Microscopic description of shape coexistence and shape transition

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Approach to large-amplitude collective motion

- Generalized Bohr-Mottelson collective Hamiltonian

recent review: Próchniak and Rohoziński, J. Phys. G **36** 123101 (2009)

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

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

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

V(β, γ)	collective potential
D(β, γ)	vibrational collective mass
J(β, γ)	rotational moment of inertia

- Classical Hamiltonian for adiabatic quadrupole collective motion of five dimensions (quadrupole deformations β,γ, three Euler angles)
- Small-amplitude motion (surface vib. rotation, β-vib., γ-vib)
- Requantization of Hamiltonian: experimental observables

Kumar and Baranger NPA **92**, 608 (1967)

- Potential and inertial functions should be determined from microscopic theory

Inertial functions in Bohr-Mottelson Hamiltonian

Microscopic derivation of inertial functions (ATDHFB)

- **Inglis-Belyaev inertia (cranking approx.)**

  microscopic, derived from adiabatic perturbation theory
  contribution from time-odd mean-field ignored
  too small to explain vib. 0_2^+ energies, Dudek et al., Z Phys **A294**, 341(1980)
  20-30% overestimate rotational 2_1^+ energies

- **Thouless-Valatin inertia**

  microscopic, contribution from time-odd mean-field included
  rotational MOI: QRPA/adiabatic limit of cranked mean field.
  vibrational mass: QRPA (small-amplitude)
  ATDHFB (axial) Dobaczewski and Skalski, NPA**369**,123(1981)

no calculation with full βγ dependence
(large-amplitude shape vibration)

Microscopic derivations of functions in collective Hamiltonian

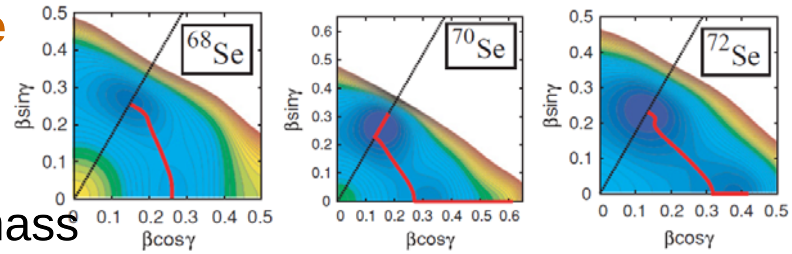
Microscopic theory of large-amplitude collective motion

“**Adiabatic self-consistent collective coordinate (ASCC) method**”

Matsuo, Nakatsukasa, Matsuyanagi, Prog.Theor.Phys.**103**,959 (2000)

Theory to determine **“collective path/subspace**

Application to 1dim collective coordinate



- ☐ time-odd mean field contribution to collective mass

Prog. Theor. Phys. **115**, 567 (2006)

- ☐ Extraction of collective path for shape coexistence ($^{68\text{-}72}$Se, ^{72}Kr)

PTP**113**, 129 (2005), PTP**119**,59(2008), PRC**80**, 014305(2009)

ASCC for two-dimensional collective subspace (q_1,q_2,p_1,p_2)

Moving-frame HFB equations (0th order in p)

$$\delta \langle \phi(\boldsymbol{q})| \hat{H}_M(\boldsymbol{q}) |\phi(\boldsymbol{q})\rangle = 0$$

$$\hat{H}_M(\boldsymbol{q}) = \hat{H} - \sum_\tau \lambda^{(\tau)}(\boldsymbol{q})\tilde{N}^{(\tau)} - \sum_i \frac{\partial V}{\partial q^i}\hat{Q}^i(\boldsymbol{q})$$

Moving-frame QRPA equations (1st and 2nd order in p)

$$\delta \langle \phi(\boldsymbol{q})| [\hat{H}_M(\boldsymbol{q}), \hat{Q}^i(\boldsymbol{q})] - \frac{1}{i}\sum_k B^{ik}(\boldsymbol{q})\hat{P}_k(\boldsymbol{q}) + \frac{1}{2}\left[\sum_k \frac{\partial V}{\partial q^k}\hat{Q}^k(\boldsymbol{q}), \hat{Q}^i(\boldsymbol{q})\right] |\phi(\boldsymbol{q})\rangle = 0$$

$$\delta \langle \phi(\boldsymbol{q})| [\hat{H}_M(\boldsymbol{q}), \frac{1}{i}\hat{P}_i(\boldsymbol{q})] - \sum_j C_{ij}(\boldsymbol{q})\hat{Q}^j(\boldsymbol{q}) - \frac{1}{2}\left[\left[\hat{H}_M(\boldsymbol{q}), \sum_k \frac{\partial V}{\partial q^k}\hat{Q}^k(\boldsymbol{q})\right], \sum_j B_{ij}(\boldsymbol{q})\hat{Q}^j(\boldsymbol{q})\right]$$

$$- \sum \frac{\partial \lambda^{(\tau)}}{\partial q^i}\tilde{N}^{(\tau)} |\phi(\boldsymbol{q})\rangle = 0$$

Microscopic derivations of functions in collective Hamiltonian

ASCC for two-dimensional collective subspace (q_1,q_2,p_1,p_2)

- one-to-one correspondence between (q_1,q_2) and (β,γ)
- $|\varphi(q_1,q_2)\rangle \sim |\varphi(\beta,\gamma)\rangle$
- curvature term omitted
- moving-frame Hamiltonian → CHFB Hamiltonian

NH et al., PRC**82**, 064313(2010)

Constrained Hartree-Fock-Bogoliubov equation

$$\delta \langle \phi(\beta,\gamma)| \hat{H}_{\mathrm{CHFB}} |\phi(\beta,\gamma)\rangle = 0$$

→ **V(β, γ)**

Local QRPA equations (for vibration)

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

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

→ **D(β, γ)**

Local QRPA equations for rotation

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

$$\langle \phi(\beta,\gamma)| [\Psi_k(\beta,\gamma), \hat{I}_k] |\phi(\beta,\gamma)\rangle = i$$

→ **J(β, γ)**

- QRPA on top of CHFB state
- Hamiltonian used in QRPA contains constraint terms

Calculation of LQRPA vibrational collective mass D(β,γ)

kinetic energy obtained from LQRPA

$$\mathcal{H}_{\text{vib}} = \frac{1}{2}\sum_{\alpha=1,2} \dot{q}_\alpha^2(\beta,\gamma)$$

(scaling: collective mass = one)

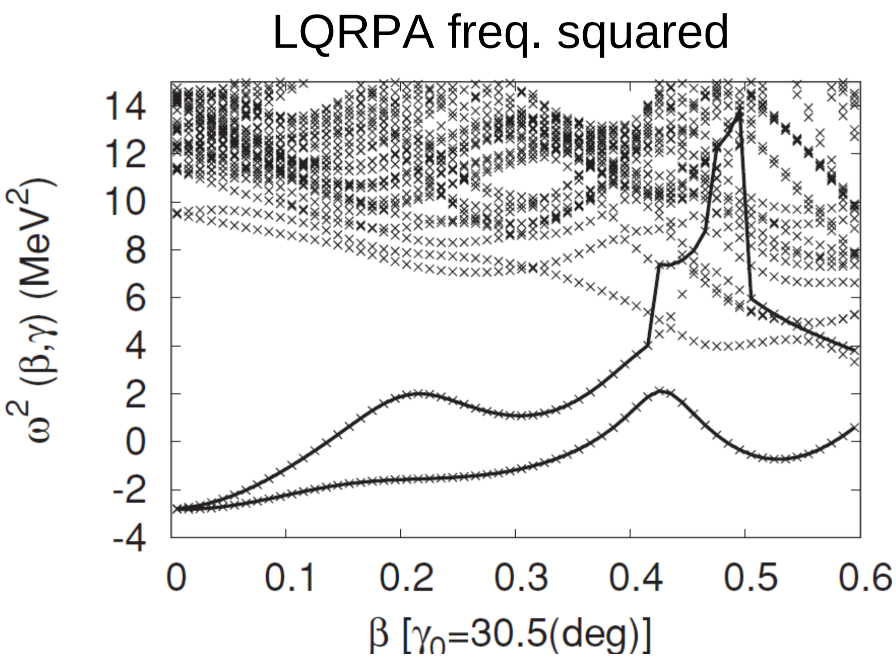
one-to-one correspondence between (q_1,q_2) and (β,γ)

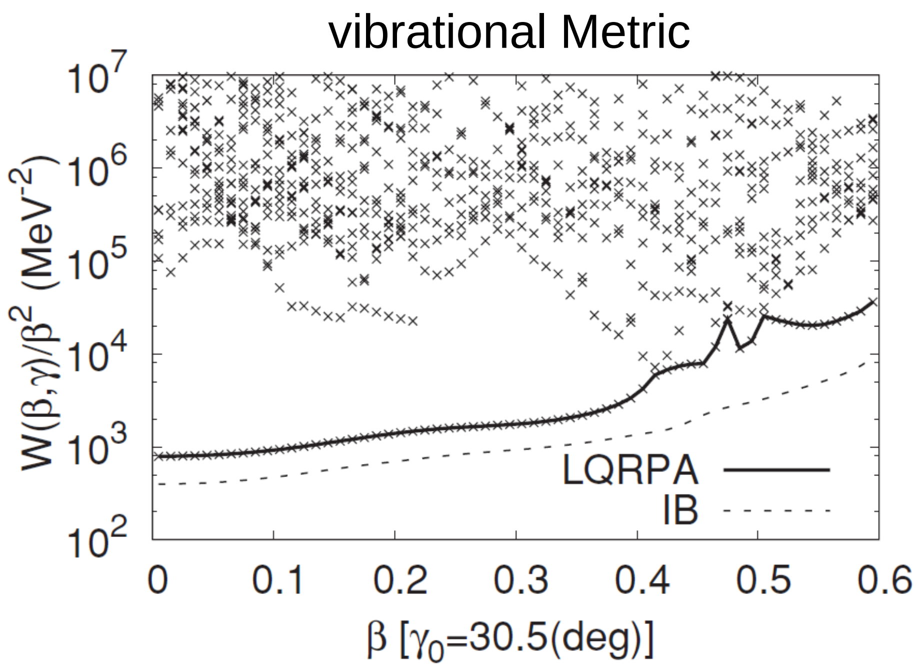
$$T_{\text{vib}} = \frac{1}{2}D_{\beta\beta}(\beta,\gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta,\gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2}D_{\gamma\gamma}(\beta,\gamma)\dot{\gamma}^2$$

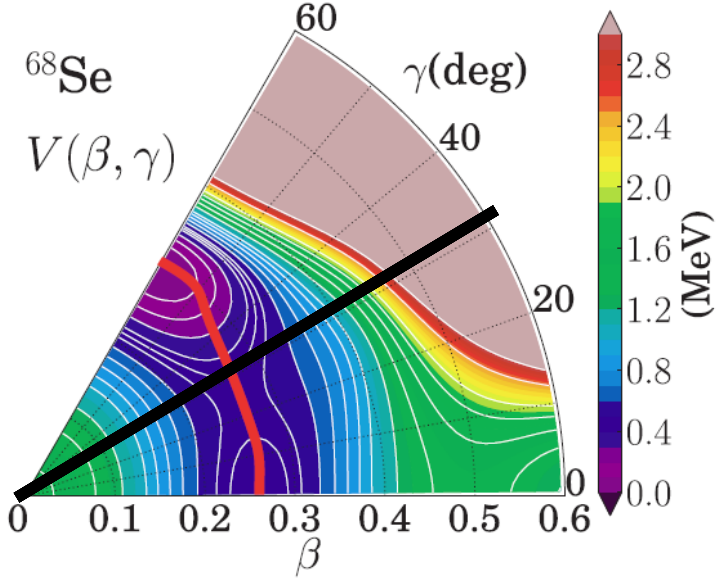
Metric: $W(\beta,\gamma) = \left\{D_{\beta\beta}(\beta,\gamma)D_{\gamma\gamma}(\beta,\gamma) - [D_{\beta\gamma}(\beta,\gamma)]^2\right\}\beta^{-2}$

We choose two "collective" LQRPA modes at each non-equilibrium (CHFB) state which give smallest quadrupole vibrational metric

Choice of collective modes (^{68}Se)



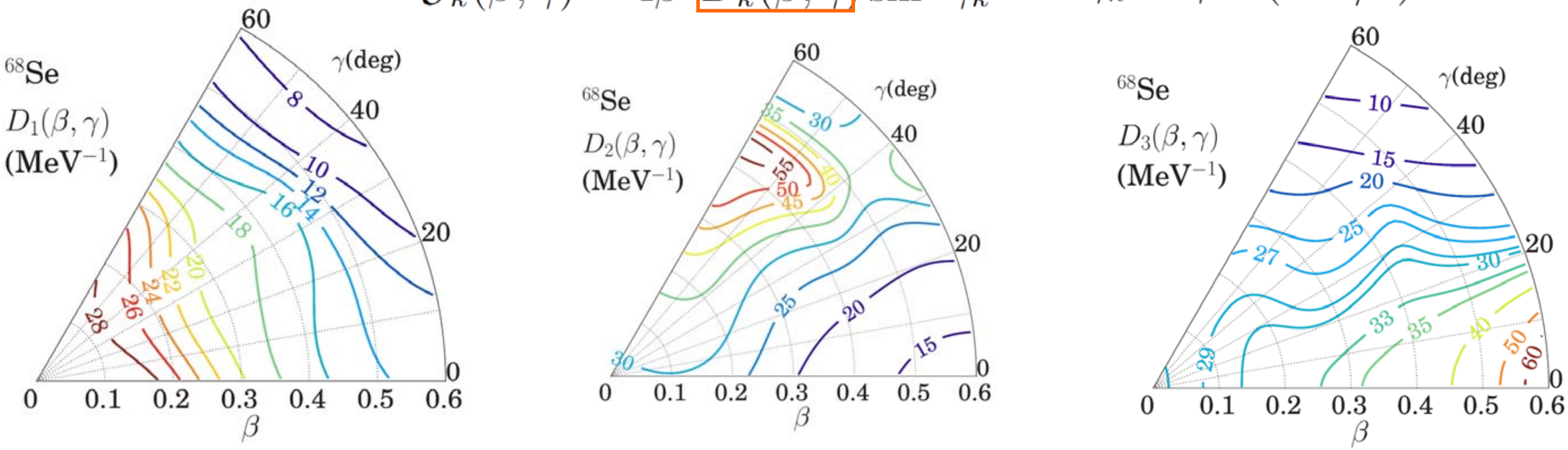




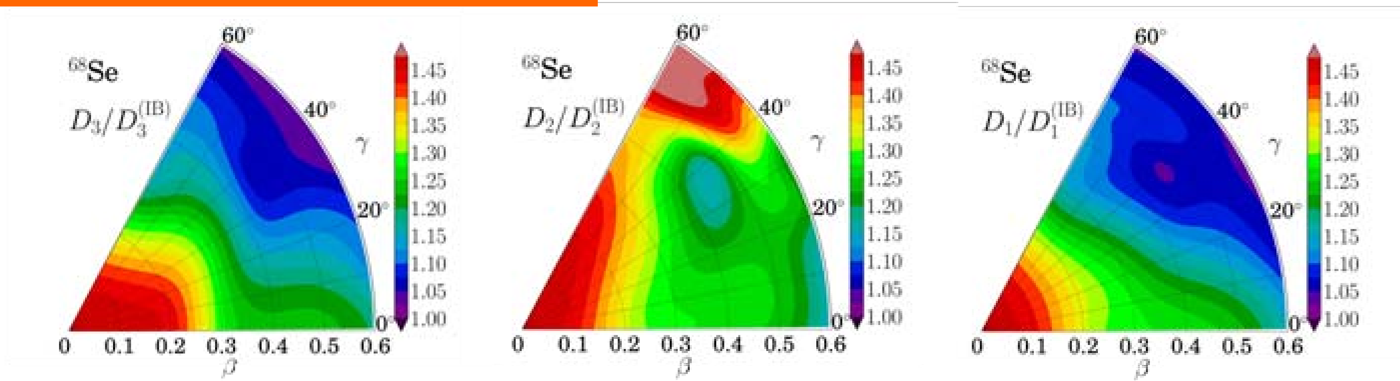
- 3,600 points in (β, γ) plane
- pairing-plus-quadrupole model including quadrupole pairing
- parameters adjusted to Skyrme SIII HFB
- two-major shell model space

Rotational moment of inertia (^{68}Se)

$$\mathcal{J}_k(\beta,\gamma) = 4\beta^2 D_k(\beta,\gamma)\sin^2\gamma_k \qquad \gamma_k = \gamma - (2\pi k/3)$$



Ratio to Inglis-Belyaev MOI



$$\frac{D^{(LQRPA)}_k(\beta,\gamma)}{D^{(IB)}_k(\beta,\gamma)}$$

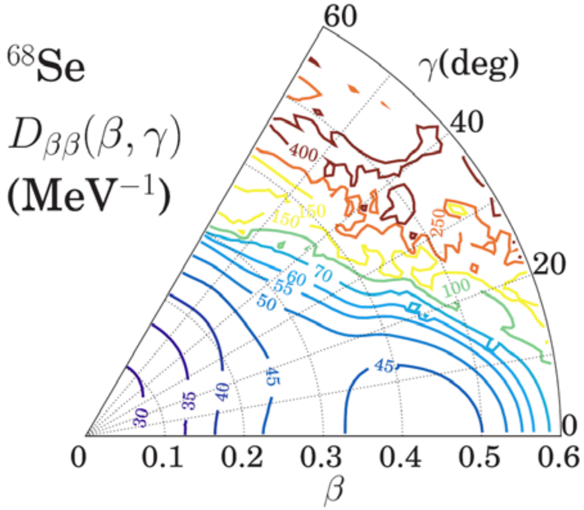
1.5

1.0

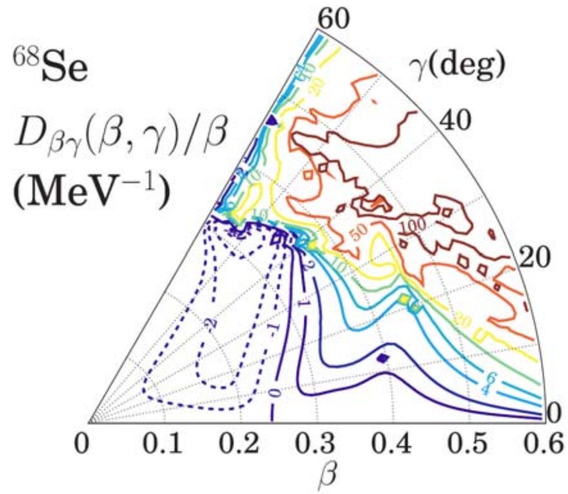
- LQRPA MOI: 1~1.5 times larger than Inglis-Belyaev values
- Deformation dependence is different between LQRPA and IB

Vibrational collective mass (^{68}Se)

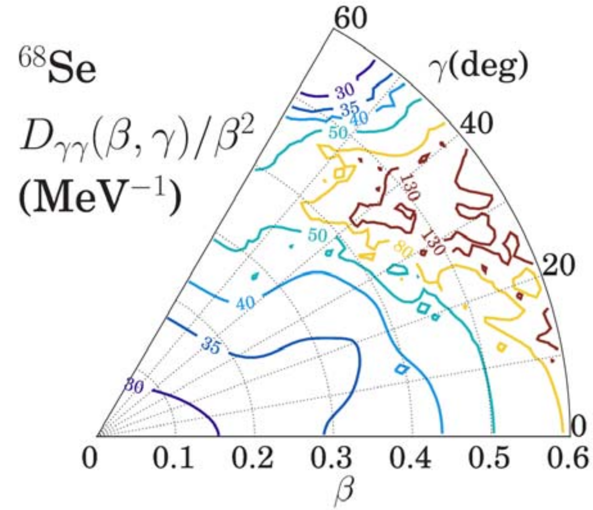
$D_{\beta\beta}$



$D_{\beta\gamma} / \beta$

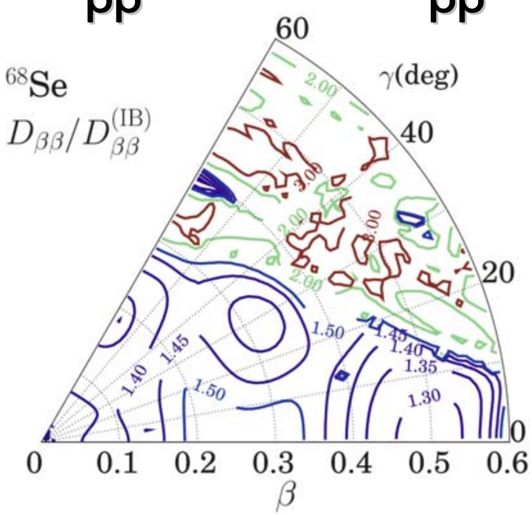


$D_{\gamma\gamma} / \beta^2$



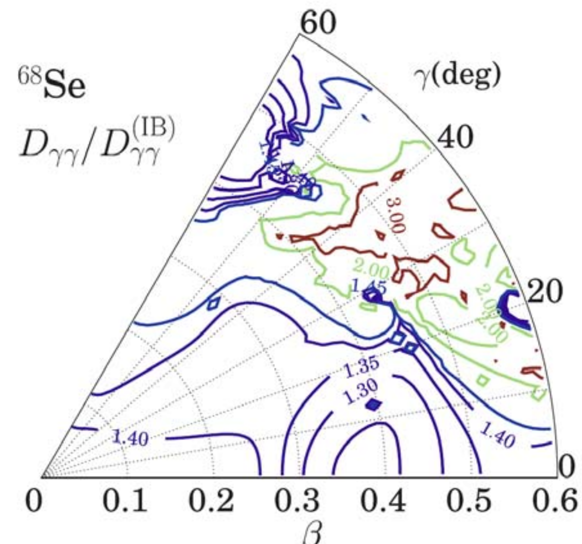
Ratio to cranking values

$D_{\beta\beta}^{(LQRPA)}/D_{\beta\beta}^{(IB)}$

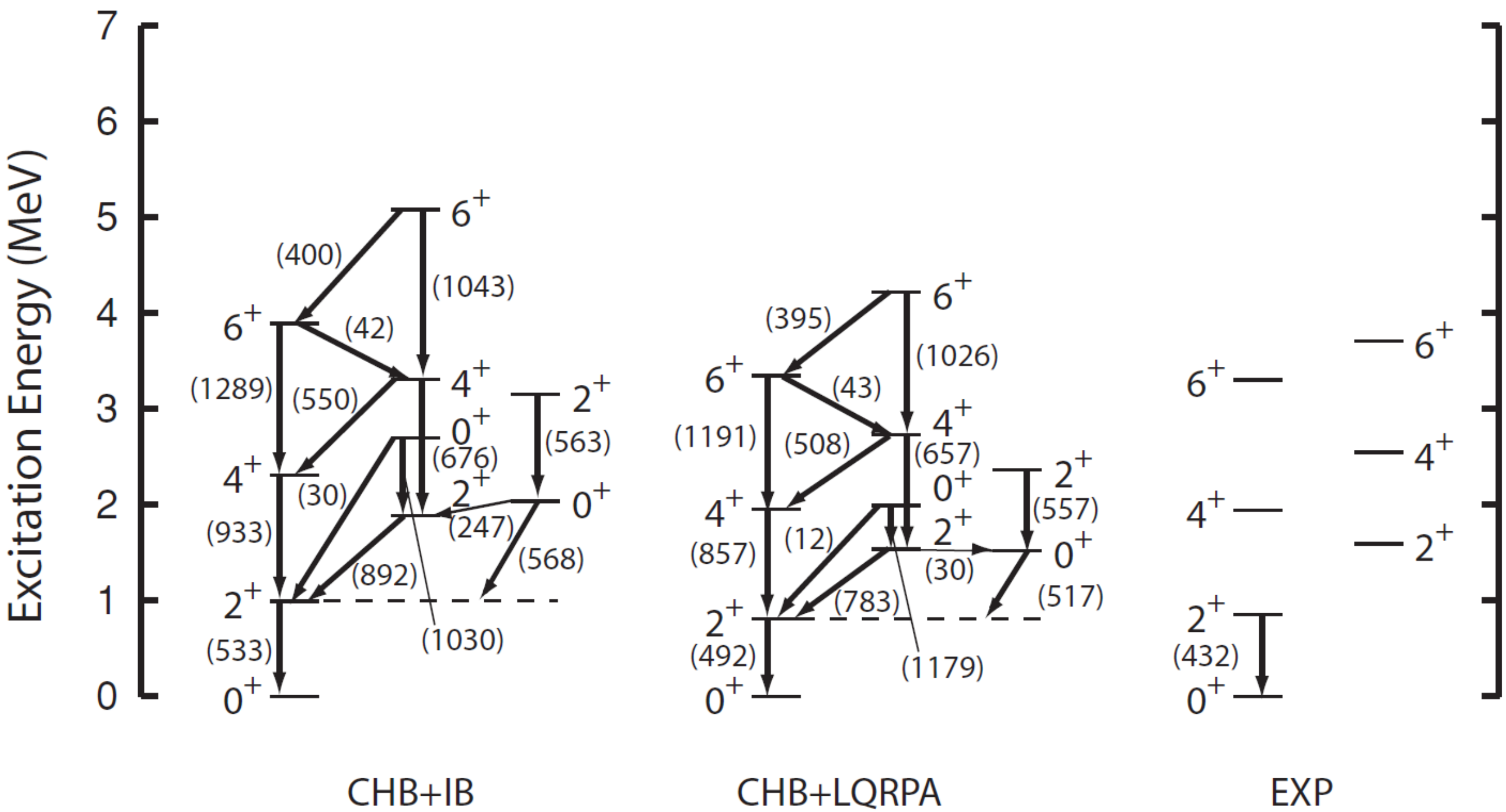


- ~3.0
- ~2.0
- 1.0~1.5

$D_{\gamma\gamma}^{(LQRPA)}/D_{\gamma\gamma}^{(IB)}$



Excitation energy of ^{68}Se



Excitation energies: lowered by contribution from time-odd mean field
0^+ energy: sensitive to inertial function

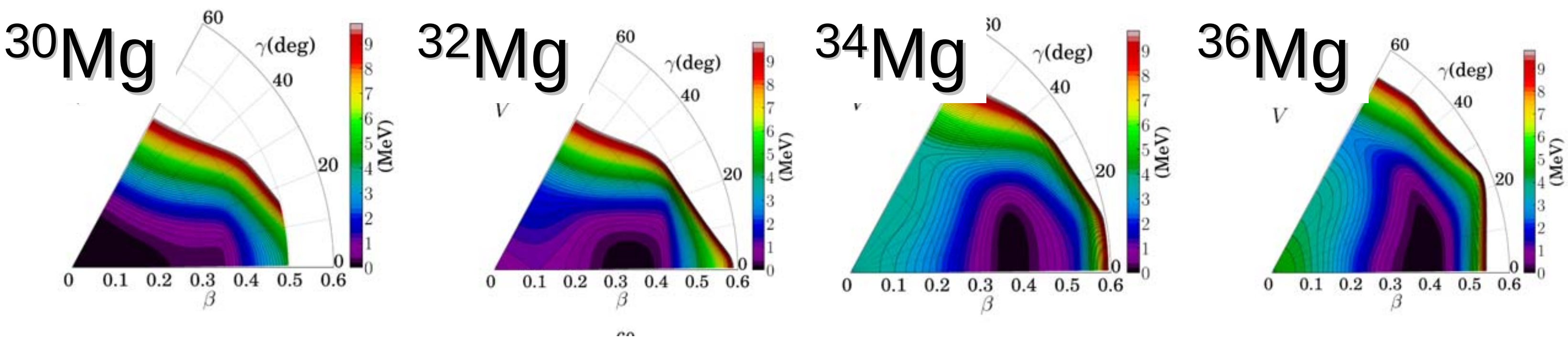
( ) .... **B(E2) e^2 fm^4**

effective charge: (en,ep)=(0.4,1.4)

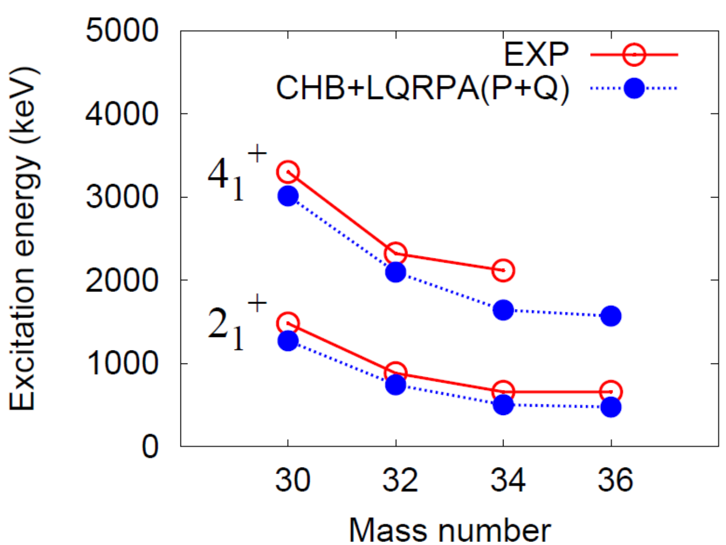
EXP：Fischer et al., Phys.Rev.**C67** (2003) 064318.
B(E2;$2_1^+ \rightarrow 0_1^+$) Obertelli et al, Phys.Rev.**C80** (2009)031304(R)

Shape coexistence in n-rich Mg isotopes

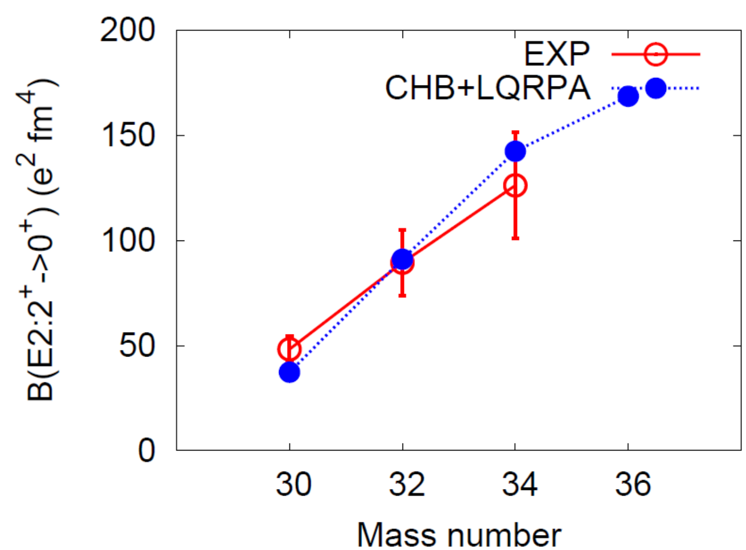
- P0+P2+Q Hamiltonian, parameters adjusted to reproduce deformations and pairing gaps (at spherical conf.) of Skyrme SkM* (HFBTHO)
- two-major oscillator shells (sd + pf), effective charge:(en,ep) = (0.5,1.5)



yrast state energies

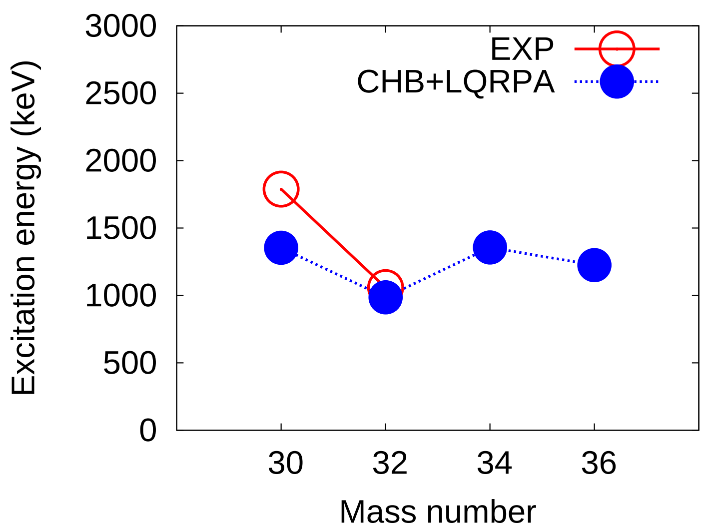


B(E2)

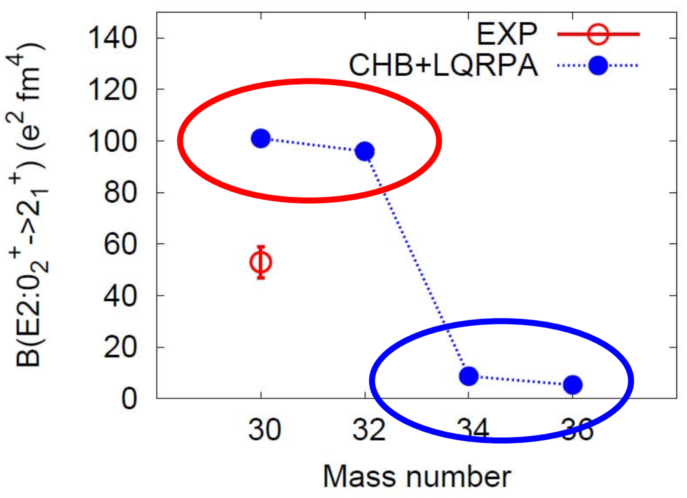


Properties of excited 0^+ states

0_2^+ energy



B(E2; $0_2^+ \rightarrow 2_1^+$)



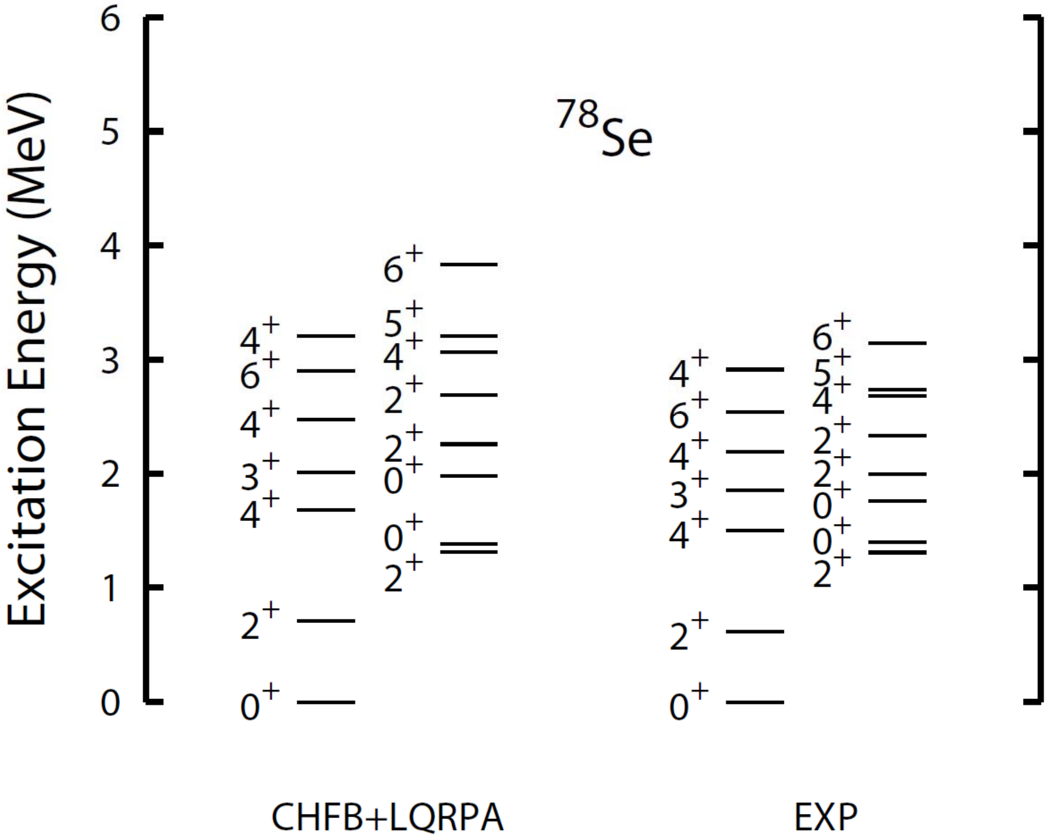
EXP

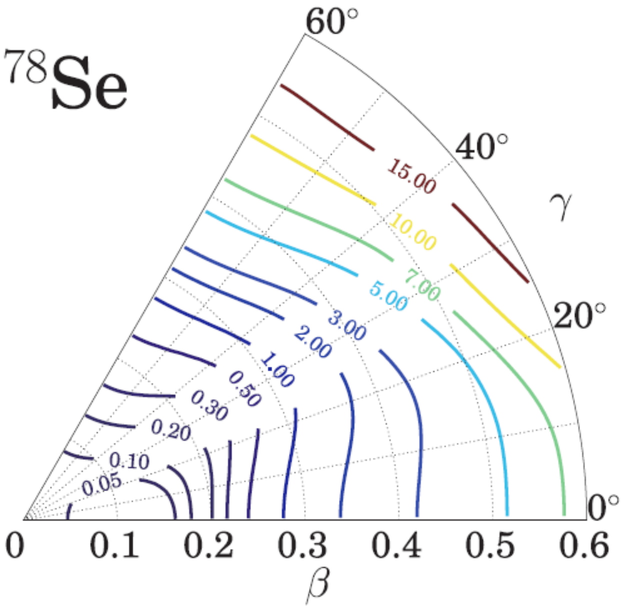
^{30}Mg W. Schwerdtfeger Phys. Rev. Lett. **103**, 012501 (2009)

^{32}Mg K. Wimmer et al. Phys. Rev. Lett. **105**, 252501 (2010)

0_2^+ changes from shape mixing to β-vibration between ^{32}Mg and ^{34}Mg

Anharmonic vibration in ^{78}Se





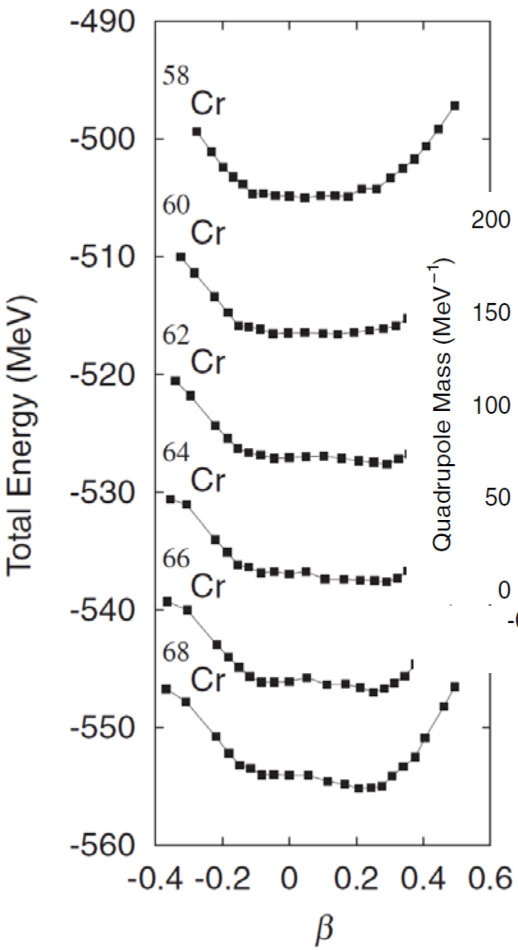
	β	⊿n(MeV)	⊿p(MeV)
SLy4	0.118	1.198	1.178
P+Q	0.116	1.180	1.161

- **Anharmonic vibrations, ordering of two-phonon states reproduced.**
- **No parameters are adjusted to the experimental data (adjusted to Skyrme-HFB)**

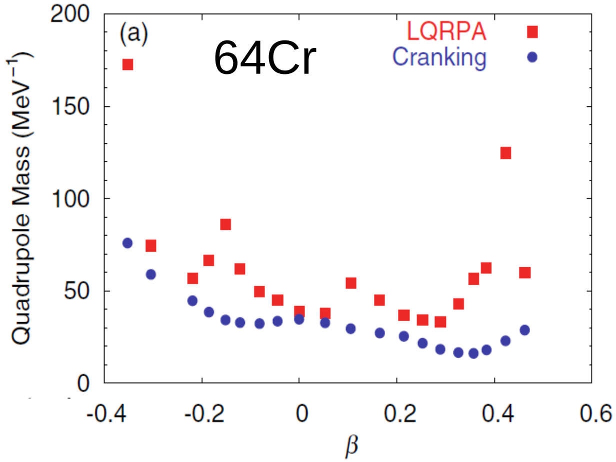
Derivation of collective Hamiltonian from Skyrme EDF

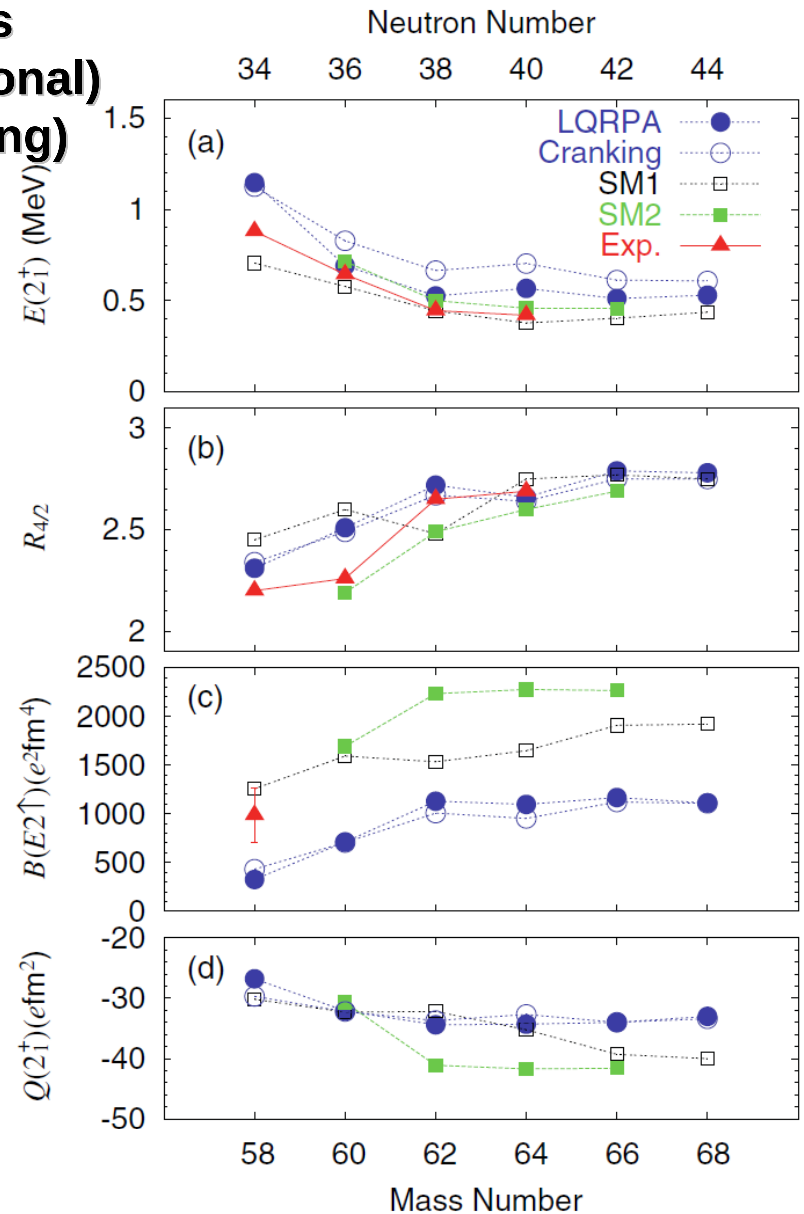
K. Yoshida and NH, Phys. Rev. C, in press.

- ☐ **Shape transition in neutron-rich Cr isotopes**
- ☐ **Axial collective Hamiltonian (three-dimensional)**
- ☐ **Skyrme CHFB+ LQRPA (SkM*, volume pairing)**



vibrational mass $M_{\beta\beta}(\beta)$





Conclusion

- We proposed a microscopic theory to construct the five-dimensional quadrupole collective Hamiltonian. (**CHFB + LQRPA method)**

- Contribution of time-odd mean field is evaluated for large-amplitude vibration and rotation, and it is shown that it increases the collective mass.

- We applied this method to shape coexistence/mixing in Se and shape phase transition in Mg isotopes.

- Axial collective Hamiltonian is constructed directly from the Skyrme EDF for neutron-rich Cr isotopes. Shape phase transition in ground band is described.