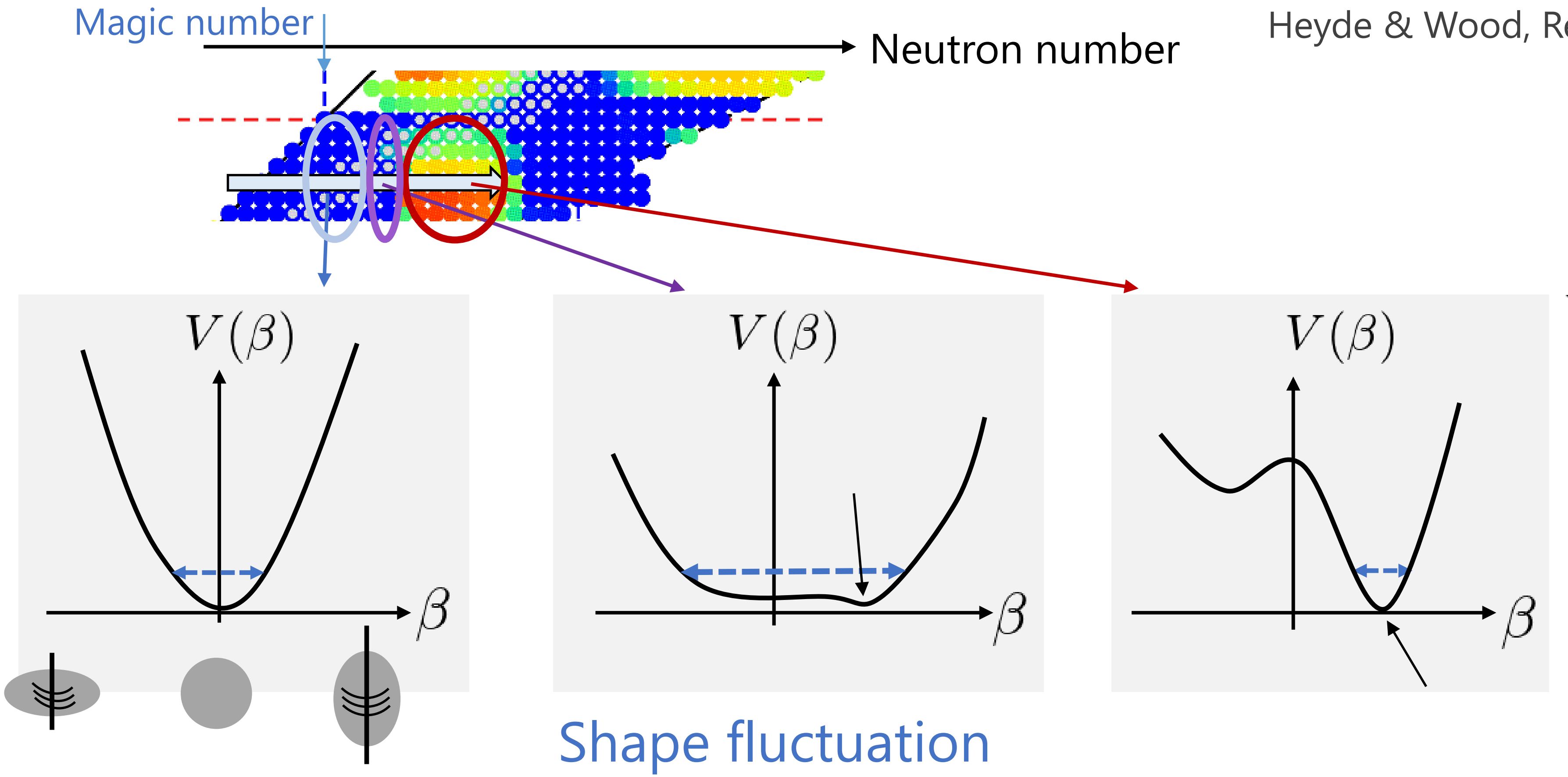
Quadrupole deformation in the nuclear chart

Ebata, Nakatsukasa, Phys. Scr. 92 (2017) 064005



Introduction: Shape of atomic nuclei

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



$$V(\beta) = E[\rho; \langle \hat{Q} \rangle = \beta]$$

Constrained DFT for shapes

Shape fluctuation

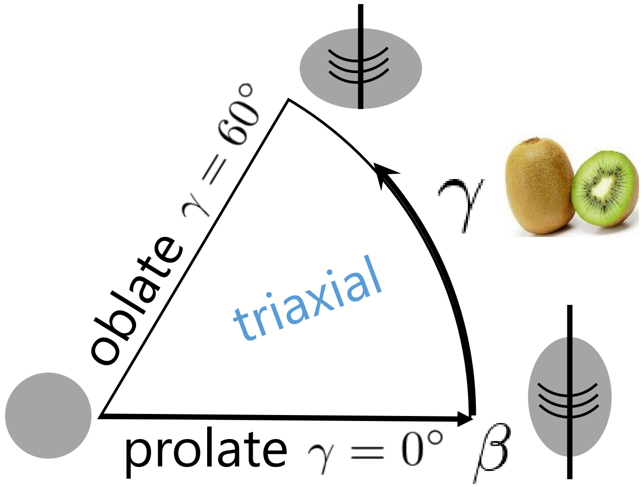
DFT for single reference state is not enough
Multi reference states for shapes are necessary

Large-amplitude collective dynamics

Bohr collective model -- Large-amplitude collective dynamics

Quadrupole deformations are described by β and γ

→ β–γ plane

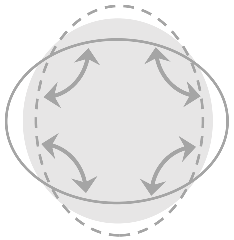


Bohr collective Hamiltonian for quadrupole dynamics

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

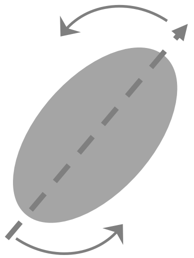
Vibrational inertia

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



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

Moment of inertia



Quantize Hamiltonian

$$\hat{H}\Psi_{\alpha IM} = E_{\alpha I}\Psi_{\alpha IM}$$

Excitation energies

Transition probabilities

Previous works on DFT-based Bohr model

Constrained DFT $V(\beta, \gamma)$

+ Cranking approximation $D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma}, \mathcal{J}_k$

Prochniak et al., NPA730 (2004) 59
Niksic et at., PRC79 (2009) 034303
Delaroche et al., PRC81 (2010) 014303, etc.

Neglect dynamical effects (time-odd terms)

Underestimate the collective inertias

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

Constrained DFT + Local QRPA

Hinohara et al., PRC82 (2010) 064313

Include dynamical effects by QRPA

High computation cost

P + Q force, β–γ plane

Skyrme DFT, axial symmetry

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

Our Method: Skyrme DFT + Local QRPA, full β–γ plane

Aim of this talk

Goal

To understand shape fluctuations and large-amplitude collective motions in nuclei by developing suitable models

Aim of this talk

To develop Skyrme DFT + Local QRPA for β–γ deformation space for the collective Hamiltonian model

To evaluate the collective inertias $D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma}, \mathcal{J}_k$ with dynamical effects that have been neglected in most previous works

Relation between QRPA and collective inertia

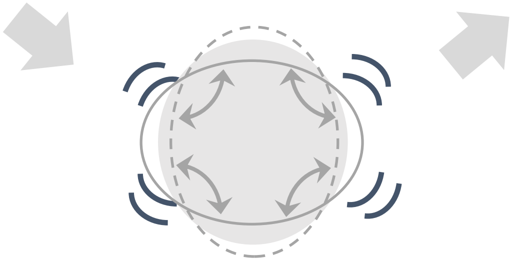
$$T_{\mathrm{vib}} = \frac{1}{2} D_{\beta\beta}(\beta,\gamma) \left(\frac{d\beta}{dt}\right)^2 + \dots$$

Collective surface vibrations

QRPA: linear response to an external field

External field

Response (collective vibrations)



Response (energy, strength) → Inertia $D_{\beta\beta}(\beta,\gamma)$

Local QRPA equations

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

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

→ $\hat{Q}^i,\ \hat{P}^i,\ C_i = \Omega_i^2$ → $M_{mn} \to D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma}$

Finite amplitude method (FAM)

Previous DFT-based works used cranking approximation for inertia

QRPA (or Adiabatic TDHFB) needs huge computational cost

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

N^2 x N^2 ~ 10^{12}

N: Number of basis (~10^3)

Finite amplitude method (FAM)

Nakatsukasa et al., PRC76 (2007) 024318
Avogadro & Nakatsukasa, PRC84(2011)014314
Stoitsov et al., PRC84 (2011) 041305
Liang et al., PRC87 (2013) 054310
Niksic et al., PRC88 (2013) 044327

Equivalent to QRPA response

Smaller computational cost

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

N x N ~ 10^6

Linear response to triaxial shape nuclei

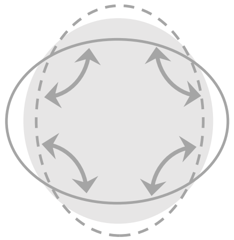
Washiyama, Nakatsukasa, PRC96, 041304(R) (2017)
Washiyama, Nakatsukasa, JPS Conf. Proc. 23, 013012 (2018)

Collective inertia in spontaneous fission

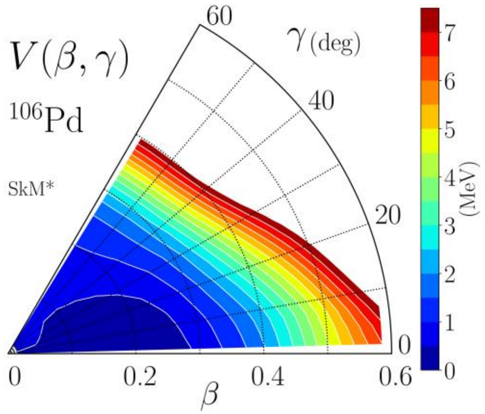
Washiyama, Hinohara, Nakatsukasa, PRC103, 014306 (2021)

Result: Vibrational inertia in ^{106}Pd

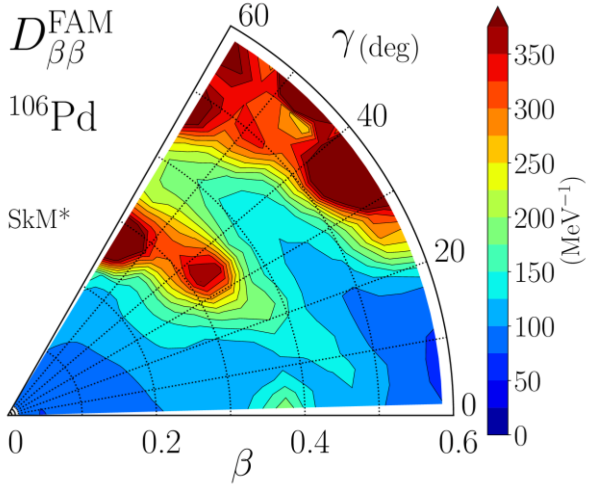
$$T_{\text{vib}} = \frac{1}{2}D_{\beta\beta}(\beta,\gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta,\gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2}D_{\gamma\gamma}(\beta,\gamma)\dot{\gamma}^2$$



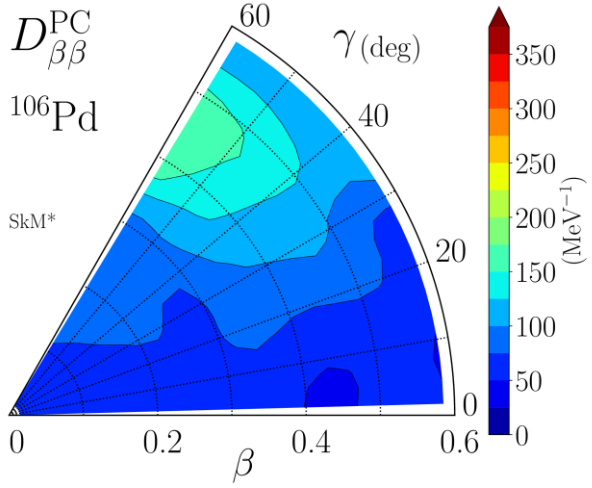
Constrained DFT



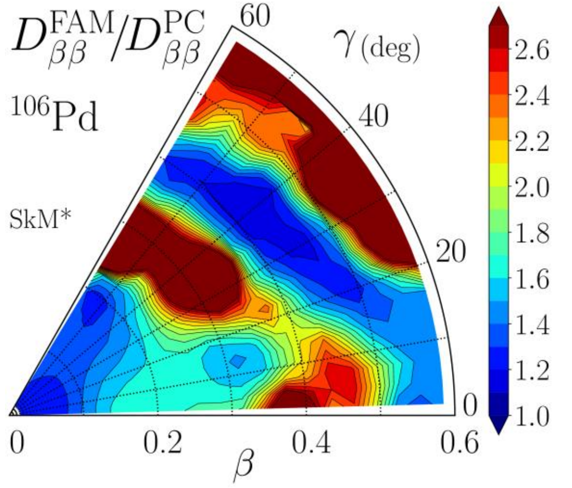
QRPA



Cranking



Ratio: QRPA/cranking



- Small at prolate side, large at oblate side
- $D_{\text{FAM}} > D_{\text{cranking}}$
- Strong variation of $D_{\text{FAM}}/D_{\text{cranking}}$

Washiyama, Hinohara, Nakatsukasa, in preparation

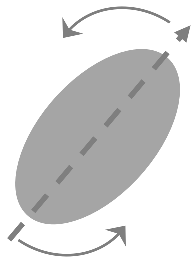
Result: Rotational moment of inertia in ^{106}Pd

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

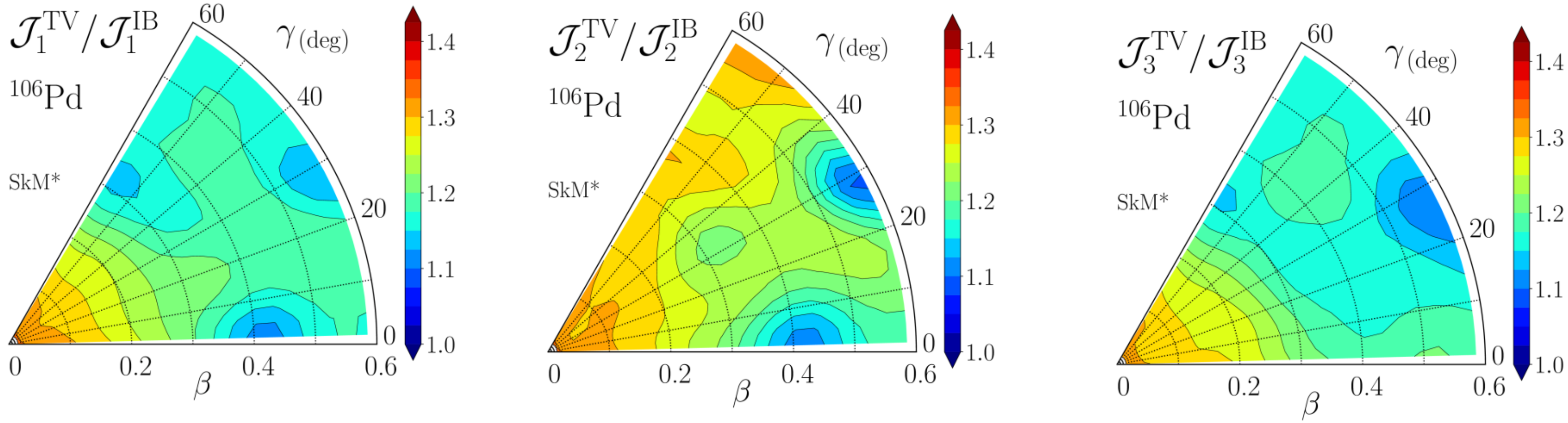
FAM + Nambu-Goldstone mode

$$S^{\mathrm{FAM}}(\hat{J}_k,\omega=0) = \sum_{\mu<\nu}[J_{\mu\nu}^{20*}X_{\mu\nu}(\omega=0) + J_{\mu\nu}^{02*}Y_{\mu\nu}(\omega=0)] = -\mathcal{J}_k$$

Hinohara, PRC92, 034321 (2015)



Ratio: QRPA/cranking

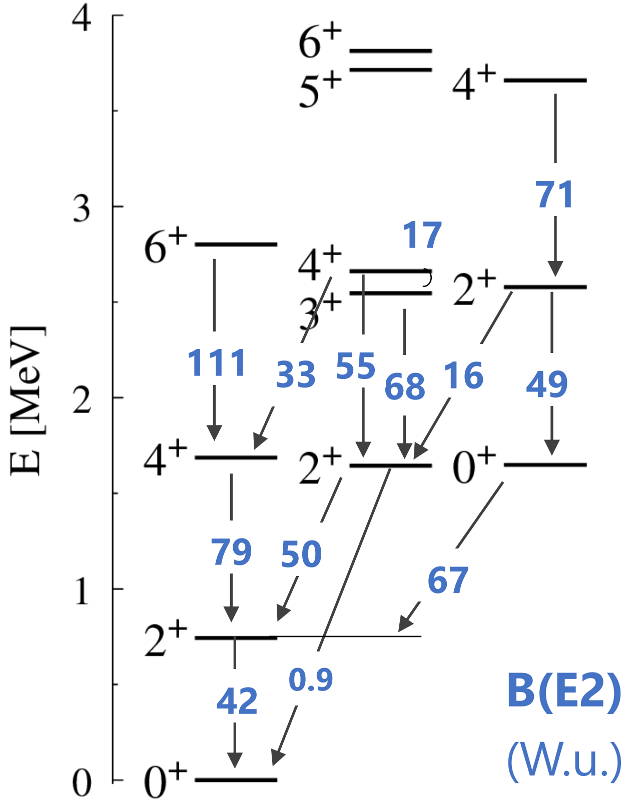


$\mathcal{J}_k^{\mathrm{QRPA}} > \mathcal{J}_k^{\mathrm{cranking}}$ (ratio = 1.1 – 1.35)

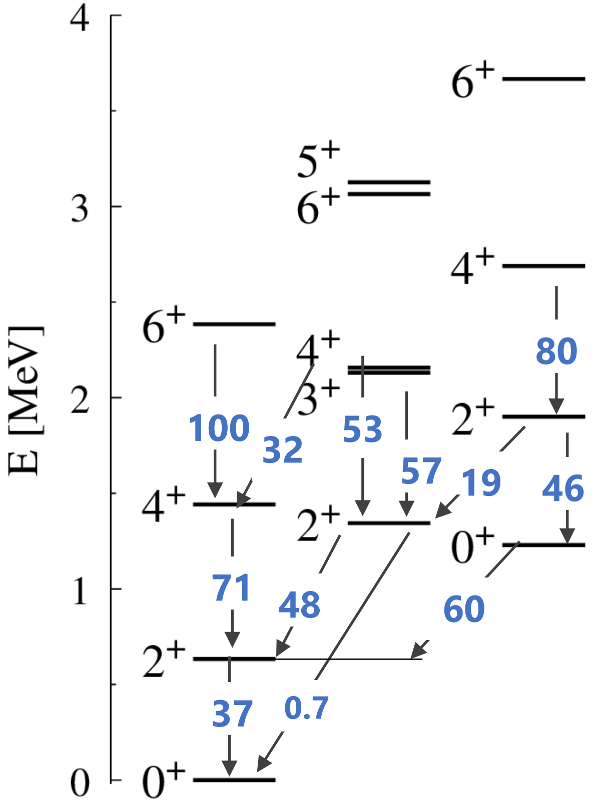
Strong β–γ dependence

Result: Low-lying levels in ^{106}Pd

^{106}Pd, **Cranking**

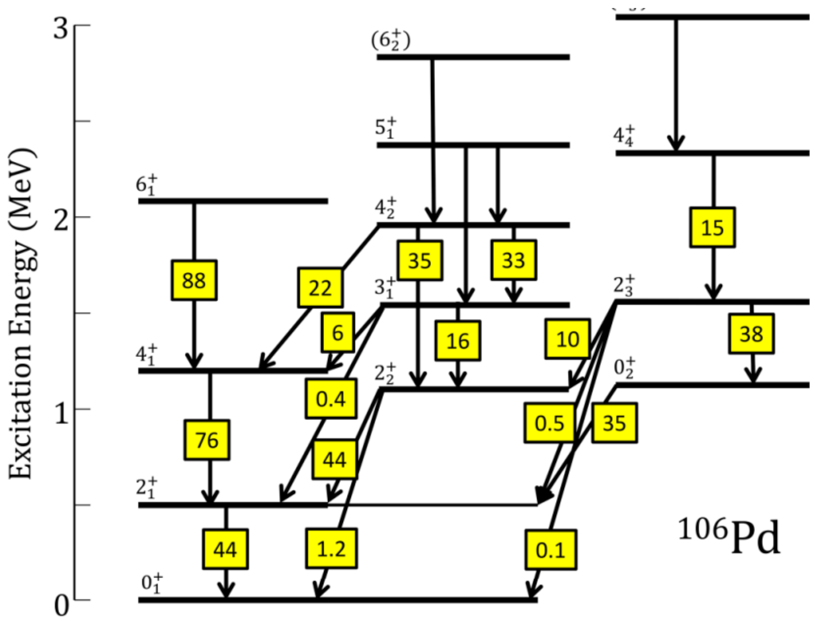


^{106}Pd, **Local QRPA**



Experiment

Prados-Estevez et al., PRC95,034328 (2017)



- Level spacing: $E_{cranking}$ > E_{QRPA}
- Quasi γ-band
- B(E2) values are reproduced

Summary

Collective inertia in Bohr Hamiltonian by DFT

Strong β–γ dependence in inertia by QRPA

Dynamical effects in QRPA increases the inertia

Better reproduction in energies of low-lying levels

Future

Pairing functionals

Systematic study