Extraction of collective coordinates by means of adiabatic theory of large-amplitude collective motion

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Collective coordinates in nuclear collective motion

Collective motion and collective coordinates

- small-amplitude collective motion
  - β vibration, γ vibration, pairing vibration, surface quadrupole vibration ...
  - approximate collective coordinates are given by known parameters, quadrupole moments, pairing gaps...
  - quasiparticle RPA(QRPA) provides optimal collective coordinates

- large-amplitude collective motion
  - symmetry restoration: translation, rotation, pairing rotation
  - -> coordinates are known
  - shape coexistence (shape vibration connecting two equilibrium shapes)
  - transitional nuclei (large shape fluctuation)
  - nuclear fission
  - nuclear fusion (reaction)
  - -> coordinates unknown, change during the motion

Adiabatic time-dependent Hartree-Fock (ATDHF(B))

- adiabatic approximation to collective motion
- goal: determination of collective coordinate / collective path
- collective Hamiltonian, collective mass

ATDHF(B)

Adiabatic approximation to time-dependent variational principle (TDVP)

$$\delta \langle \phi(t) | \, i\hbar \frac{\partial}{\partial t} - \hat{H} \, | \phi(t) \rangle = 0$$

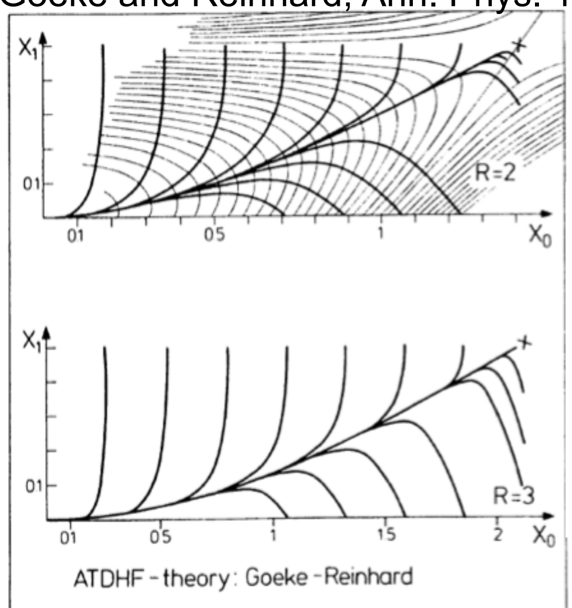
$|\phi(t)\rangle$: Slater determinant

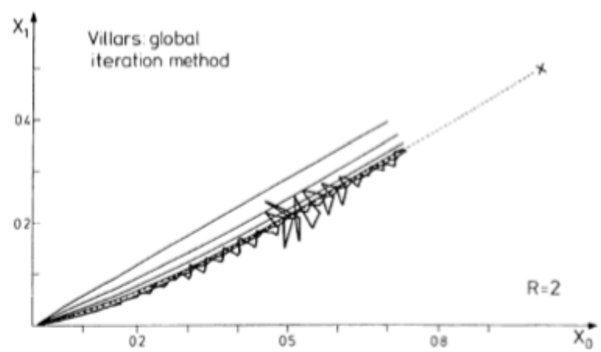
1. introduce of a few collective variables (reduction of d.o.f)
   (q: collective coordinate, p:collective momentum)
2. expand TDVP in terms of collective momenta (adiabatic exp.)
3. determine collective path and collective Hamiltonian

$$|\phi(q)\rangle \qquad \mathcal{H}(q,p) = \frac{p^2}{2M(q)} + V(q)$$

Goeke, Reinhard, Rowe NPA359,408 (1981)

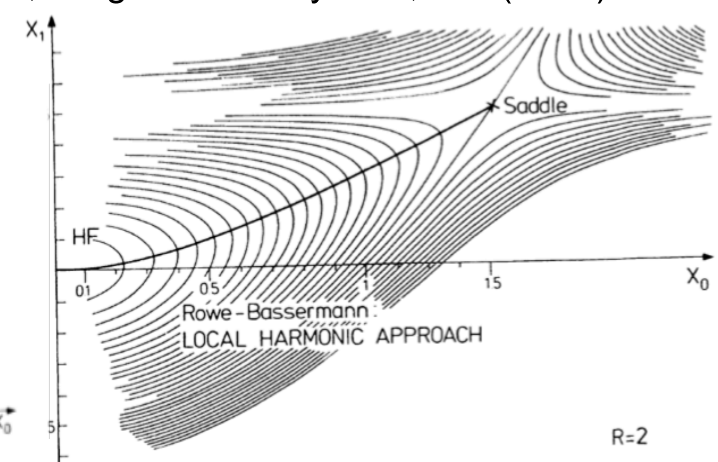
Goeke and Reinhard, Ann. Phys. 112, 328 (1978)





Villars, Nucl. Phys. A285, 269 (1977)

Rowe and Basserman, Can. Phys. 54, 1941 (1976)
Marumori, Prog. Theor. Phys. 57, 112 (1977)



Self-consistent collective coordinate (SCC) method

Marumori et al., Prog. Theor. Phys. **64**, 1294 (1980).
Matsuo et al., Prog.Theor.Phys. **76** (1986) 372.

- extract the collective subspace (path) from TDHFB manifold
- TDHFB: symplectic structure, equivalent to classical dynamics
- canonical variables for collective motion introduced
- reduction of degrees of freedom, decoupling with non-collective d.o.f.

- Time-dependent variational principle

$$\delta\langle\phi(t)|\, i\hbar\frac{\partial}{\partial t} - \hat{H}\,|\phi(t)\rangle = 0$$

$$|\phi(t)\rangle = |\phi(q,p,\varphi,n)\rangle = e^{-i\varphi\tilde{N}}\,|\phi(q,p,n)\rangle$$

collective subspace (path)

classical eq. of motion

$$\dot{q} = \frac{\partial\mathcal{H}}{\partial p} \qquad \dot{p} = -\frac{\partial\mathcal{H}}{\partial q}$$

$$\dot{\varphi} = \frac{\partial\mathcal{H}}{\partial n} \qquad \dot{n} = -\frac{\partial\mathcal{H}}{\partial \varphi} = 0$$

(q,p) :collective coordinates and momenta
(φ,n): angle in gauge space, number fluctuation

$\tilde{N} \equiv \hat{N} - N_0$ fluctuation part of number operators

SCC equation I: equation of collective submanifold

$$\delta\,\langle\phi(q,p,n)|\,\hat{H} - i\left(\frac{\partial\mathcal{H}}{\partial p}\frac{\partial}{\partial q} - \frac{\partial\mathcal{H}}{\partial q}\frac{\partial}{\partial p} + \frac{1}{i}\frac{\partial\mathcal{H}}{\partial n}\tilde{N}\right)|\phi(q,p,n)\rangle = 0$$

time-independent equation

Self-consistent collective coordinate (SCC) method

SCC equation II: canonical variable condition

$$\langle\phi(q,p,n)|\, i\frac{\partial}{\partial q}\,|\phi(q,p,n)\rangle = p + \frac{\partial S}{\partial q} \qquad \langle\phi(q,p,n)|\,\frac{\partial}{i\partial p}\,|\phi(q,p,n)\rangle = -\frac{\partial S}{\partial p}$$

$$\langle\phi(q,p,n)|\,\tilde{N}\,|\phi(q,p,n)\rangle = n + \frac{\partial S}{\partial \varphi} \qquad \langle\phi(q,p,n)|\,\frac{\partial}{i\partial n}\,|\phi(q,p,n)\rangle = -\frac{\partial S}{\partial n}$$

S: arbitrary function of q,p,φ,n

SCC equation III: collective Hamiltonian

$$\mathcal{H}(q,p,n) = \langle\phi(q,p,\varphi,n)|\,\hat{H}\,|\phi(q,p,\varphi,n)\rangle = \langle\phi(q,p,n)|\,\hat{H}\,|\phi(q,p,n)\rangle$$

- equal treatment for q and p
- original solution: (η*, η) expansion (expansion with respect to η=q+ip)
- -> applications to anharmonic phenomena, not suitable for large-amplitude collective motion

Adiabatic SCC method

Matsuo et al. Prog. Theor. Phys. **103**(2000) 959.

- alternative solution of SCC method
- expansion of the basic equations of SCC up to 2nd order in p. (adiabatic)
- no expansion with respect to collective coordinate

collective subspace Thouless th.

$$|\phi(q,p,n)\rangle = e^{ip\hat{Q}(q)+in\hat{\Theta}(q)}|\phi(q)\rangle$$

p=n=0

$$\hat{Q}(q) = \sum_{\alpha\beta}\left(Q_{\alpha\beta}(q)a^\dagger_\alpha a^\dagger_\beta + Q_{\alpha\beta}(q)^* a_\beta a_\alpha\right),$$

$$\hat{\Theta}(q) = i\sum_{\alpha\beta}\left(\Theta_{\alpha\beta}(q)a^\dagger_\alpha a^\dagger_\beta - \Theta_{\alpha\beta}(q)^* a_\beta a_\alpha\right)$$

(a(q),a⁺(q)):quasiparticle operators locally defined with a(q)|φ(q)> = 0

Collective Hamiltonian

$$\mathcal{H}(q,p,n) = V(q) + \frac{1}{2}B(q)p^2 + \lambda(q)n$$

Collective potential $V(q) = \mathcal{H}(q,p,n)|_{p=0,n=0} = \langle\phi(q)|\,\hat{H}\,|\phi(q)\rangle\,,$

(collective mass)$^{-1}$ $B(q) = \dfrac{\partial^2\mathcal{H}(q,p,n)}{\partial p^2}\Big|_{p=0,n=0} = -\langle\phi(q)|\,[[\hat{H},\hat{Q}(q)],\hat{Q}(q)]\,|\phi(q)\rangle$

chemical potential $\lambda(q) = \dfrac{\partial\mathcal{H}(q,p,n)}{\partial n}\Big|_{p=0,n=0} = \langle\phi(q)|\,[\hat{H},i\hat{\Theta}(q)]\,|\phi(q)\rangle\,.$

Adiabatic SCC method

equation of collective path (submanifold) expanded up to 2nd order in p

moving-frame HFB equation from 0th order

Moving-frame Hamiltonian

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

$$\hat{H}_M(q) = \hat{H} - \lambda(q)\hat{N} - \frac{\partial V}{\partial q}\hat{Q}(q)$$

moving-frame QRPA (quasiparticle RPA) equations from 1st and 2nd order

$$\delta\langle\phi(q)|\,[\hat{H}_M(q), \hat{Q}(q)] - \frac{1}{i}B(q)\hat{P}(q)\,|\phi(q)\rangle = 0$$

$$\delta\,\langle\phi(q)|\,[\hat{H}_M(q), \hat{P}(q)] - iC(q)\hat{Q}(q) - \frac{1}{2B(q)}[[\hat{H}_M(q), \frac{\partial V}{\partial q}\hat{Q}(q)], i\hat{Q}(q)] - i\frac{\partial \lambda}{\partial q}\tilde{N}\,|\phi(q)\rangle = 0$$

$$C(q) = \frac{\partial^2 V}{\partial q^2} + \frac{1}{2B(q)}\frac{\partial B}{\partial q}\frac{\partial V}{\partial q} \qquad \hat{P}(q)\,|\phi(q)\rangle = i\frac{\partial}{\partial q}\,|\phi(q)\rangle$$

- collective coordinate is determined locally by moving-frame QRPA eigenmode
- constrained operator Q(q) changes along the path (function of q)
- constrained operator Q(q) is a solution of moving-frame QRPA equations
- self-consistency required between moving-frame HFB and QRPA at each q

Adiabatic SCC method

canonical variable conditions

expanded up to 1st order in p

$$\langle\phi(q)|\,[\hat{Q}(q),\hat{P}(q)]\,|\phi(q)\rangle = i,$$
$$\langle\phi(q)|\,[\tilde{N},\hat{P}(q)]\,|\phi(q)\rangle = 0.$$

$$\langle\phi(q)|\,\hat{P}(q)\,|\phi(q)\rangle = 0,$$
$$\boxed{\langle\phi(q)|\,\hat{Q}(q)\,|\phi(q)\rangle = 0,}$$
$$\langle\phi(q)|\,\tilde{N}\,|\phi(q)\rangle = 0,$$
$$\langle\phi(q)|\,\hat{\Theta}(q)\,|\phi(q)\rangle = 0,$$
$$\langle\phi(q)|\,[\hat{\Theta}(q),\tilde{N}]\,|\phi(q)\rangle = i,$$
$$\langle\phi(q)|\,[\hat{Q}(q),\hat{\Theta}(q)]\,|\phi(q)\rangle = 0,$$
$$\boxed{\langle\phi(q)|\,\frac{\partial\hat{Q}}{\partial q}\,|\phi(q)\rangle = -1}$$

$$\Downarrow$$

$$\langle\phi(q)|\hat{Q}(q-\delta q)|\phi(q)\rangle = \delta q$$

scaling of the collective coordinate

gauge invariance

All ASCC equations are invariant under transformation

$$\hat{Q}(q) \to \hat{Q}(q) + \alpha\tilde{N} \qquad \lambda(q) \to \lambda(q) - \alpha\frac{\partial V}{\partial q}(q)$$
$$\hat{\Theta}(q) \to \hat{\Theta}(q) + \alpha\hat{P}(q) \qquad \frac{\partial\lambda}{\partial q}(q) \to \frac{\partial\lambda}{\partial q}(q) - \alpha C(q)$$

need to impose gauge fixing condition

NH et al., Prog. Theor. Phys. 117 (2007) 451.

Algorithm to construct the collective path (1-dim)

1. HFB and QRPA (solutions at q=0, QRPA mode with lowest frequency is chosen)
2. solve moving-frame HFB at q=q using Q(q-dq) (or combinations of operators) as an initial guess of Q(q)
3. solve moving-frame QRPA and update Q(q) (choose the lowest $\omega^2(q)=B(q)C(q)$ mode)
4. repeat 2. and 3. until the solution converges at q=q.

Moving-frame HFB equation

$$\delta\langle\phi(q)|\,\hat{H}_M(q)\,\boxed{|\phi(q)\rangle} = 0 \qquad \hat{H}_M(q) = \hat{H} - \lambda(q)\hat{N} - \frac{\partial V}{\partial q}\boxed{\hat{Q}(q)}$$

the constrained operator in the moving-frame Hamiltonian changes as a function of q (cf. constrained HFB)

constraints: neutron and proton numbers, and $\langle\phi(q)|\hat{Q}(q-\delta q)|\phi(q)\rangle = \delta q$

Moving-frame QRPA equations

$$\boxed{\delta\langle\phi(q)|}\left[\hat{H}_M(q), \boxed{\hat{Q}(q)}\right] - \frac{1}{i}B(q)\hat{P}(q)\boxed{|\phi(q)\rangle} = 0$$

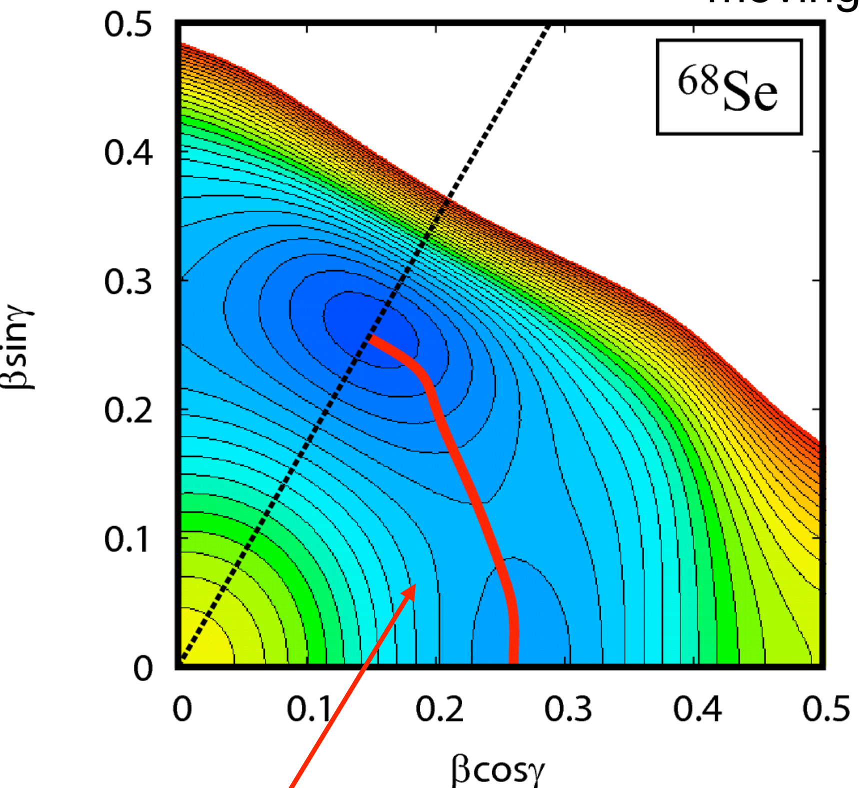
$$\boxed{\delta\langle\phi(q)|}\left[\hat{H}_M(q), \frac{1}{i}\hat{P}(q)\right] - C(q)\boxed{\hat{Q}(q)} - \frac{\partial\lambda}{\partial q}\hat{N} - \frac{1}{2B(q)}\left[\left[\hat{H}_M(q), \frac{\partial V}{\partial q}\boxed{\hat{Q}(q)}\right], \boxed{i\hat{Q}(q)}\right]\boxed{|\phi(q)\rangle} = 0$$

- self-consistency between moving-frame HFB and moving-frame QRPA

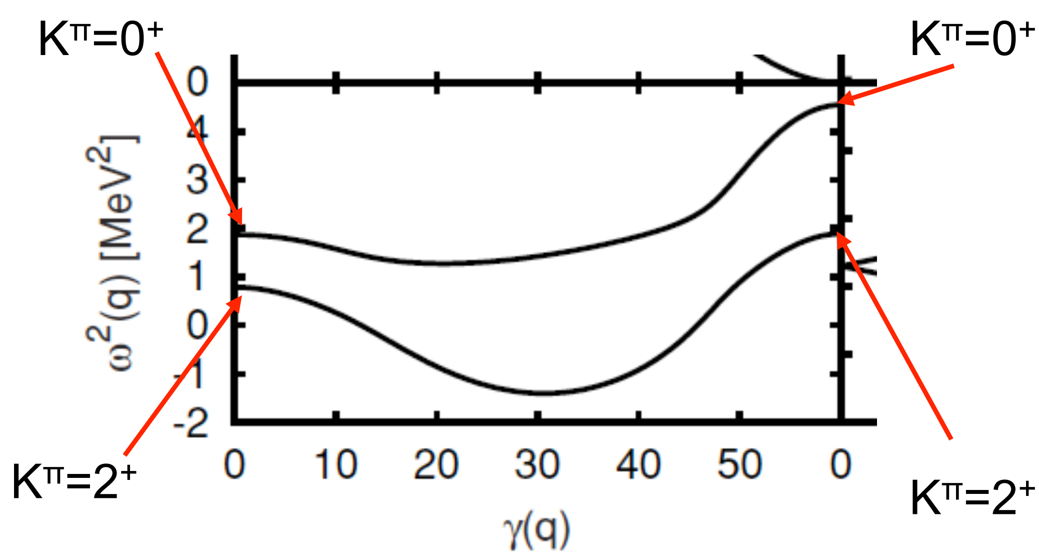
applications to oblate-prolate shape coexistence

oblate-prolate shape coexistence

NH et al., Phys. Rev. **C80**, 014305 (2009)



moving-frame QRPA frequency squared $B(q)C(q)=\omega^2(q)$



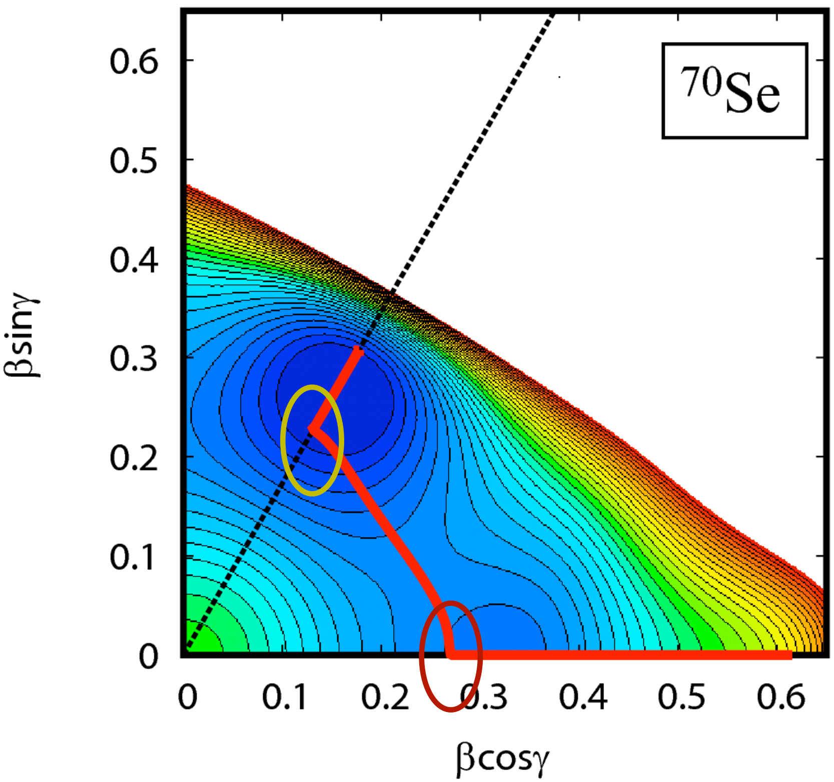
one-dimensional collective path (q) in TDHB manifold mapped onto the (β,γ) plane
($\langle\Phi(q)|Q_{20}|\Phi(q)\rangle$, $\langle\Phi(q)|Q_{22}|\Phi(q)\rangle$)

- P+Q model, 2-major shells model space, parameters simulate Skyrme-HFB(SIII)
- one-dimensional collective coordinate for oblate-prolate shape mixing
- triaxial degree of freedom is important

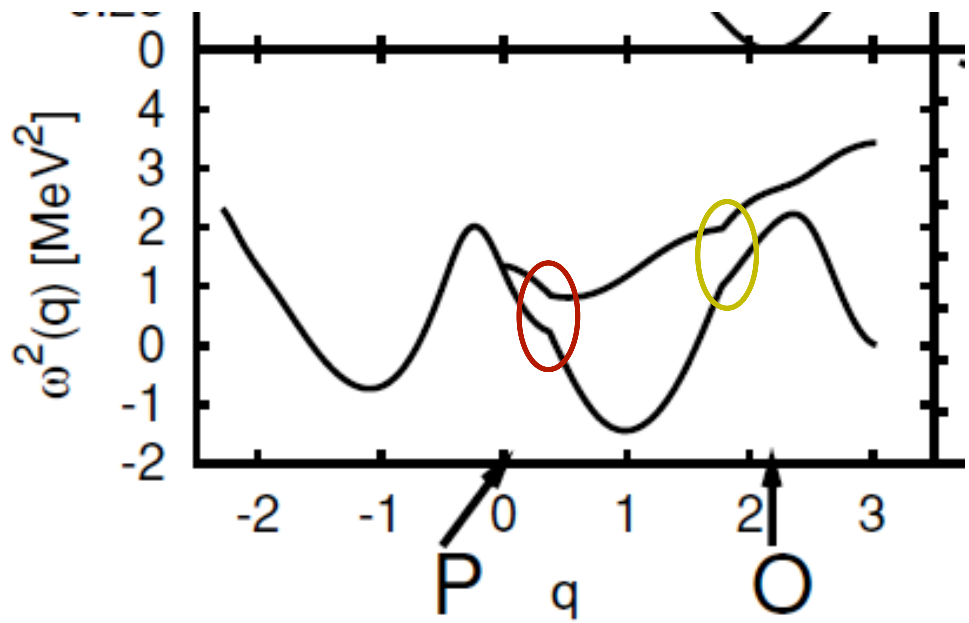
applications to oblate-prolate shape coexistence

oblate-prolate shape coexistence

NH et al., Phys. Rev. **C80**, 014305 (2009)



moving-frame QRPA frequency squared



- axial symmetry breaking path
- K-mixed operator is used for initial guess of iteration at axially symmetric region

ASCC for multi-dimensional collective subspace

Matsuo et al. Prog. Theor. Phys. **103**(2000) 959.

Collective variables

$$\boldsymbol{q} = (q^1, q^2 \cdots q^n) \qquad \boldsymbol{p} = (p_1, p_2, \cdots p_n)$$

$$|\phi(t)\rangle = |\phi(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n},\boldsymbol{\varphi})\rangle = e^{-i\varphi^{(\tau)}\widetilde{N}_{(\tau)}} |\phi(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n})\rangle$$

$$|\phi(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n})\rangle = e^{i\hat{G}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n})} |\phi(\boldsymbol{q})\rangle \qquad \hat{G}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n}) = p_i \hat{Q}^i(\boldsymbol{q}) + n_{(\tau)}\hat{\Theta}^{(\tau)}(\boldsymbol{q})$$

Collective Hamiltonian

$$\mathcal{H}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n}) = \langle\phi(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n})| \hat{H} |\phi(\boldsymbol{q},\boldsymbol{p},\boldsymbol{n})\rangle = V(\boldsymbol{q}) + \frac{1}{2}B^{ij}(\boldsymbol{q})p_i p_j + \lambda^{(\tau)}(\boldsymbol{q})n_{(\tau)}$$

moving-frame HFB equation

$$\delta \langle\phi(\boldsymbol{q})| \hat{H}_M(\boldsymbol{q}) |\phi(\boldsymbol{q})\rangle = 0 \qquad \hat{H}_M(\boldsymbol{q}) = \hat{H} - \frac{\partial V}{\partial q^i}\hat{Q}^i(\boldsymbol{q}) - \lambda^{(\tau)}(\boldsymbol{q})\widetilde{N}_{(\tau)}$$

moving-frame QRPA equations

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

$$\delta \langle\phi(\boldsymbol{q})| \left[\hat{H}_M(\boldsymbol{q}), \frac{1}{i}\hat{P}_i(\boldsymbol{q})\right] - C_{ij}(\boldsymbol{q})\hat{Q}^j(\boldsymbol{q})$$
$$- \frac{1}{2}\left[\left[\hat{H}_M(\boldsymbol{q}), \frac{\partial V}{\partial q^k}\hat{Q}^k(\boldsymbol{q})\right], B_{ij}(\boldsymbol{q})\hat{Q}^j(\boldsymbol{q})\right] - \frac{\partial \lambda^{(\tau)}}{\partial q^i}\widetilde{N}_{(\tau)} |\phi(\boldsymbol{q})\rangle = 0$$

$$C_{ij}(\boldsymbol{q}) = \frac{\partial^2 V}{\partial q^i \partial q^j} - \Gamma^k_{ij}\frac{\partial V}{\partial q^k} \qquad \hat{P}_i(\boldsymbol{q})|\phi(\boldsymbol{q})\rangle = i\frac{\partial}{\partial q^i}|\phi(\boldsymbol{q})\rangle \qquad \Gamma^i_{kj} = \frac{1}{2}B^{il}\left(\frac{\partial B_{lk}}{\partial q^j} + \frac{\partial B_{lj}}{\partial q^k} - \frac{\partial B_{kj}}{\partial q^l}\right)$$

Bohr Mottelson collective Hamiltonian

- full 2D ASCC solution: future task
- mapping collective subspace (q_1, q_2) to geometrical (β,γ) plane
- determine the inertial functions in Bohr-Mottelson collective Hamiltonian

- Generalized Bohr-Mottelson collective Hamiltonian

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

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

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

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

CHFB+LQPRA

- one-to-one correspondence between (q_1,q_2) and (β,γ)
- |φ(q_1,q_2)>~|φ(β,γ)>
- curvature term omitted
- moving-frame Hamiltonian → CHFB Hamiltonian

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

Constrained Hartree-Fock-Bogoliubov equation

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

collective potential → **V(β, γ)**

Local QRPA equations (for large-amplitude vibration)

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

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

vibrational mass → **D(β, γ)**

Local QRPA equations for rotation

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

rotational moment of inertia → **J(β, γ)**

- QRPA on top of CHFB state
- calculations at different (β,γ) is individual. easy to parallelize.
- vibrational mass and moment of inertia includes the time-odd contribution

Derivation of D(β,γ) from local normal mode

Kinetic energy of two LQRPA modes

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

scaled in collective mass = 1

(q_1,q_2) <-> (β,γ)

$$dq_\alpha = \sum_{m=0,2} \frac{\partial q_\alpha}{\partial D_{2m}^{(+)}} dD_{2m}^{(+)}$$

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

LQRPA phonon operator

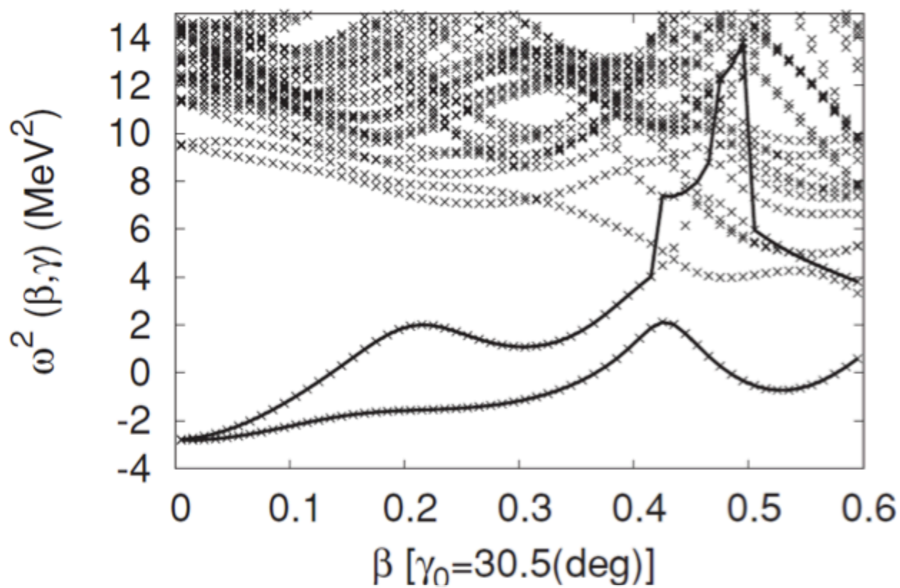
$$\frac{\partial D_{2m}^{(+)}}{\partial q_\alpha} = \frac{\partial}{\partial q_\alpha}\langle\phi(\beta,\gamma)|\,\hat{D}_{2m}^{(+)}\,|\phi(\beta,\gamma)\rangle = \langle\phi(\beta,\gamma)|\,[\hat{D}_{2m}^{(+)}, \frac{1}{i}\hat{P}^\alpha(\beta,\gamma)]\,|\phi(\beta,\gamma)\rangle$$

vib. part of metric $W(\beta,\gamma) = \{D_{\beta\beta}(\beta,\gamma)D_{\gamma\gamma}(\beta,\gamma) - [D_{\beta\gamma}(\beta,\gamma)]^2\}\beta^{-2}$

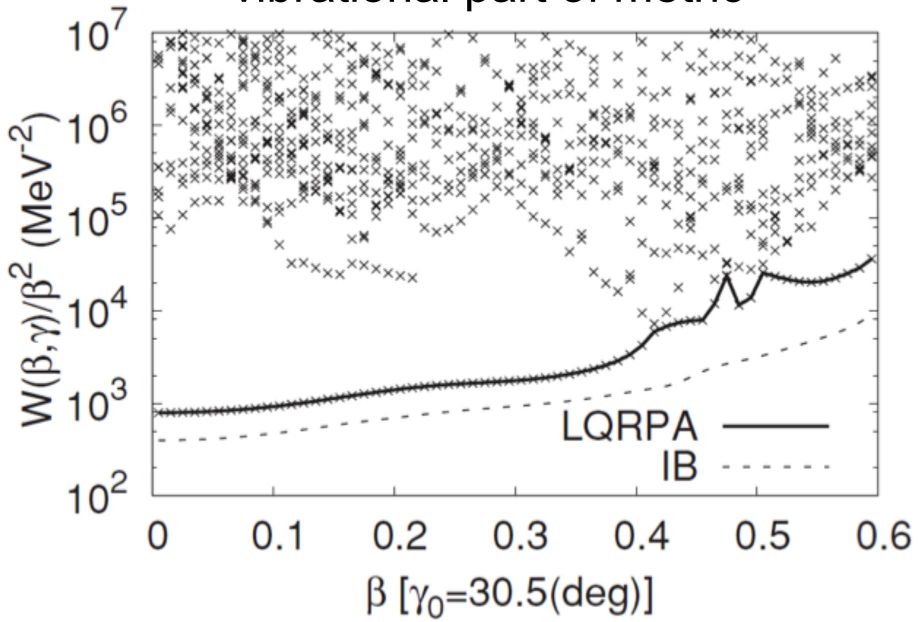
criterion to choose two LQRPA modes:
at each (β,γ) point, choose a pair which gives smallest W(β,γ)
(displacement in β-γ direction is largest)

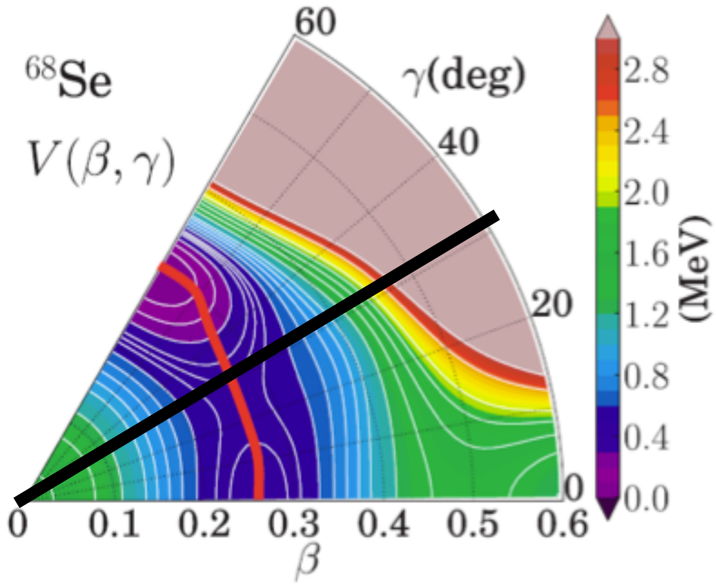
Choice of collective LQRPA modes (^{68}Se)

LQRPA frequencies squared



vibrational part of metric





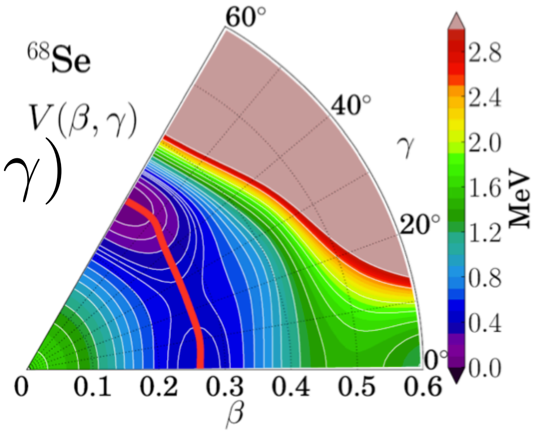
- 3,600 points in (β,γ) plane
- lines: collective modes chosen

Application to oblate-prolate shape coexistence (^{68}Se)

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

collective potential

$V(\beta,\gamma)$

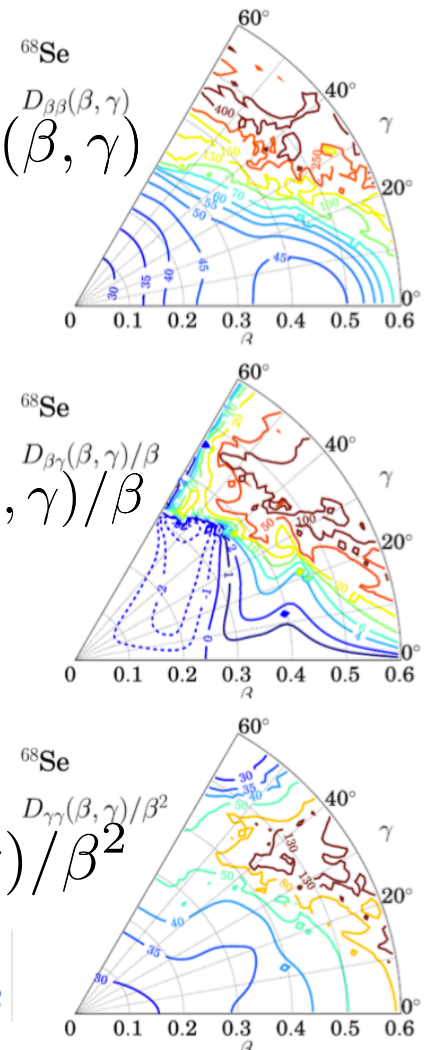


vibrational mass

$D_{\beta\beta}(\beta,\gamma)$

$D_{\beta\gamma}(\beta,\gamma)/\beta$

$D_{\gamma\gamma}(\beta,\gamma)/\beta^2$

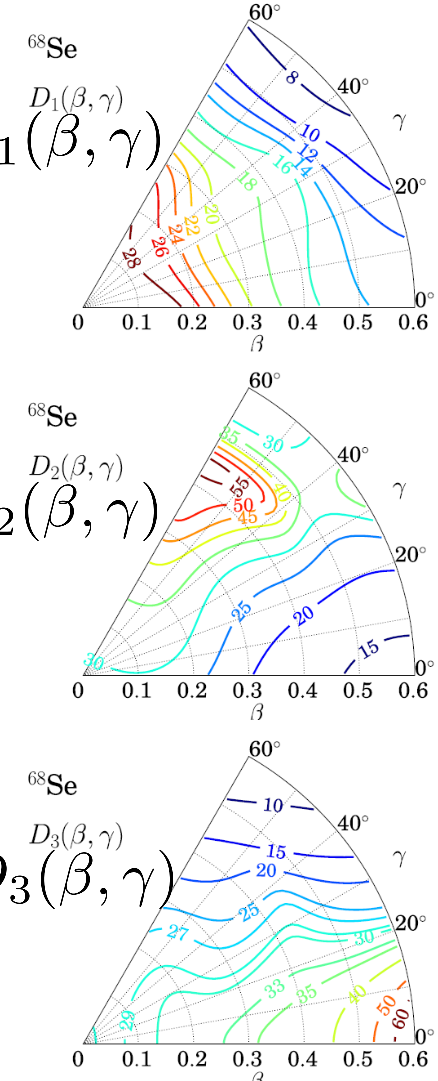


rotational mass

$D_1(\beta,\gamma)$

$D_2(\beta,\gamma)$

$D_3(\beta,\gamma)$



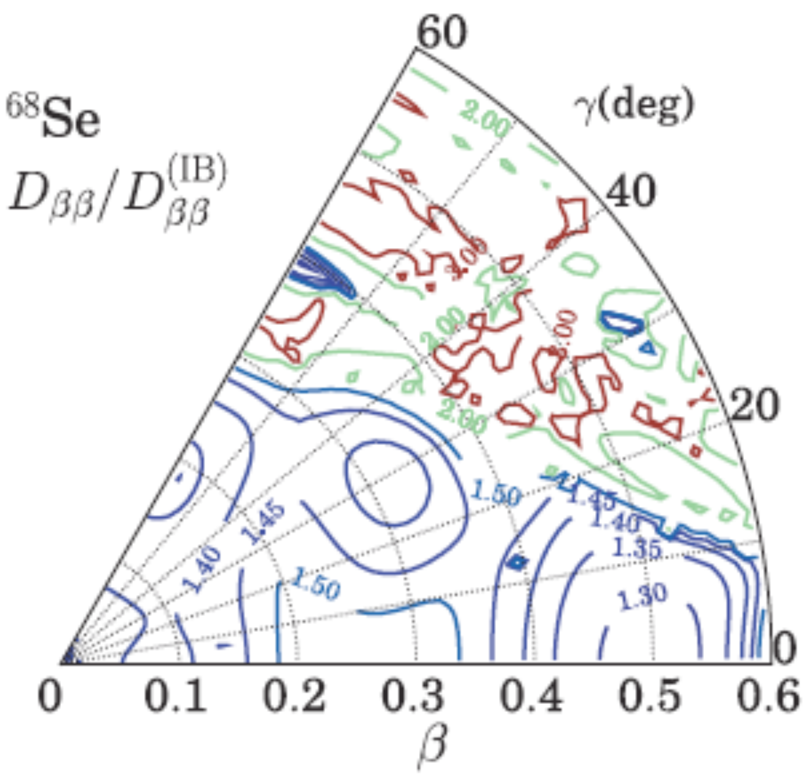
$$\mathcal{J}_k(\beta,\gamma) = 4\beta^2 \boxed{D_k(\beta,\gamma)} \sin^2\gamma_k$$

$$\gamma_k = \gamma - (2\pi k/3)$$

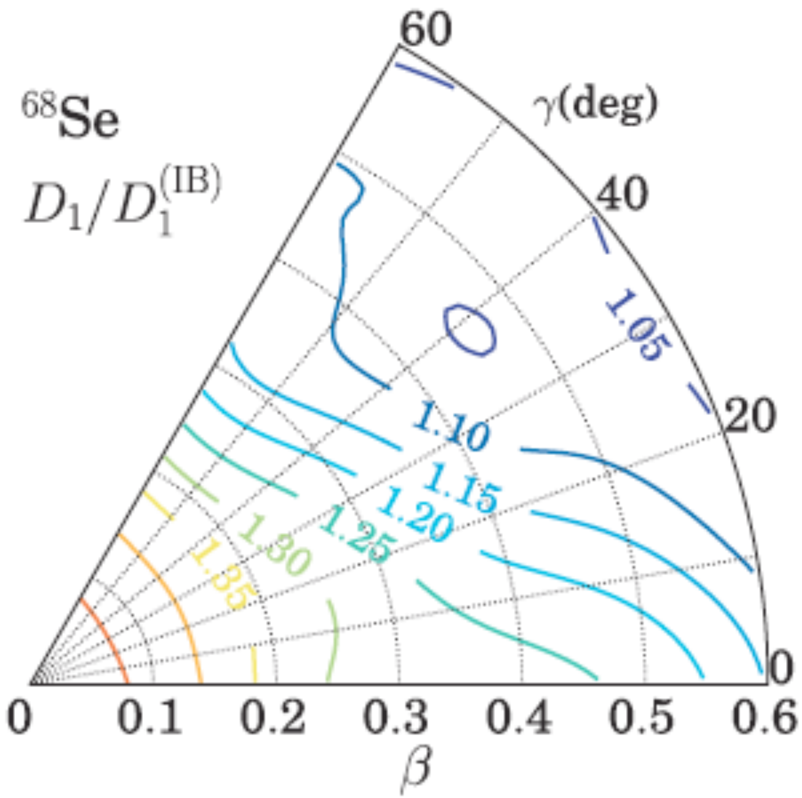
Effect of time-odd component

Ratio to Inglis-Belyaev cranking vibrational/rotational mass

vibrational mass



rotational mass

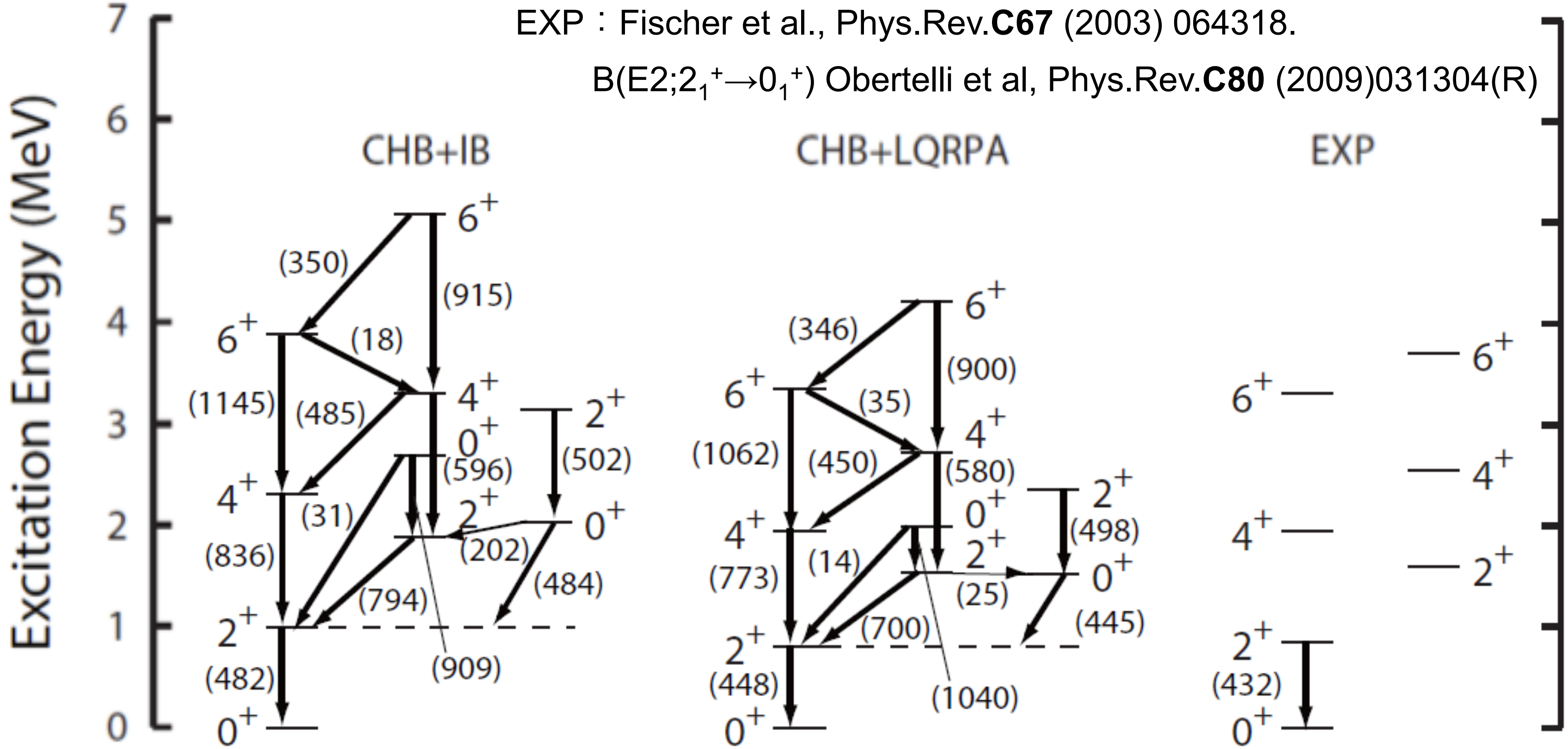


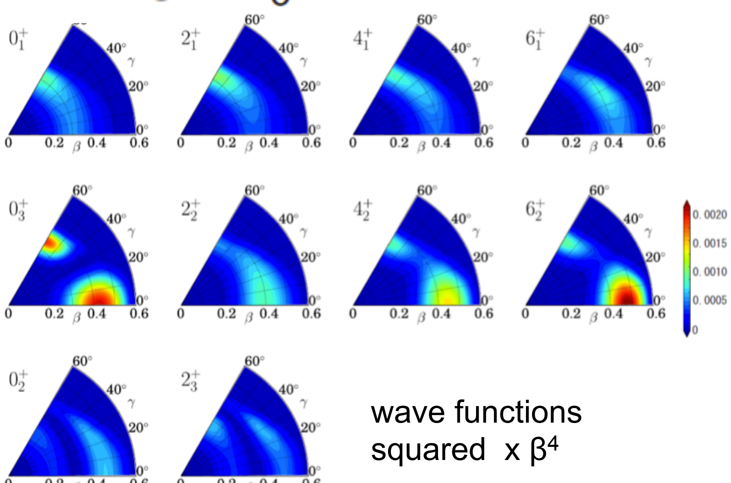
- time-odd component generated by quadrupole-pairing
- LQRPA MOI: 1~1.5 times larger than Inglis-Belyaev values
- Deformation dependence is different between LQRPA and IB

Excitation energy of ^{68}Se

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)

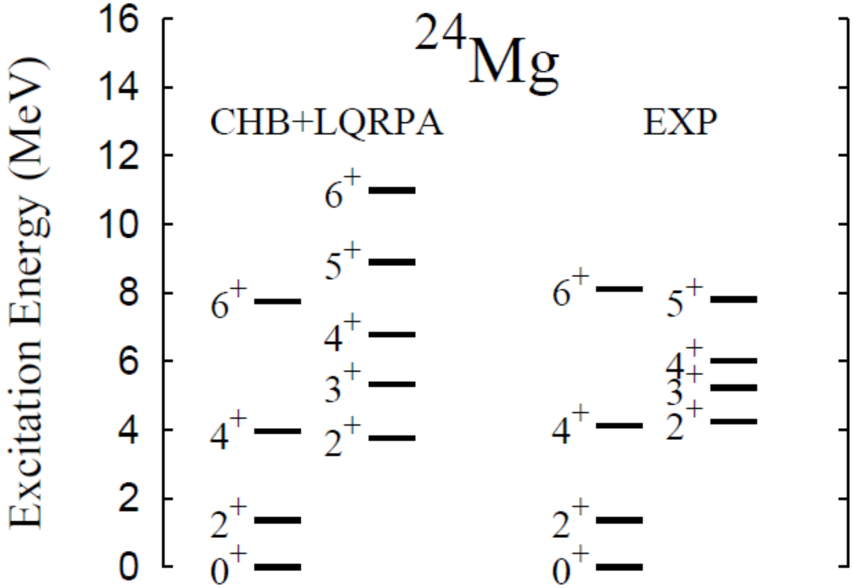




wave functions squared x β^4

- Time-odd mean field contribution lowers excitation energies.
- large-amplitude γ-dynamics
- 0_2^+ , 2_3^+ states: large-amplitude γ vibration coupling with β-vibration
- effective charge (e_n, e_p) = (0.4, 1.4)

^{24}Mg

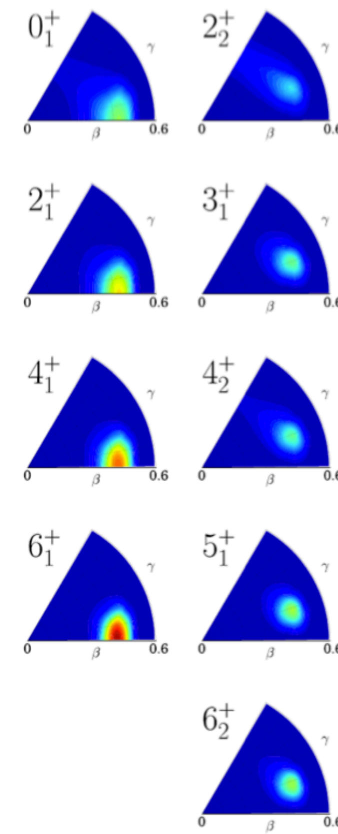


NH and Kanada-En'yo, PRC83, 034321 (2011)

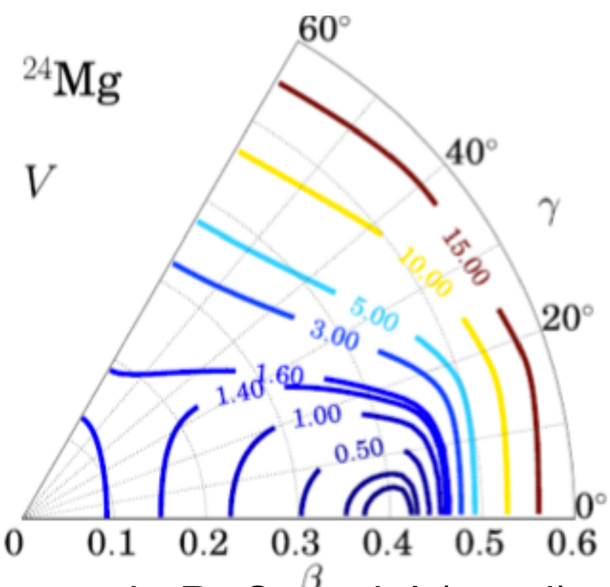
B(E2) (e^2 fm^4)

	EXP	CHB+LQRPA
$2_1^+ \to 0_1^+$	88	63.026
$4_1^+ \to 2_1^+$	160	96.171
$6_1^+ \to 4_1^+$	155	108.032
$3_1^+ \to 2_2^+$	239	103.484
$4_2^+ \to 3_1^+$	-	80.216
$5_1^+ \to 4_2^+$	-	57.085
$6_2^+ \to 5_1^+$	-	47.575
$4_2^+ \to 2_2^+$	64	44.673
$5_1^+ \to 3_1^+$	149	65.981
$6_2^+ \to 4_2^+$	-	83.500
$4_1^+ \to 2_2^+$	-	0.011
$2_2^+ \to 2_1^+$	15	17.197
$2_2^+ \to 0_1^+$	8	4.911
$3_1^+ \to 4_1^+$	-	5.091
$3_1^+ \to 2_1^+$	10	8.180
$4_2^+ \to 4_1^+$	-	12.100
$6_1^+ \to 4_2^+$	-	0.018
$4_2^+ \to 2_1^+$	5	3.493
$5_1^+ \to 6_1^+$	-	4.217
$5_1^+ \to 4_1^+$	-	7.618
$6_2^+ \to 6_1^+$	-	9.756
$6_2^+ \to 4_1^+$	-	3.534

vibrational wave function squared β^4 multiplied



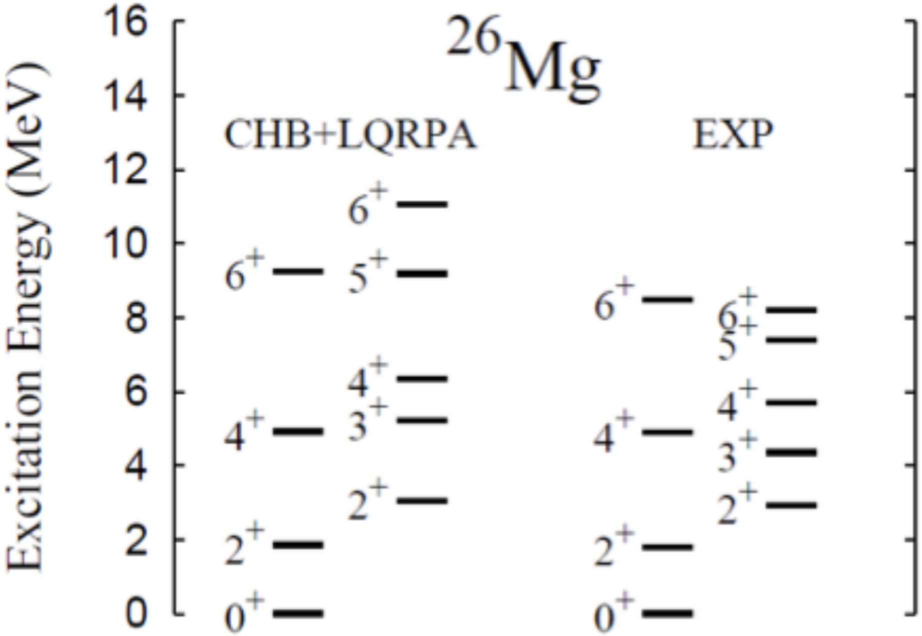
prolate ground band (K=0)
γ-vibrational side band (K=2)

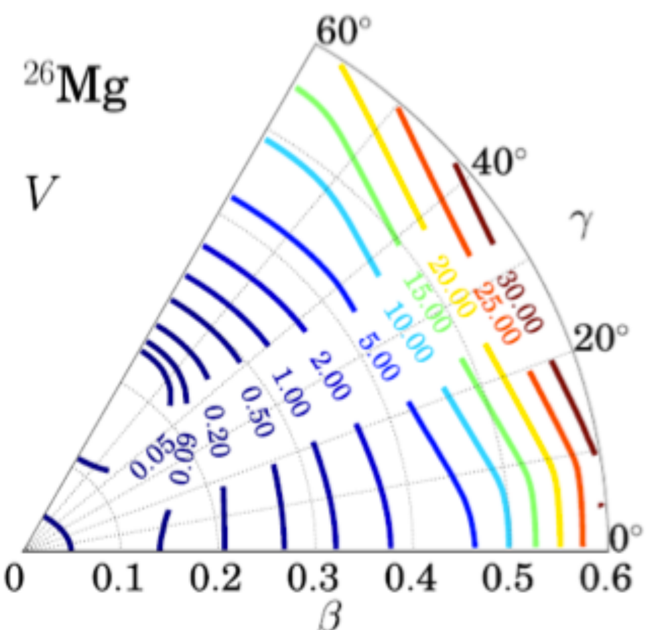


parameters in P+Q model (p+sd): adjusted to results of Skyrme HFB(SkM*, mixed)

Losa et al. Phys. Rev. C81, 064307 (2010)

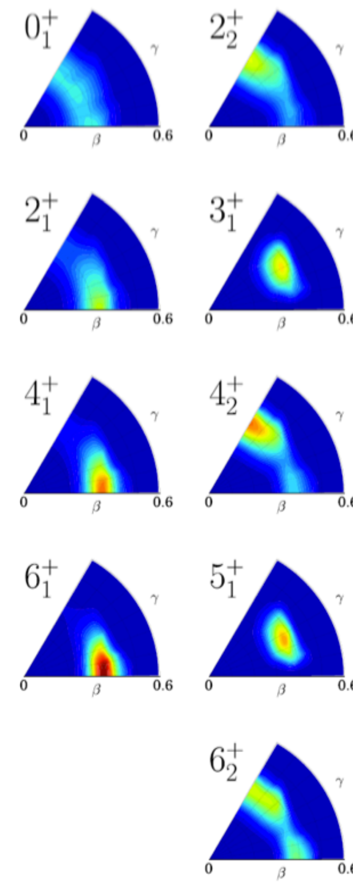
^{26}Mg (γ-soft case)





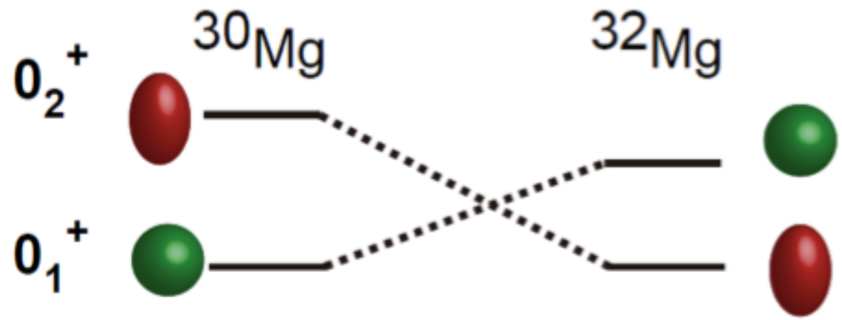
B(E2) (e^2 fm^4)

	Expt.	CHB + LQRPA
$2_1^+ \to 0_1^+$	61.3	52.870
$4_1^+ \to 2_1^+$	64.1	90.302
$6_1^+ \to 4_1^+$	–	112.596
$3_1^+ \to 2_2^+$	41.2	74.890
$4_2^+ \to 3_1^+$	37.0[a]	20.437
$5_1^+ \to 4_2^+$	–	32.073
$6_2^+ \to 5_1^+$	–	19.052
$4_2^+ \to 2_2^+$	23.8[a]	58.789
$5_1^+ \to 3_1^+$	–	70.150
$6_2^+ \to 4_2^+$	–	88.693
$4_1^+ \to 2_2^+$	16.0[a]	2.073
$2_2^+ \to 2_1^+$	28.4	62.940
$2_2^+ \to 0_1^+$	1.60	0.765
$3_1^+ \to 4_1^+$	–	18.259
$3_1^+ \to 2_1^+$	0.23[a]	0.456
$4_2^+ \to 4_1^+$	–	28.948
$6_1^+ \to 4_2^+$	–	0.635
$4_2^+ \to 2_1^+$	–	1.536
$6_1^+ \to 5_1^+$	–	13.227
$5_1^+ \to 4_1^+$	–	0.773
$6_2^+ \to 6_1^+$	–	18.167
$6_2^+ \to 4_1^+$	–	1.113



Shape fluctuations in 0^+ states of ^{30}Mg and ^{32}Mg

NH et al., submitted to PRC, arXiv:1109.2060.



^{30}Mg: ground state: **spherical** ?
"**deformed**" 1st excited 0^+ state found at 1789 keV
W. Schwerdtfeger et al.
Phys. Rev. Lett. **103**, 012501 (2009)

^{32}Mg: ground state **deformed** ?
"**spherical**" 1st excited 0^+ state found at 1058 keV
K. Wimmer et al.,
Phys. Rev. Lett. **105**, 252501 (2010)

What about shape mixing?
Do spherical and prolate shapes mix in ^{30}Mg and ^{32}Mg ?
Simple two-level model does hold ? $|0\rangle = a|sph\rangle + b|def\rangle$

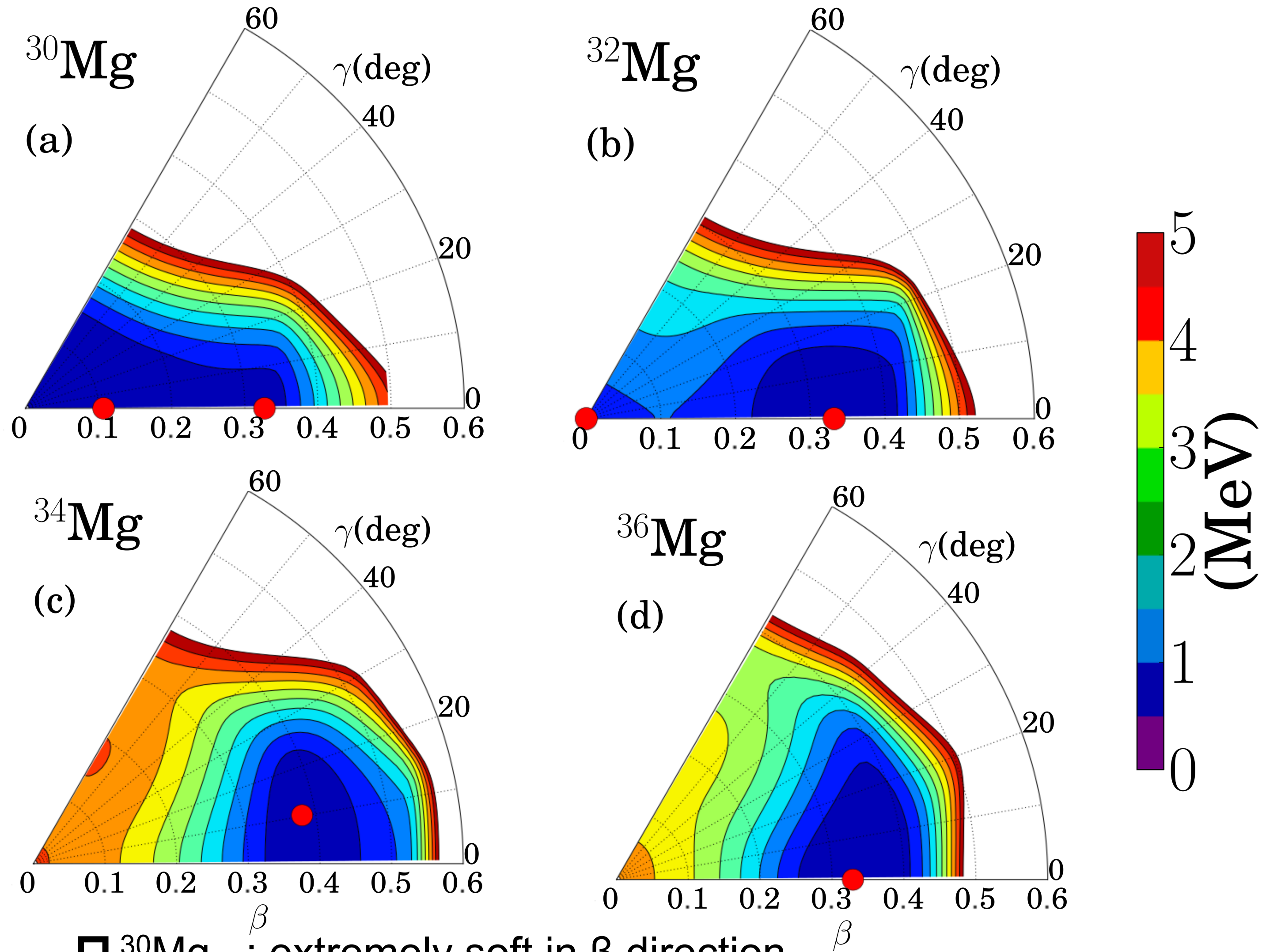
Quantum correlation beyond mean-field (HFB) + small-amplitude vibration (QRPA) plays essential role in low-lying states (**large-amplitude collective motion**)

Calculation Details (Mg)

- Microscopic Hamiltonian (Pairing + Quadrupole Model)
  Single-particle + pairing (Monopole, Quadrupole) + quadrupole (ph) force
- Single-particle model space
  harmonic oscillator two major shells (sd + pf)
- Parameters in microscopic Hamiltonian
  - adjusted to simulate the Skyrme HFB (HFBTHO, SkM*)
    with surface pairing (V_0=-374 MeV fm^{-3}, 60MeV cut off)
    which reproduce experimental Δ_n = 1.34 MeV of ^{30}Ne

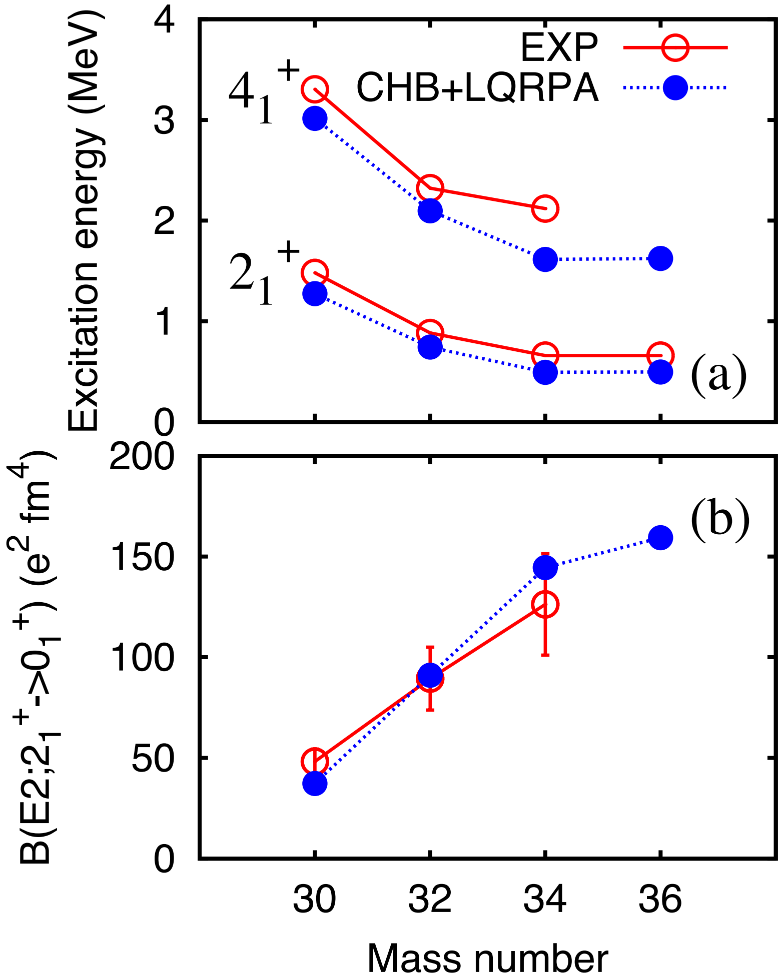
  For each nucleus,
  - single-particle energies:
    - Skyrme canonical energies after effective mass scaling (m*/m=0.79)
  - pairing interaction strengths:
    adjusted to reproduce Skyrme pairing gaps at spherical points
  - quadrupole interaction strength:
    - adjusted to reproduce deformation of Skyrme HFB states
  - quadrupole pairing strength G_2:
    - self-consistent value Sakamoto and Kishimoto PLB245 (1990) 321
- effective charges (e_n, e_p) = (0.5, 1.5)
- mesh: (β, γ) mesh with 60x60 points ($0<\beta<\beta_{max}$, β_{max}=0.5 for ^{30}Mg, 0.6 for others)

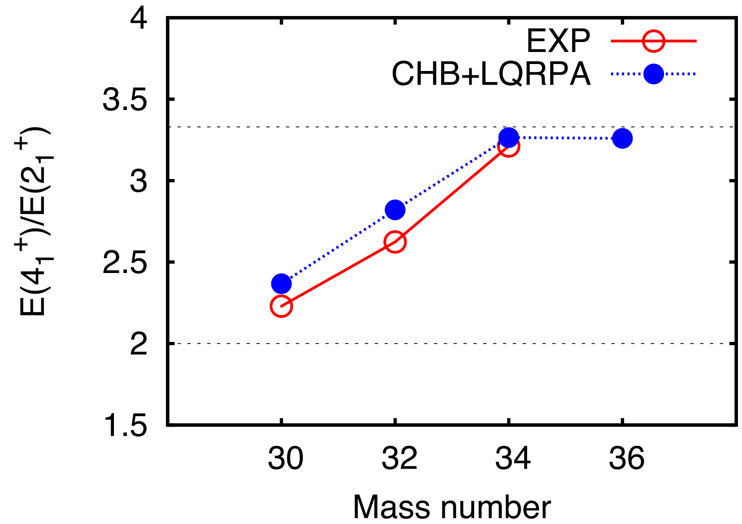
Potential energy surfaces

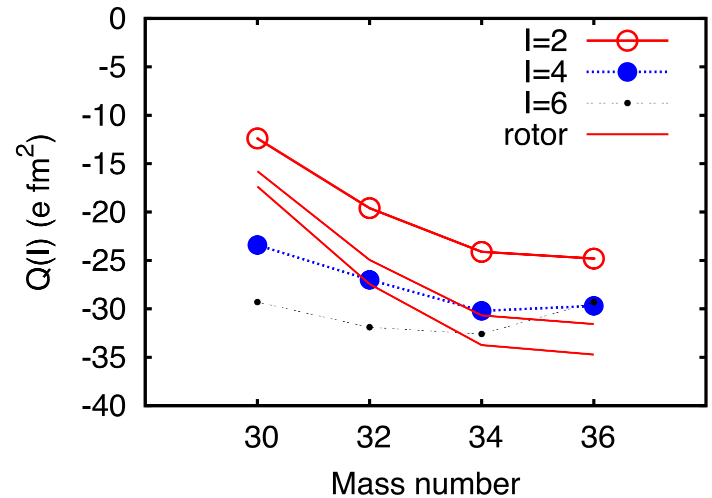


- ^{30}Mg : extremely soft in β direction
- ^{32}Mg : spherical and prolate shape coexistence
- ^{34,36}Mg: prolate, soft in γ direction

Ground bands







^{30}Mg: Deacon et al. PRC82(2010) 034305
^{32}Mg: Takeuchi et al. PRC79 (2009) 054319
^{34}Mg: Yoneda et al. PLB499 (2001) 233
^{36}Mg: Gade et al. PRL99 (2007) 072502

B(E2)

^{30}Mg: Niedermaier et al. PRL**94** (2005) 172501
^{32}Mg: Motobayashi et al. PLB**346** (1995) 9
^{34}Mg: Iwasaki et al. PLB**522** (2001) 227.

Shape changes and shape mixing in ground bands

- vibrational wave functions squared of yrast states

$$\int d\beta d\gamma \boxed{\sum_K |\Phi_{\alpha IK}(\beta,\gamma)|^2} |G(\beta,\gamma)|^{\frac{1}{2}} = 1$$

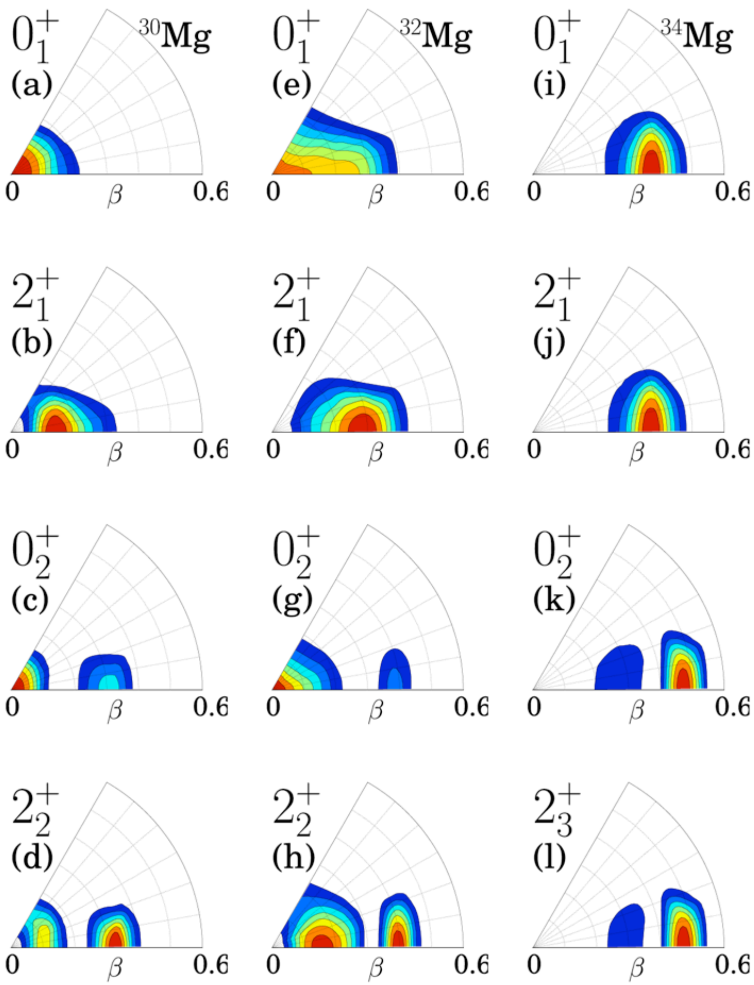
$$|G(\beta,\gamma)|^{\frac{1}{2}} d\beta d\gamma = 2\beta^4 \sqrt{W(\beta,\gamma)R(\beta,\gamma)} \sin 3\gamma d\beta d\gamma$$

$$R(\beta,\gamma) = D_1(\beta,\gamma)D_2(\beta,\gamma)D_3(\beta,\gamma),$$
$$W(\beta,\gamma) = \{D_{\beta\beta}(\beta,\gamma)D_{\gamma\gamma}(\beta,\gamma) - [D_{\beta\gamma}(\beta,\gamma)]^2\}\beta^{-2}$$

$$\mathcal{J}_k(\beta,\gamma) = 4\beta^2 D_k(\beta,\gamma) \sin^2 \gamma_k$$

$$\gamma_k = \gamma - (2\pi k/3)$$

^{30}Mg ^{32}Mg ^{34}Mg



0_1^+

2_1^+

0_2^+

$2_{2,3}^+$

transition from ^{30}Mg to ^{34}Mg in 0_1^+ state

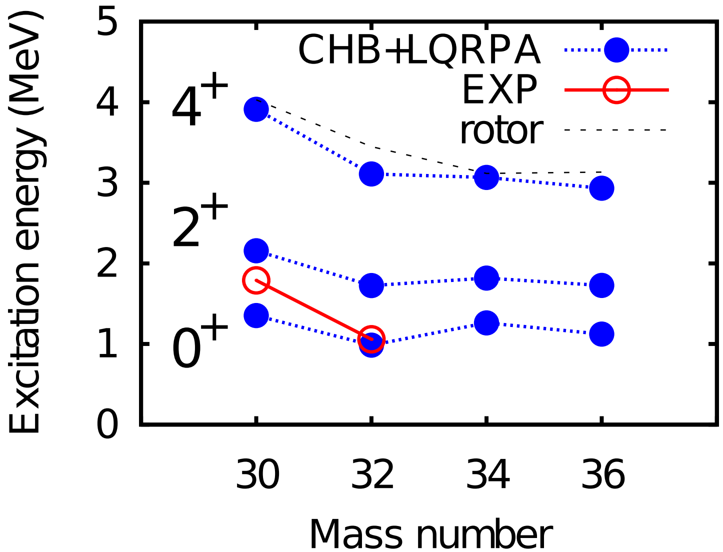
shape fluctuation is largest in 0_1^+ state of ^{32}Mg

change of structure in yrast band of ^{30}Mg and ^{32}Mg

β-vibrational 0_2^+ and 2_3^+ in ^{34}Mg

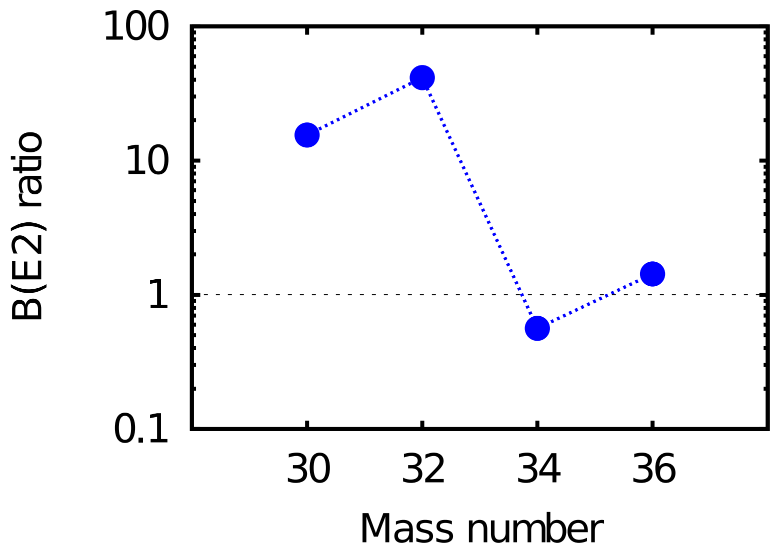
Properties of K=0 excited band

energies of excited K=0 band



B(E2) ratio between K=0 bands

$B(E2;0_2^+ \to 2_1^+)/B(E2;0_1^+ \to 2_{2,3}^+)$



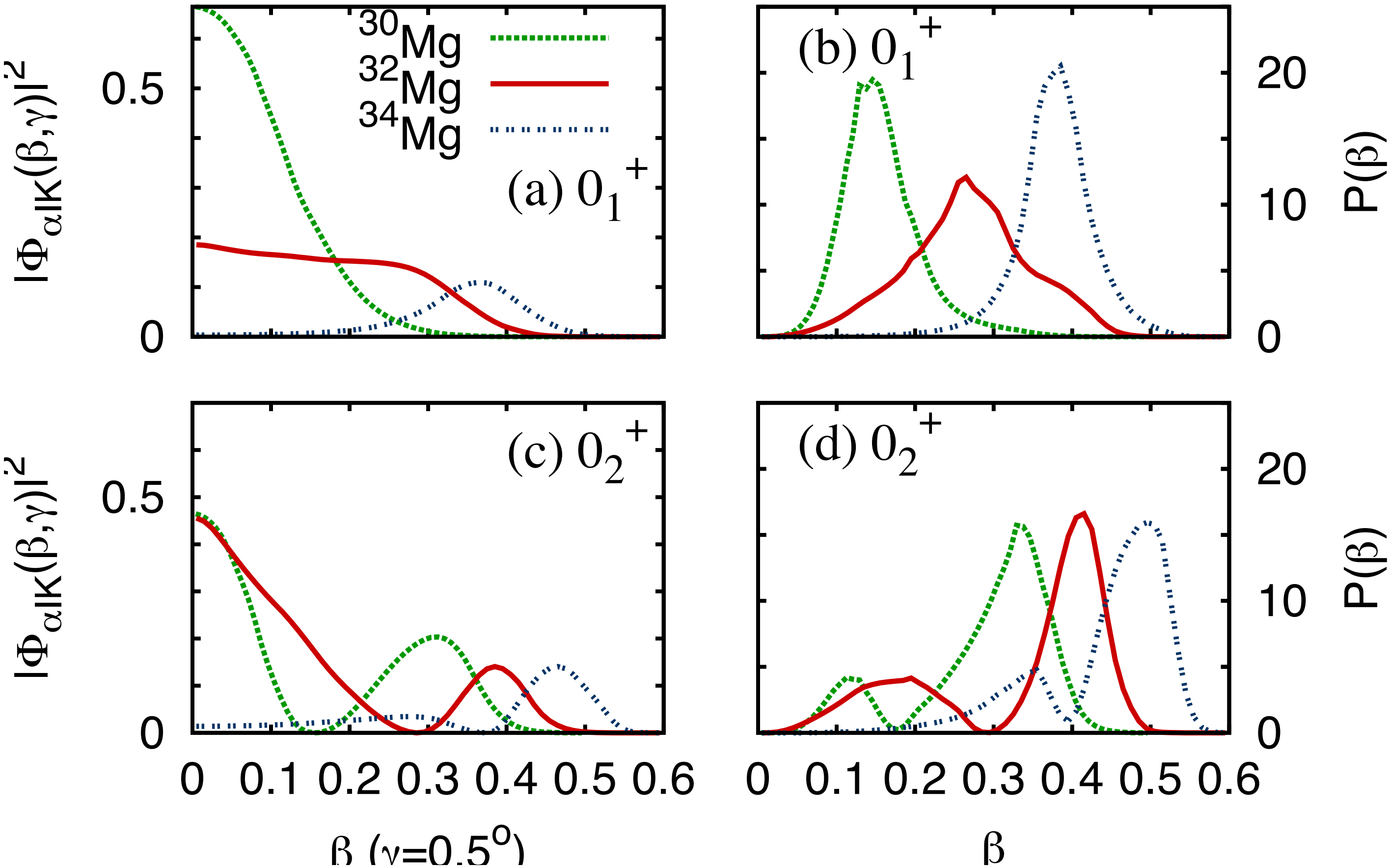
- K=0 excited band: well deformed, deviation from rotor is largest at ^{32}Mg
- The calculation reproduce experimental 0+ energy. Shell model and beyond mean-field calculations predict higher energies for 0_2+ energy of ^{32}Mg (1.4 – 3.1 MeV)
- B(E2) ratio (right figure) should be one if 0+ and 2+ states of the same band have same intrinsic structure
- Shape mixing properties changes between ^{32}Mg and ^{34}Mg

Collective wave function

$$\int d\beta d\gamma \boxed{\sum_K |\Phi_{\alpha IK}(\beta,\gamma)|^2} |G(\beta,\gamma)|^{\frac{1}{2}} = 1$$

Probability density

$$P(\beta) = \int d\gamma \sum_K |\Phi_{\alpha IK}(\beta,\gamma)|^2 |G(\beta,\gamma)|^{\frac{1}{2}}$$



spherical peak disappears in probability density, due to β^4 factor in $G(\beta,\gamma)$

- For ^{30}Mg, the shape coexistence picture with spherical ground and deformed excited states holds. (shape mixing is small.)
- For ^{32}Mg large-amplitude quadrupole fluctuation dominates both in ground and excited 0^+ states.

Skyrme CHFB+LQRPA

K. Yoshida and NH et al., Phys. Rev. **C83**, 061302 (2011)

Skyrme HFB (SkM*) + volume pairing t_0=-200 MeV fm^{-3}

Code:

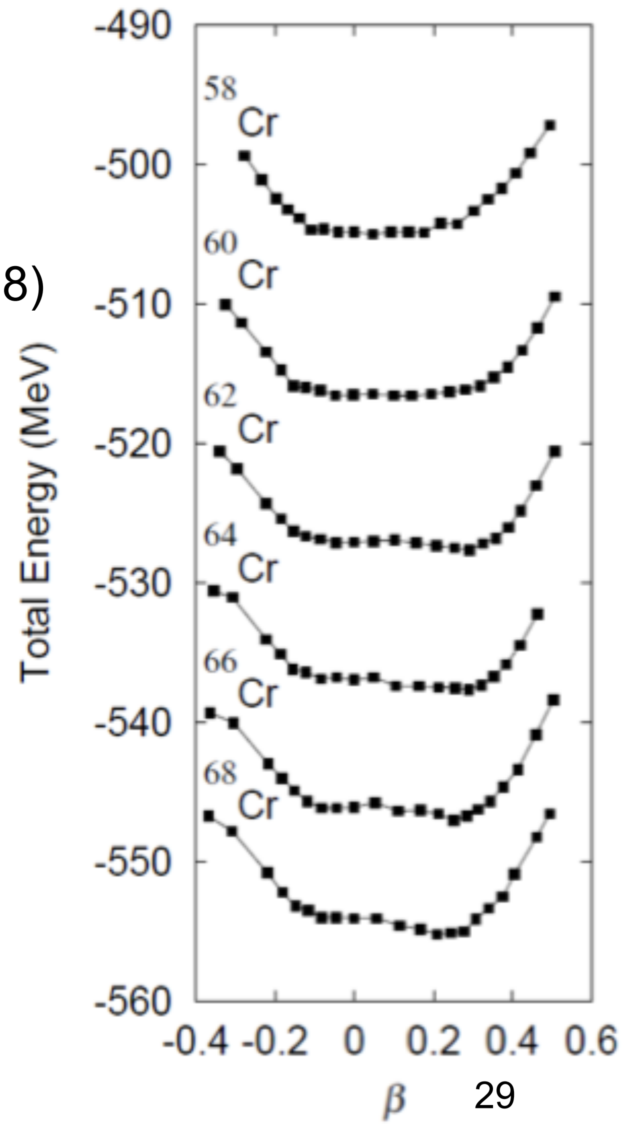
- 2D lattice (axially symmetric)
  - 12.25 fm x 12 fm (0.5 fm mesh)
- Yoshida and Giai, Phys. Rev. **C78**, 064316 (2008)

Collective Hamiltonian for axial deformation (3D)

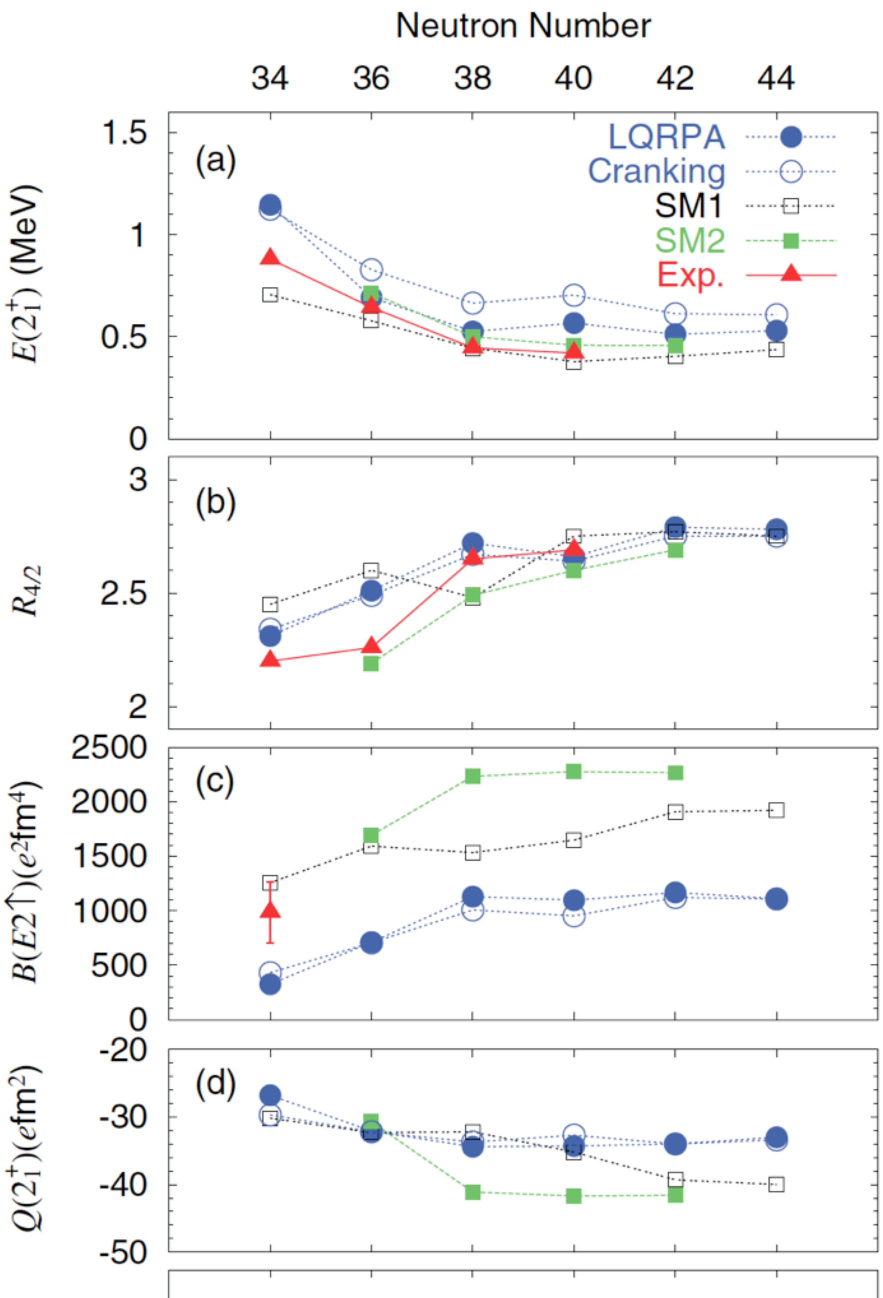
$$\mathcal{H}_{\mathrm{coll}} = \frac{1}{2}\boxed{\mathcal{M}_\beta(\beta)}\dot{\beta}^2 + \frac{1}{2}\sum_{i=1}^{2}\boxed{\mathcal{J}_i(\beta)}\omega_i^2 + \boxed{V(\beta)}$$

calculated from Skyrme-CHFB

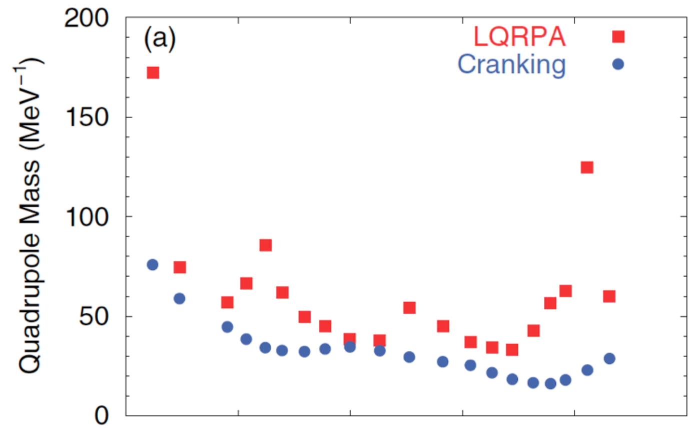
calculated from Skyrme-LQRPA



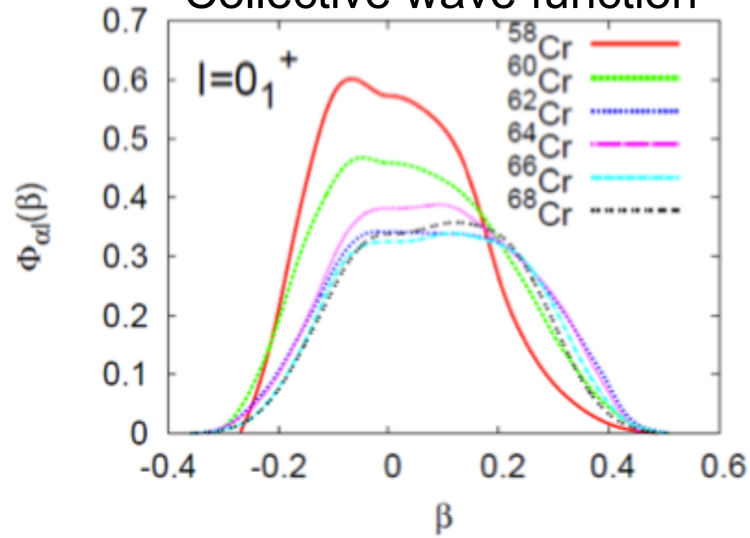
Collectivity of neutron-rich Cr isotopes



vibrational collective mass



Collective wave function



SM1: Kaneko et al., PRC78, 064312 (2008)
SM2: Lenzi, et al., PRC82, 054301 (2010)

Summary

- extraction of collective coordinates (1D collective path)

  adiabatic self-consistent collective coordinate (ASCC) method

  applications to Se isotopes

- Derivation of inertial functions in 5D collective Hamiltonian

  constrained HFB + local QRPA (2D ASCC)

  time-odd contribution in the vibrational and rotational collective masses

  applications to various phenomena
  shape coexistence in ^{68}Se
  γ-soft dynamics around ^{26}Mg
  shape phase transition around ^{32}Mg and ^{64}Cr

  Implementation using Skyrme EDF