On the microscopic theory of large-amplitude collective motion

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Microscopic theory of LACM

Open problems in GCM

- choice of optimal generator coordinates
  for low-lying excitation, quadrupole moments, q_{20} and q_{22}, pairing gaps Δ_n,Δ_p
  How about for fission and fusion ?

- reliability of collective mass with real generator coordinates
  complex generator coordinates (collective momenta) are necessary to obtain correct mass for center of motion (Ring-Schuck)

TDHF(B)

- semi-classical, need requantization for quantum process
- small-amplitude limit: (Q)RPA

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

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

Overview of ATDHF (1)

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

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

Versions of ATDHF theories

Villars, Nucl. Phys. A285, 269 (1977)
Baranger and Veneroni, Ann. Phys. 114, 123 (1978), Ring-Schuck
Goeke and Reinhard, Ann. Phys. 112, 328 (1978)
Rowe and Basserman, Can. Phys. 54, 1941 (1976)
Marumori, Prog. Theor. Phys. 57, 112 (1977)
A. Bulgac, A. Klein and N.R. Walet, Phys. Rev. C40 (1989), 945.
M.J. Giannoni and P. Quentin, Phys. Rev. C21 (1980), 2060, C21 (1980), 2076.
J. Dobaczewski and J. Skalski, Nucl. Phys. A369 (1981), 123.
Klein, Walet, Dang (Ann.Phys. 208, 90 (1991))

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a review

G. Do Dang, A. Klein and N.R. Walet Phys. Rep. 335 (2000), 93.

Overview of ATDHF (2)

- How should the collective variables be introduced ?

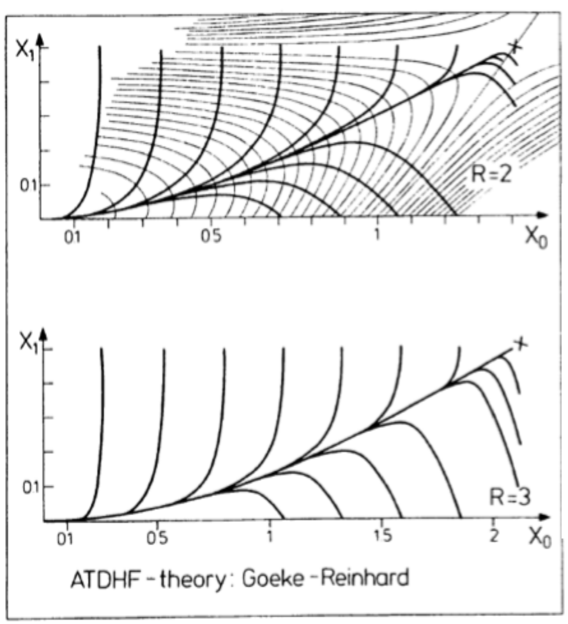
  canonical variable conditions, Yamamura,Kuriyama,Iida(PTP71,109(1984))

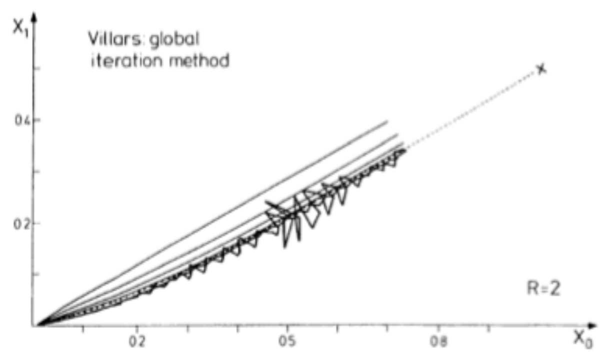
- To which order in collective momentum should the variational principle be expanded ?

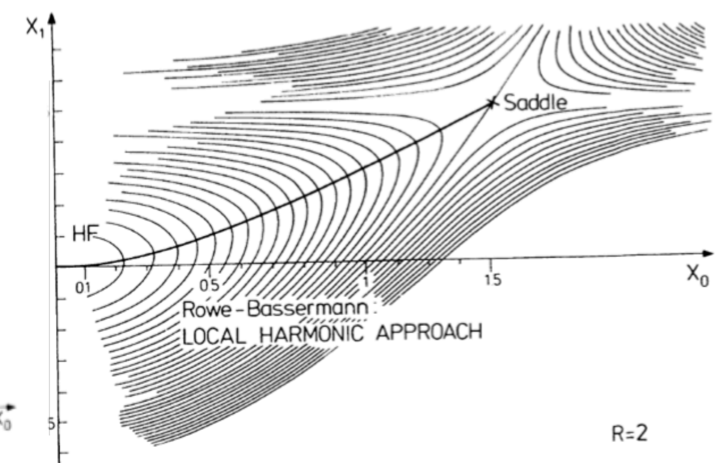
  2nd order term should be included to satisfy the RPA boundary condition, Mukherjee and Pal (PLB100,457(1982), NPA373,289(1982))

- Local harmonic approach works well (Rowe-Basserman, Marumori)

Goeke, Reinhard, Rowe NPA359,408 (1981)







Self-consistent collective coordinate (SCC) method

- TDVP

TDHFB state

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

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

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

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

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

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

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

Adiabatic SCC method

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

- one of the solutions of SCC method
- expansion of the basic equations of SCC up to 2nd order in p.

adiabatic approximation

Thouless th.

$$|\phi(q,p,n)\rangle = e^{ip\hat{Q}(q)+in\hat{\Theta}(q)}|\phi(q)\rangle \longleftarrow \text{p=n=0}$$

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

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

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

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

Adiabatic SCC method

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

moving-frame HFB equation from 0th order

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

Moving-frame Hamiltonian

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

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

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

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

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

canonical variable conditions

expanded up to 1st order in p

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

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

Algorithm to construct the collective path

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) (lowest freq. C(q))
4. repeat 2. and 3. until the solution converges.

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

$$\langle\phi(q)|\frac{\partial\hat{Q}}{\partial q}|\phi(q)\rangle = -1$$

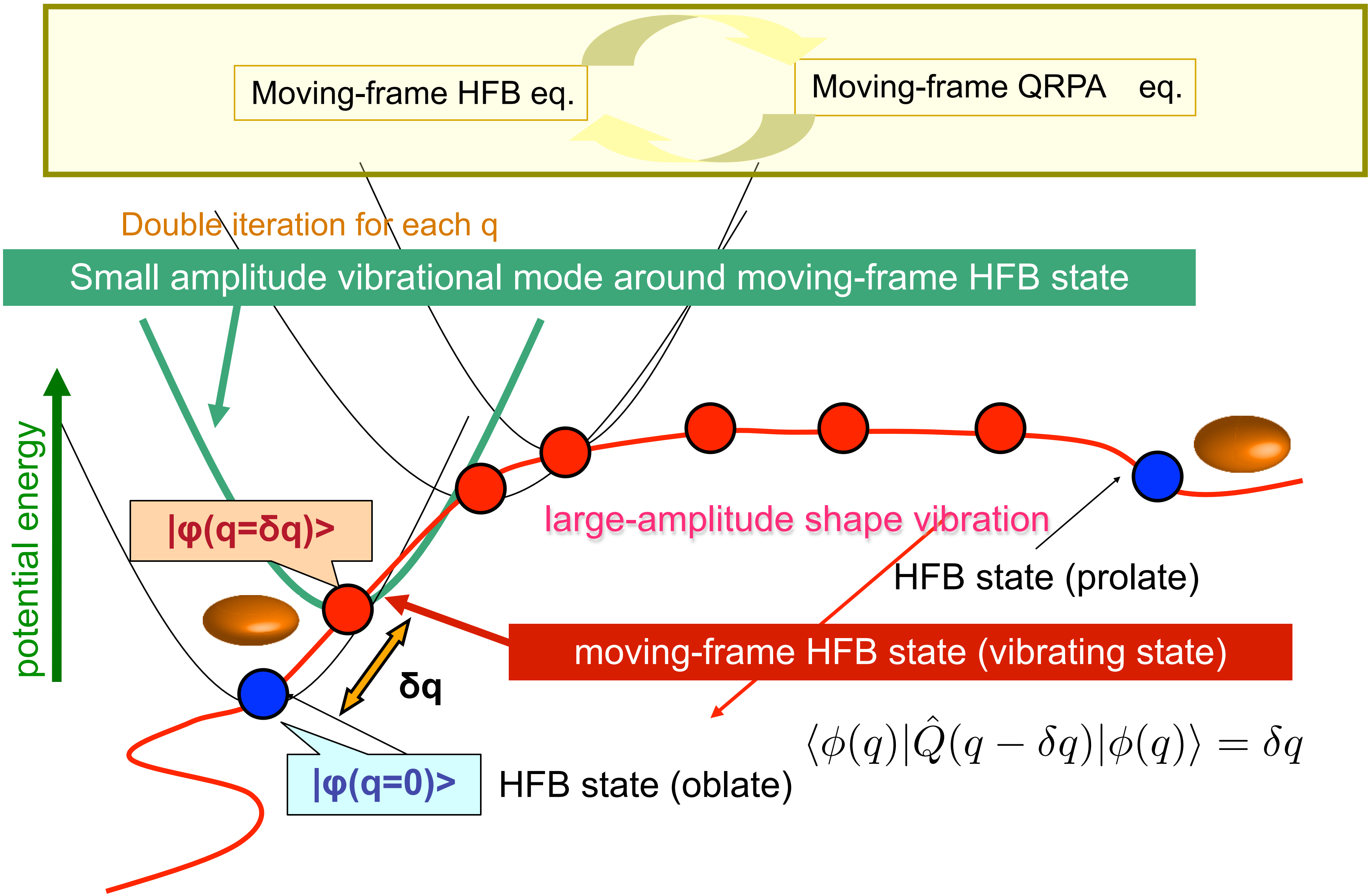
Moving-frame QRPA equations

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

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

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

Algorithm to construct the collective path



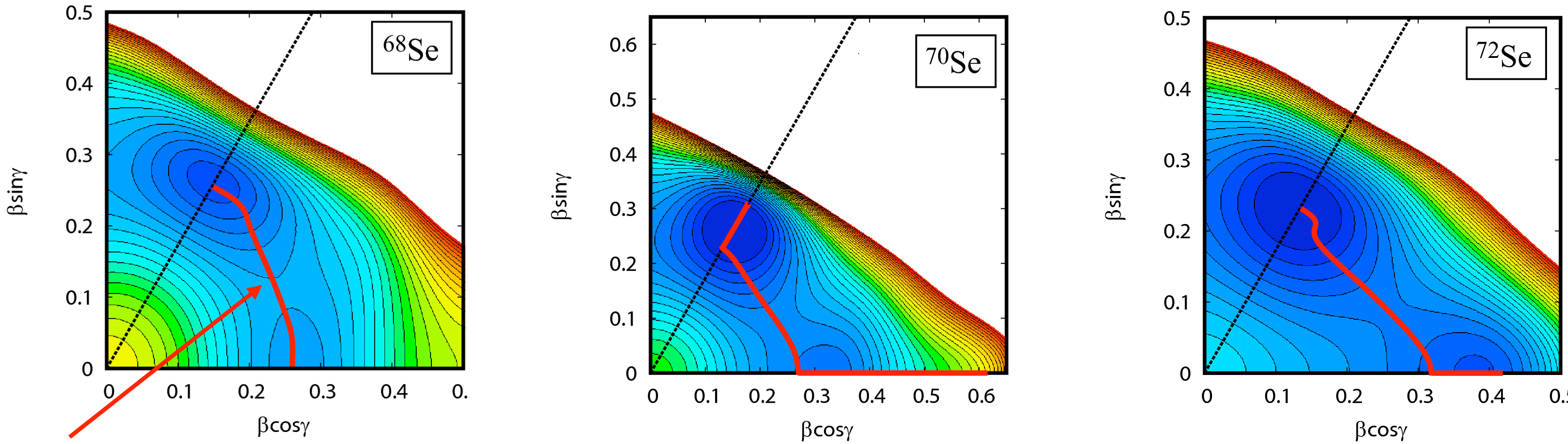
- local direction of collective coordinate is determined by moving-frame QRPA mode

1-dim collective path

oblate-prolate shape coexistence

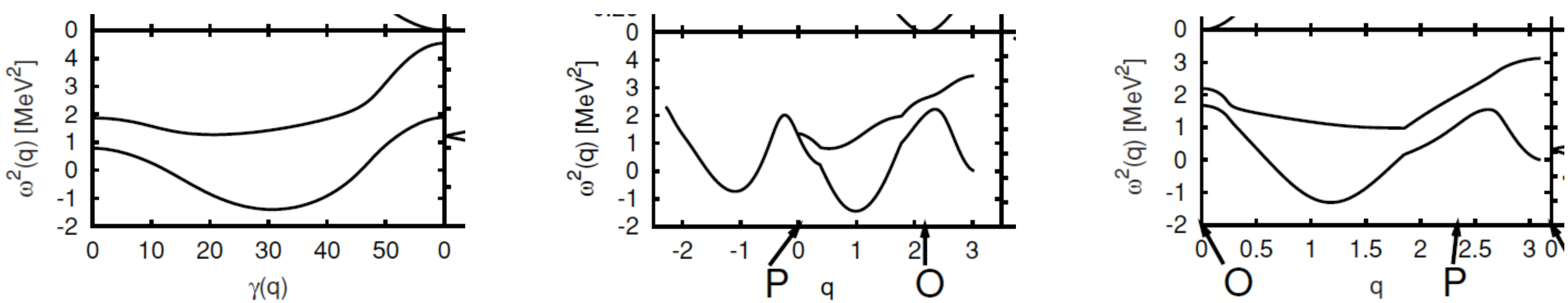
NH et al., Phys. Rev. **C80**, 014305 (2009)

^{68}Se ^{70}Se ^{72}Se



one-dimensional collective path (q) in TDHB manifold mapped onto the (β,γ) plane

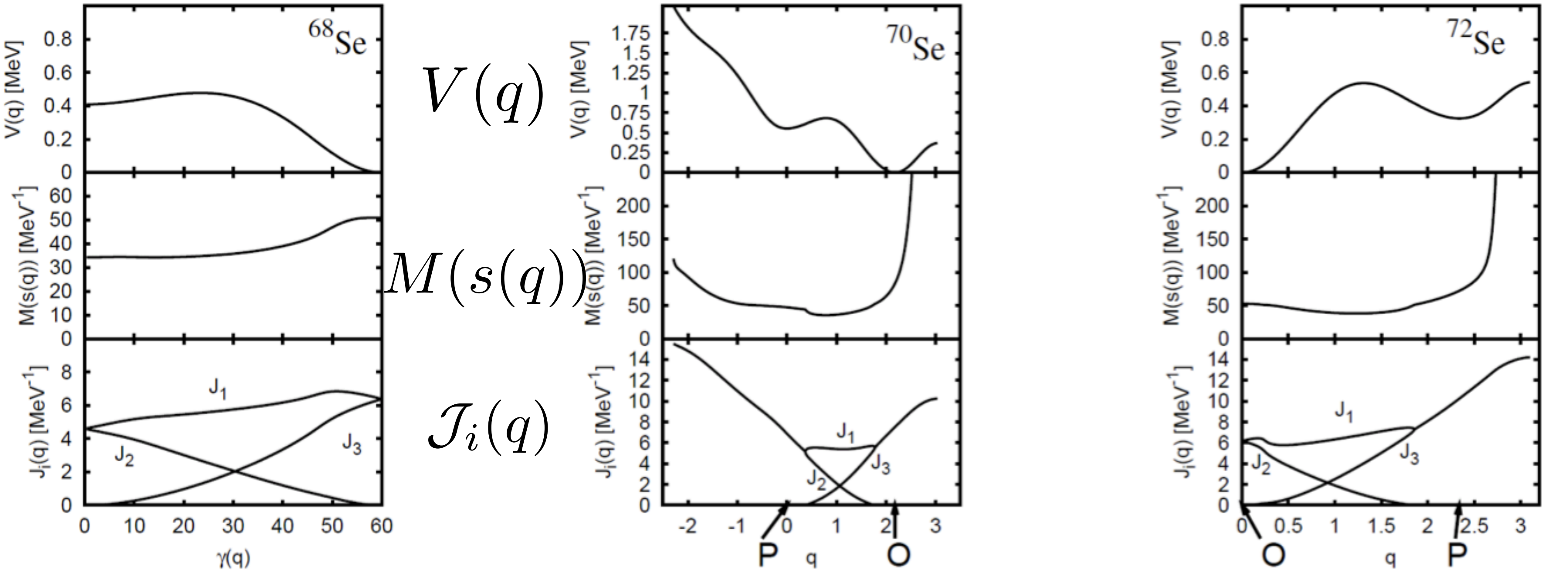
moving-frame QRPA frequency squared $B(q)C(q)=\omega^2(q)$



- P+Q model, 2-major shells model space, parameters simulate Skyrme-HFB(SIII)

Collective Hamiltonian

^{68}Se ^{70}Se ^{72}Se



vibrational collective mass

$$M(s(q)) = B^{-1}(q)\left\{\left(\frac{d\beta}{dq}\right)^2 + \beta^2(q)\left(\frac{d\gamma}{dq}\right)^2\right\}$$

$B^{-1}(q) = 1$ MeV

rotational moments of inertia

$$\delta\langle\phi(q)|\,[\hat{H}_M(q), \hat{\Psi}_i(q)] - \frac{1}{i}\mathcal{J}_i^{-1}(q)\hat{I}_i\,|\phi(q)\rangle = 0,$$

$$\langle\phi(q)|\,[\Psi_i(q), \hat{I}_i]\,|\phi(q)\rangle = i.$$

Thouless-Valatin MOI for moving-frame HFB states

ASCC for multi-dimensional collective subspace

Collective variables

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

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

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

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

Collective Hamiltonian

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

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

☐ Generalized Bohr-Mottelson collective Hamiltonian

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

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

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

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

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

☐ Zero-point energy term is absent if one derives collective Hamiltonian from TDHF.

Microscopic derivations of functions in 5D 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

collective potential

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

→ **V(β, γ)**

Local QRPA equations (for large-amplitude vibration)

vibrational mass

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

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

→ **D(β, γ)**

Local QRPA equations for rotation

rotational moment of inertia

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

→ **J(β, γ)**

- QRPA on top of CHFB state
- Hamiltonian used in QRPA contains constraint terms
- calculations at different (β,γ) is individual. easy to parallelize.

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

Kinetic energy of two LQRPA modes

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

scaled in collective mass = 1

(q1,q2) <-> (β,γ)

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

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

LQRPA phonon operator

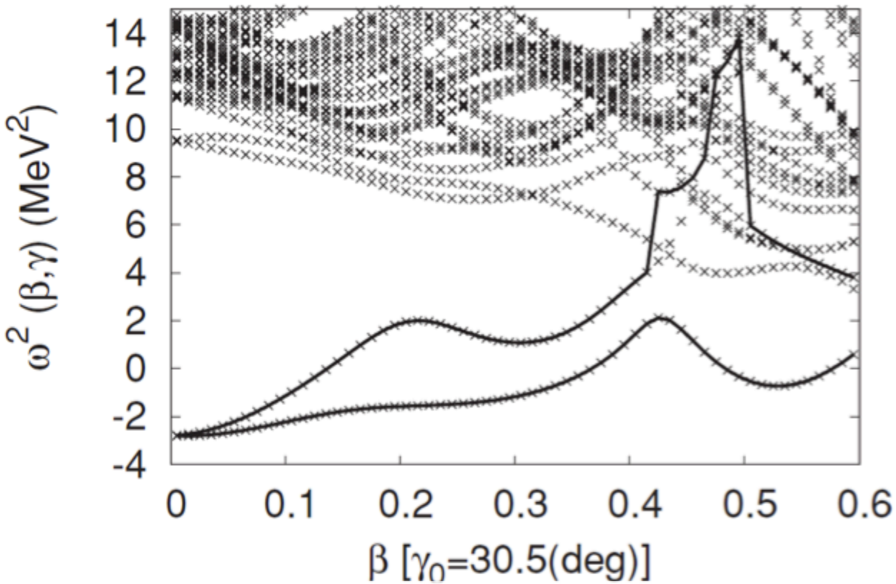
$$\frac{\partial D_{2m}^{(+)}}{\partial q_\alpha} = \frac{\partial}{\partial q_\alpha}\langle\phi(\beta,\gamma)|\,\hat{D}_{2m}^{(+)}\,|\phi(\beta,\gamma)\rangle = \langle\phi(\beta,\gamma)|\,[\hat{D}_{2m}^{(+)}, \frac{1}{i}\hat{P}^\alpha(\beta,\gamma)]\,|\phi(\beta,\gamma)\rangle$$

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

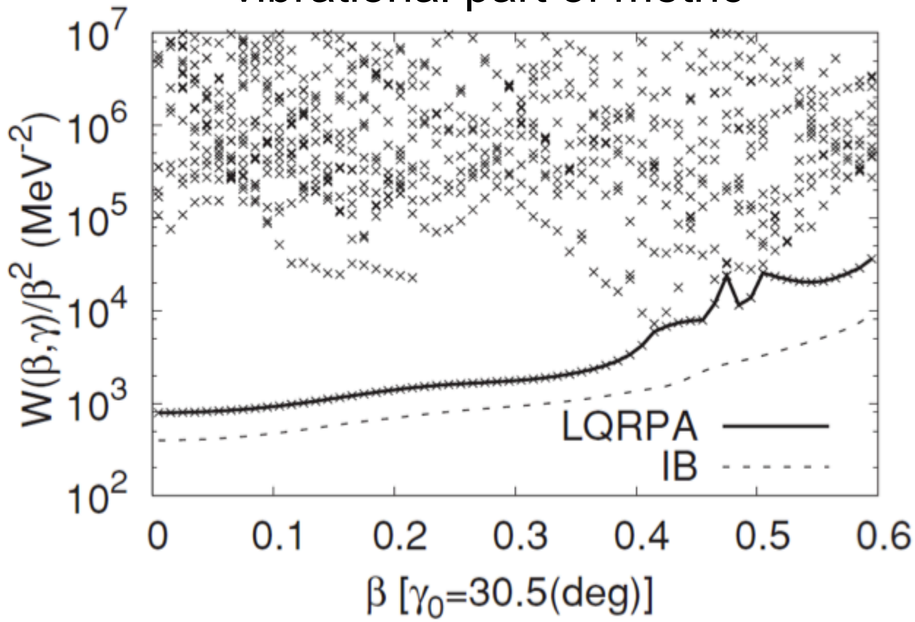
criterion to choose two LQRPA modes:
at each (β,γ) point, choose a pair which gives smallest W(β,γ)
(displacement in β-γ direction is largest)

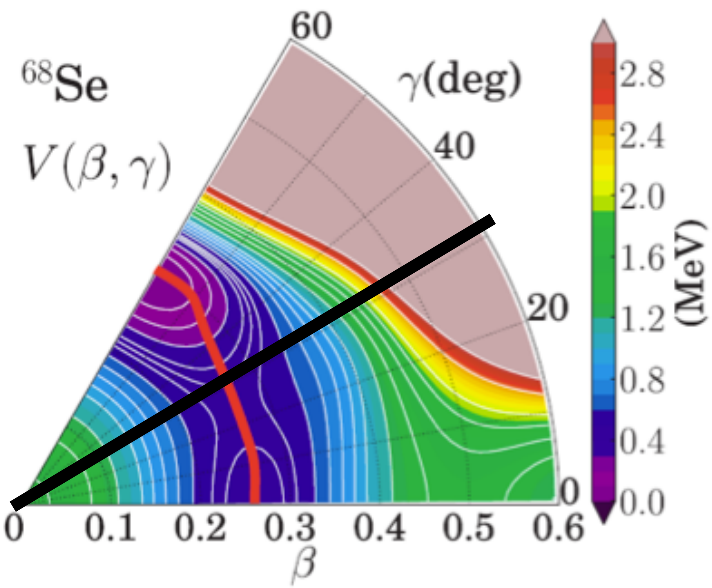
Choice of collective LQRPA modes (^{68}Se)

LQRPA frequencies squared



vibrational part of metric





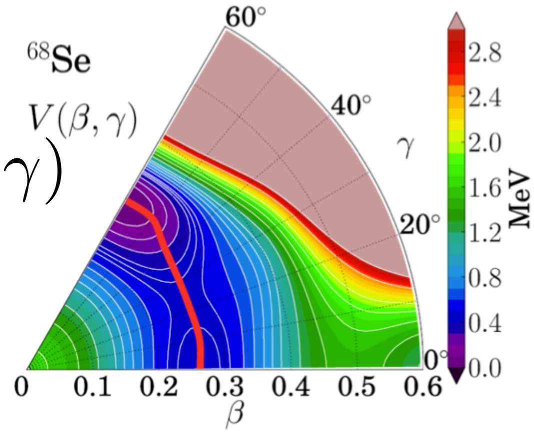
- 3,600 points in (β,γ) plane

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

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

collective potential

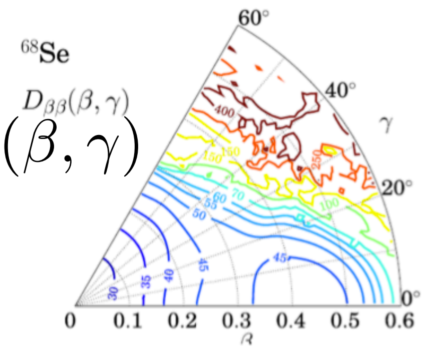
$V(\beta,\gamma)$



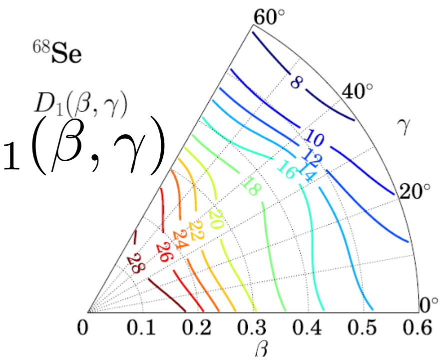
vibrational mass

rotational mass

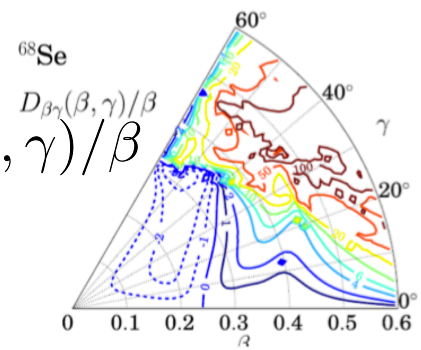
$D_{\beta\beta}(\beta,\gamma)$



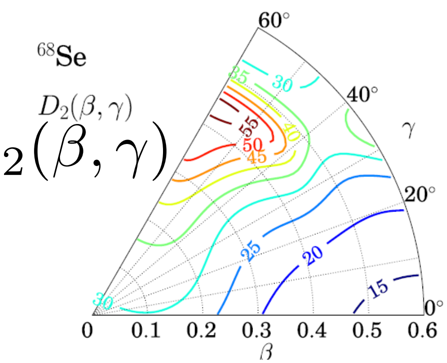
$D_1(\beta,\gamma)$



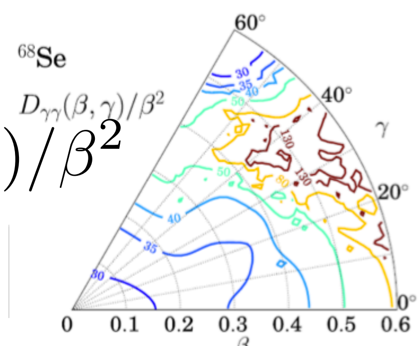
$D_{\beta\gamma}(\beta,\gamma)/\beta$



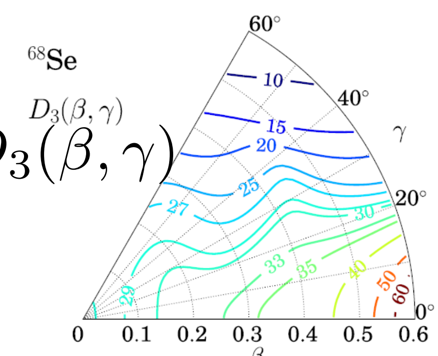
$D_2(\beta,\gamma)$



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



$D_3(\beta,\gamma)$



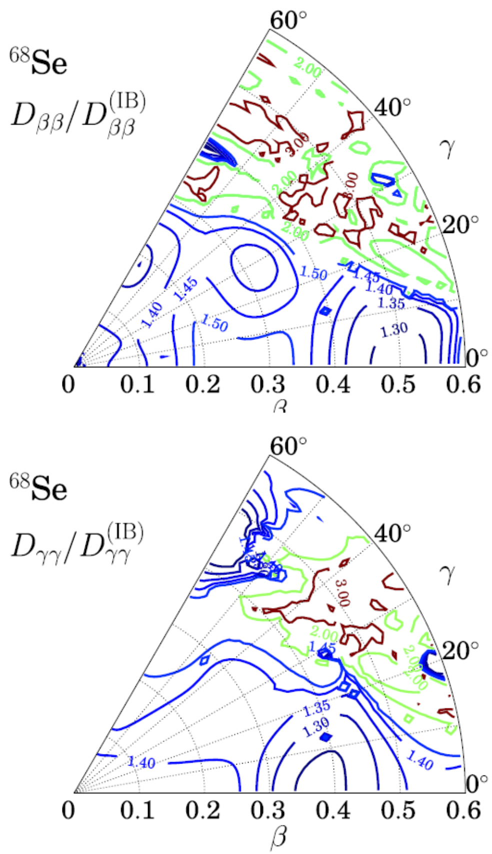
$$\mathcal{J}_k(\beta,\gamma) = 4\beta^2 \boxed{D_k(\beta,\gamma)} \sin^2\gamma_k$$

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

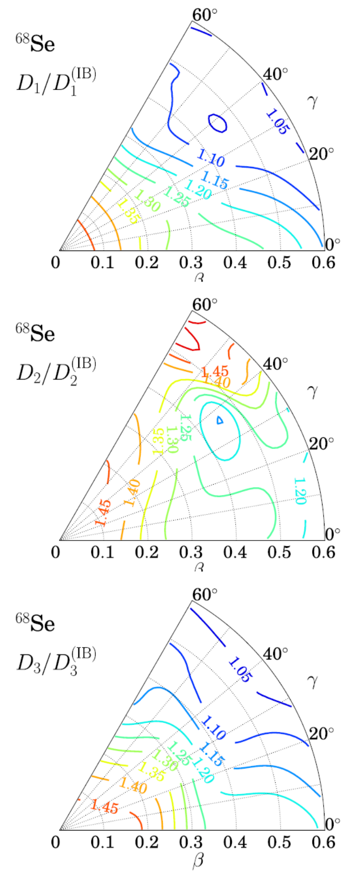
Effect of time-odd component

Ratio to Inglis-Belyaev vibrational/rotational mass

vibrational mass



rotational mass

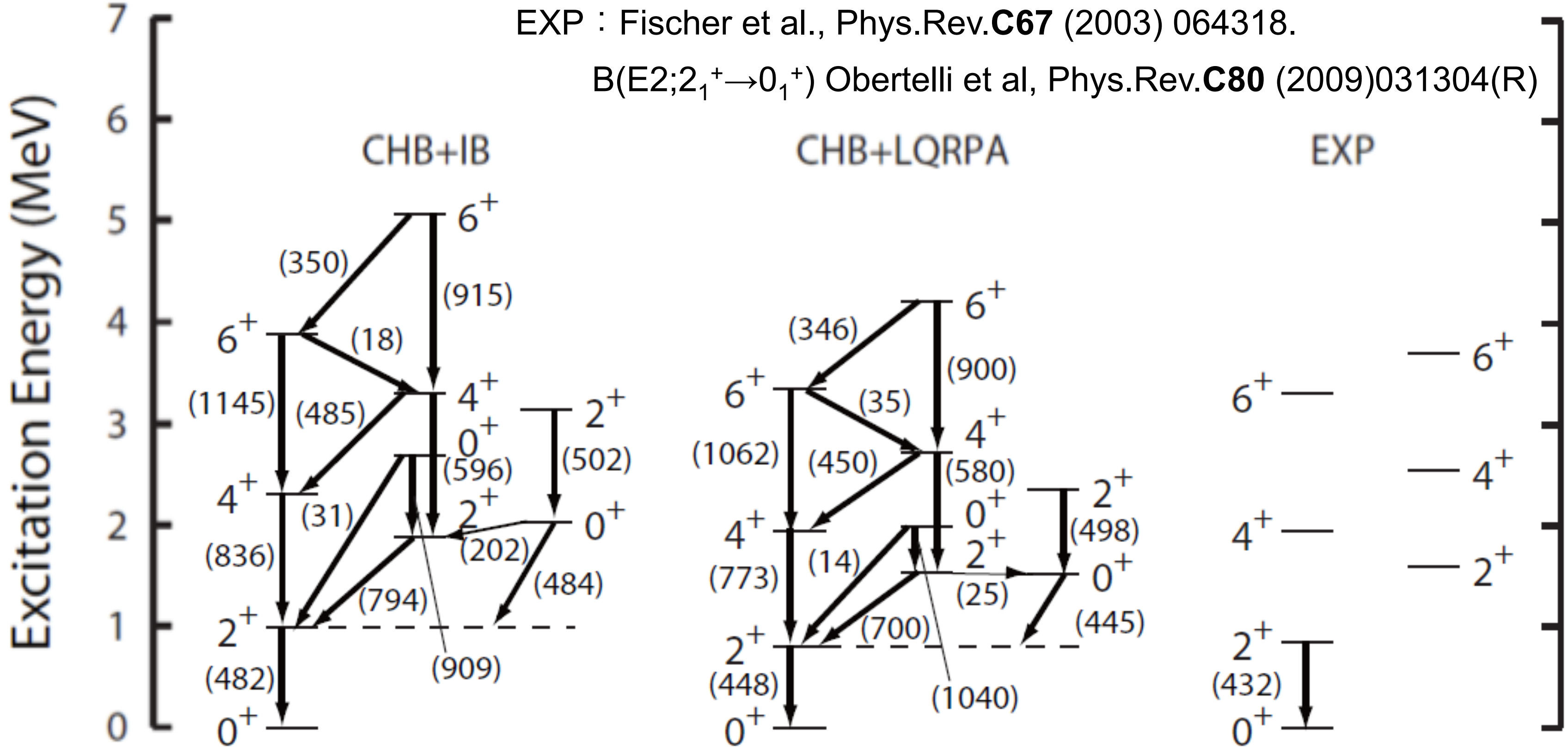


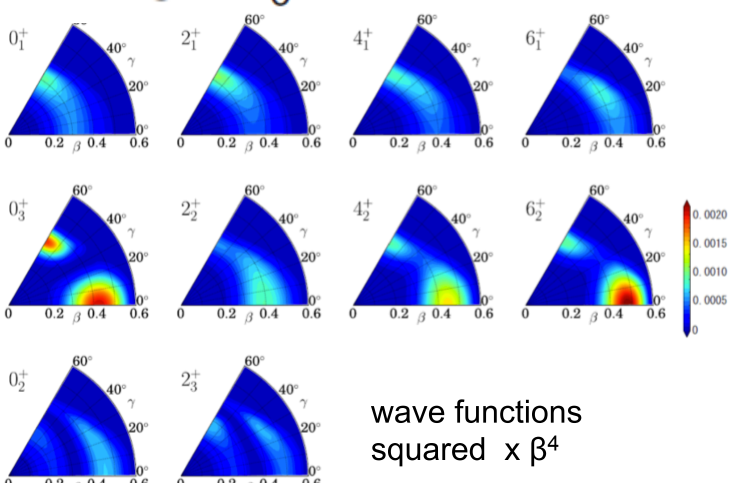
- time-odd component generated by quadrupole-pairing
- LQRPA MOI: 1~1.5 times larger than Inglis-Belyaev values
- Deformation dependence is different between LQRPA and IB

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)



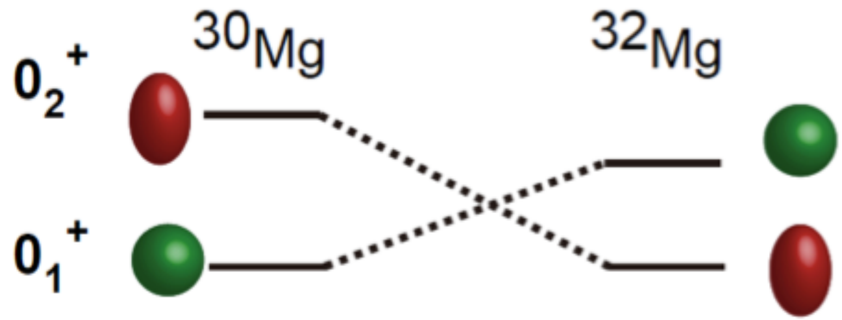


wave functions squared x β^4

- 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)

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 ? $|0\rangle = a|sph\rangle + b|def\rangle$

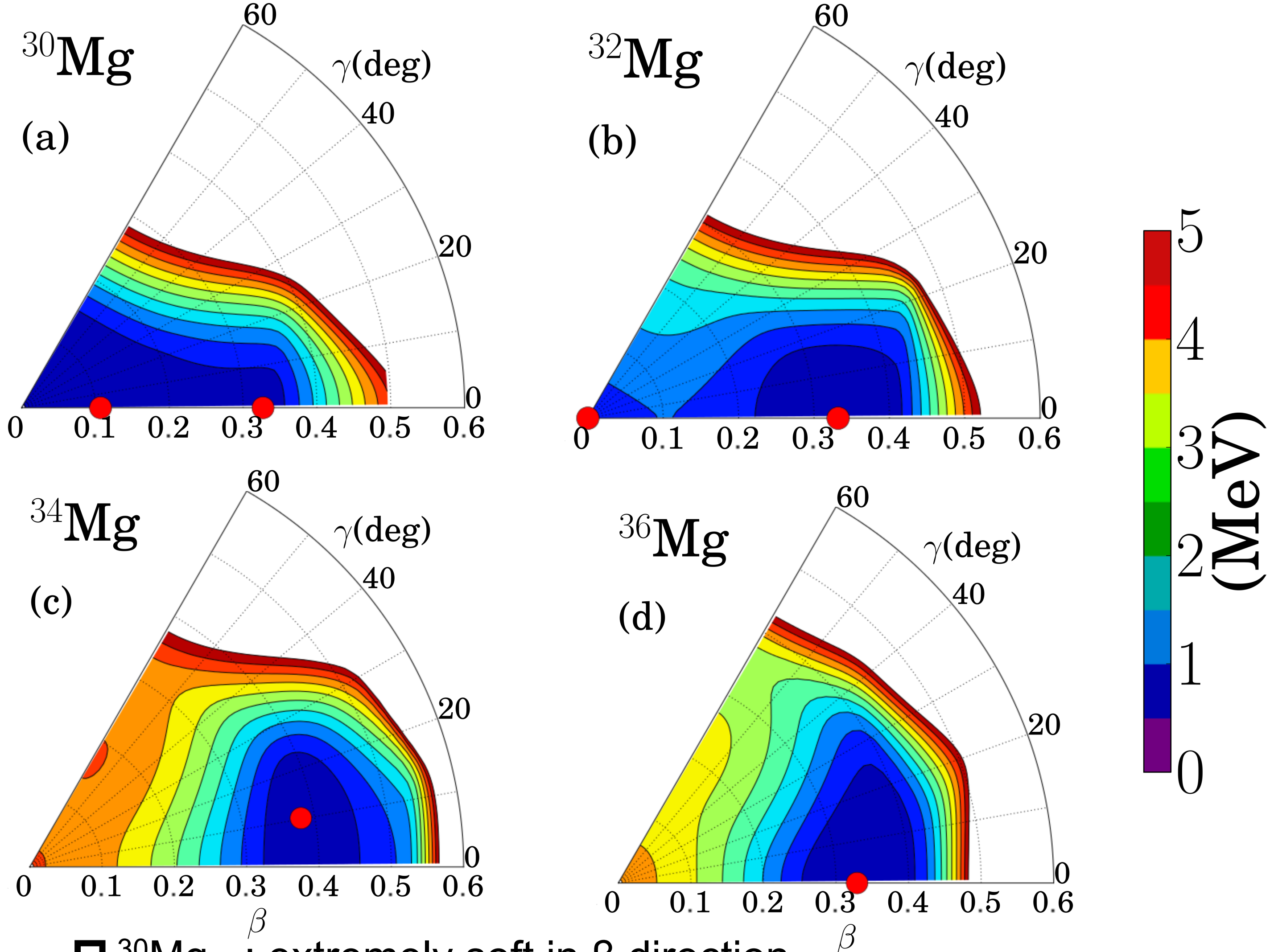
Quantum correlation beyond mean-field (HFB) + small-amplitude vibration (QRPA) plays essential role in low-lying states (**large-amplitude collective motion**)

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

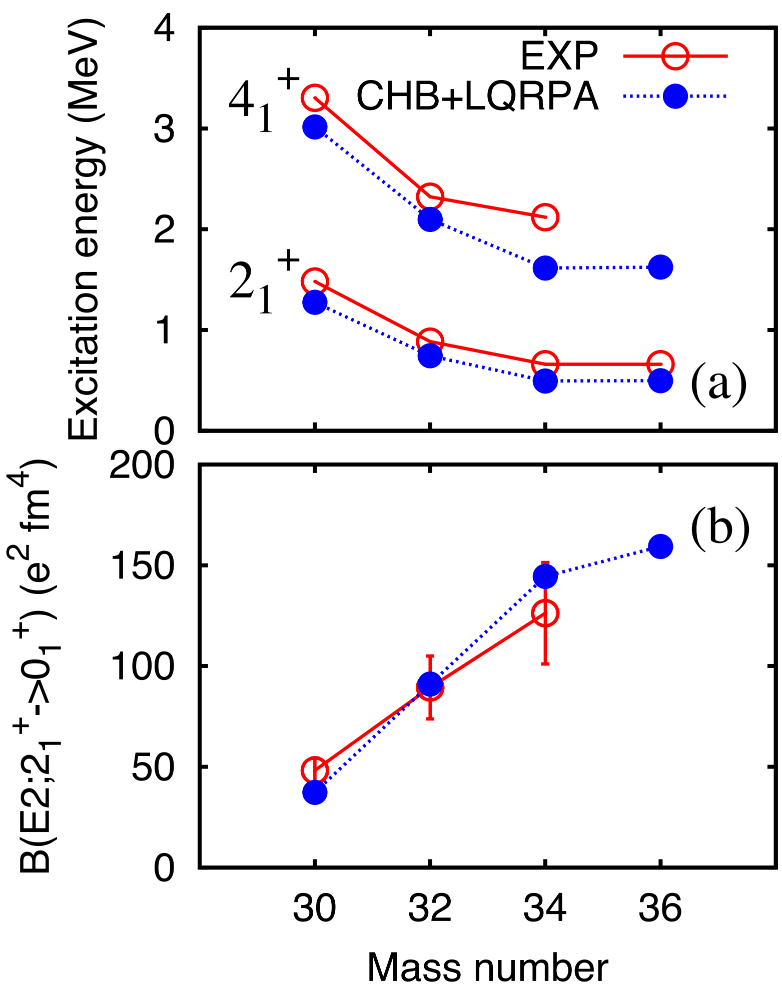
  For each nucleus,
  - single-particle energies:
    - Skyrme canonical energies after effective mass scaling (m*/m=0.79)
  - pairing interaction strengths:
    adjusted to reproduce Skyrme pairing gaps at spherical points
  - quadrupole interaction strength:
    - adjusted to reproduce deformation of 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)

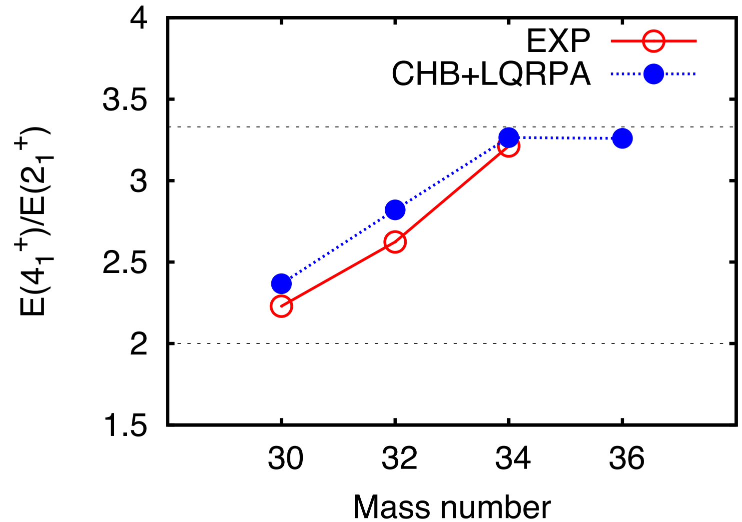
Potential energy surfaces

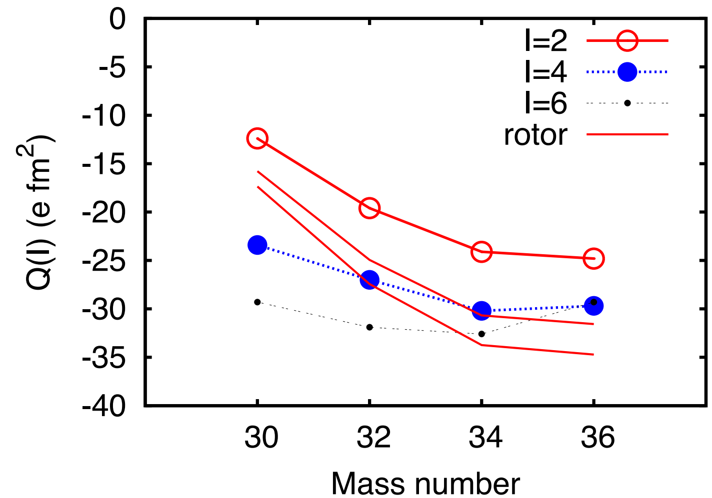


- ^{30}Mg : extremely soft in β direction
- ^{32}Mg : spherical and prolate shape coexistence
- ^{34,36}Mg: prolate, soft in γ direction

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

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

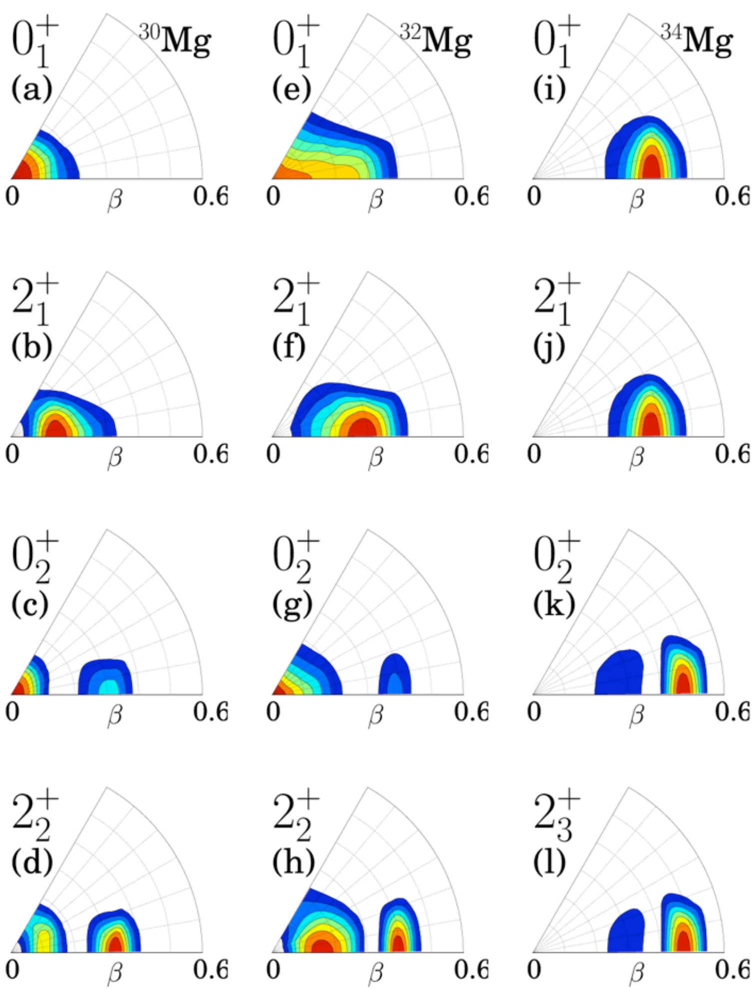
$$|G(\beta,\gamma)|^{\frac{1}{2}} d\beta d\gamma = 2\beta^4 \sqrt{W(\beta,\gamma)R(\beta,\gamma)} \sin 3\gamma \, d\beta d\gamma$$

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

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

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

^{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

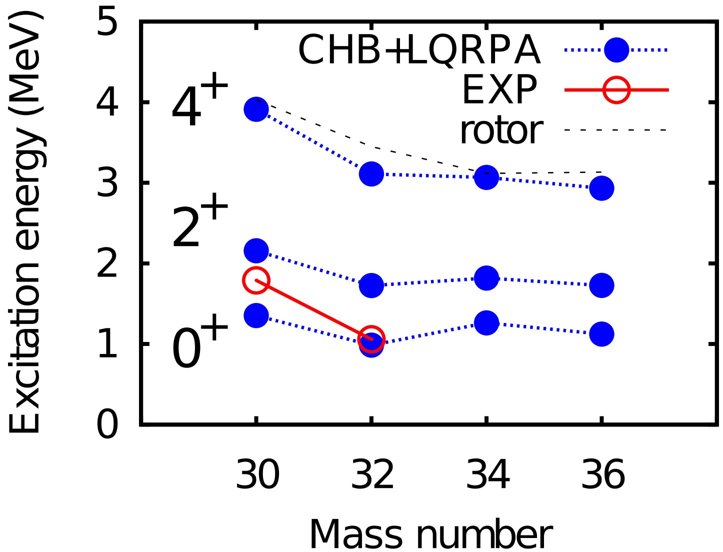
shape fluctuation is largest in 0_1^+ state of ^{32}Mg

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

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

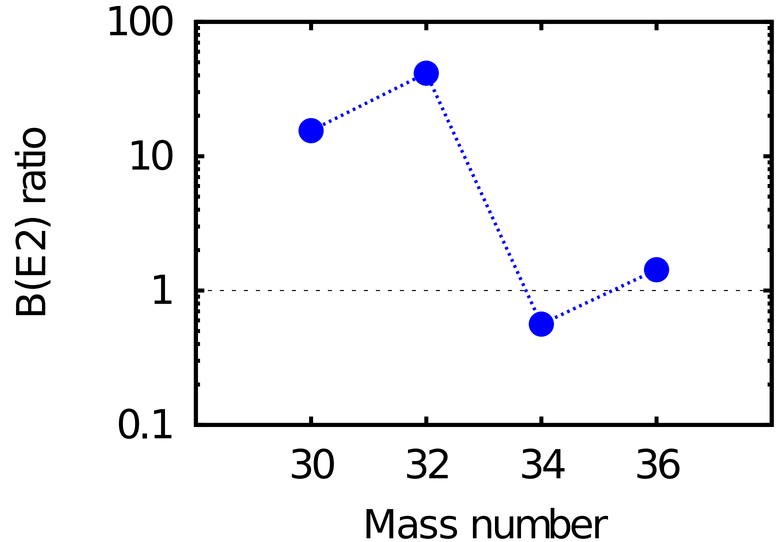
Properties of K=0 excited band

energies of excited K=0 band



B(E2) ratio between K=0 bands

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



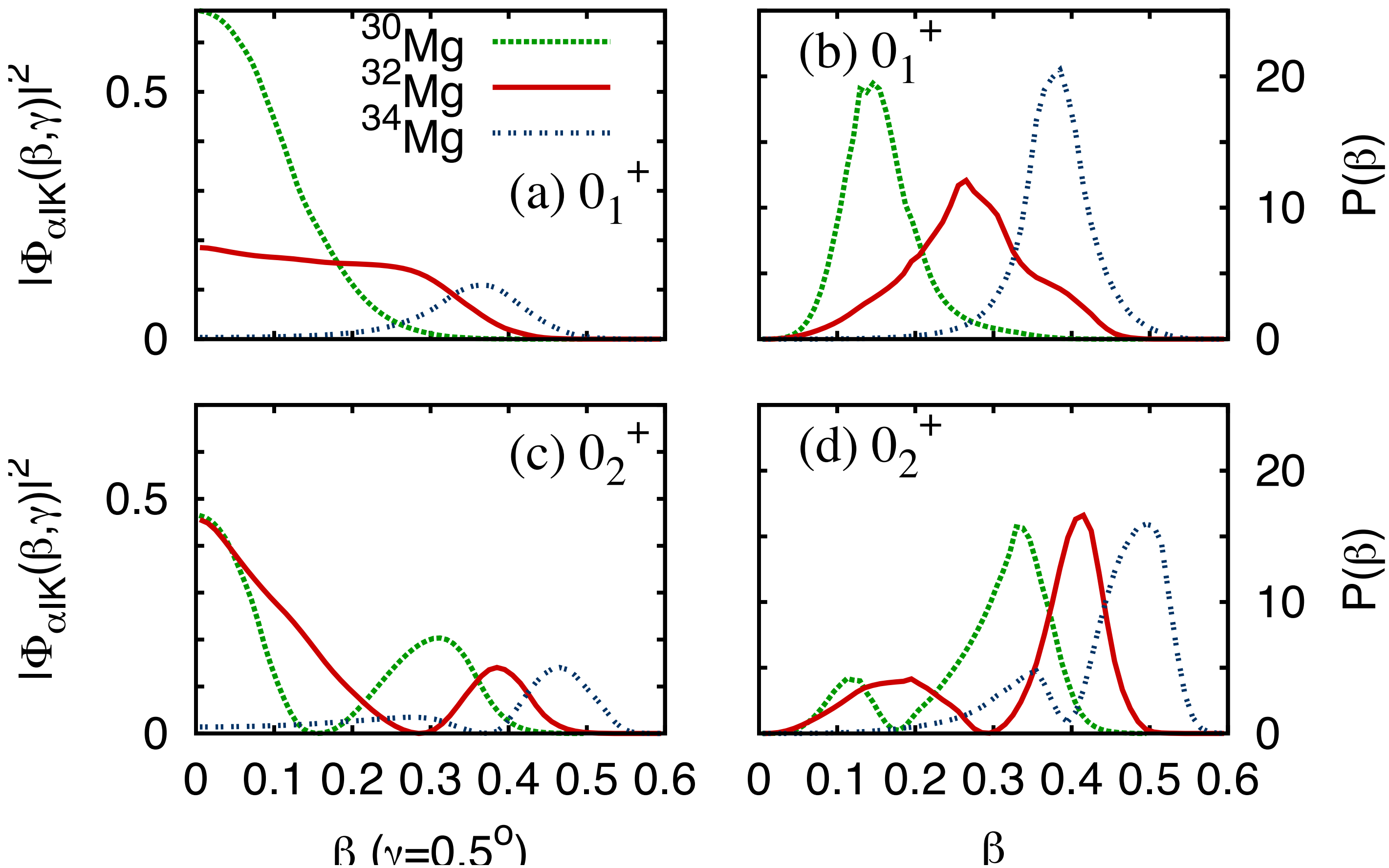
- K=0 excited band: well deformed, deviation from rotor is largest at ^{32}Mg
- The calculation reproduce experimental 0+ energy. Shell model and beyond mean-field calculations predict higher energies for 0_2+ energy of ^{32}Mg (1.4 – 3.1 MeV)
- B(E2) ratio (right figure) should be one
  if 0+ and 2+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

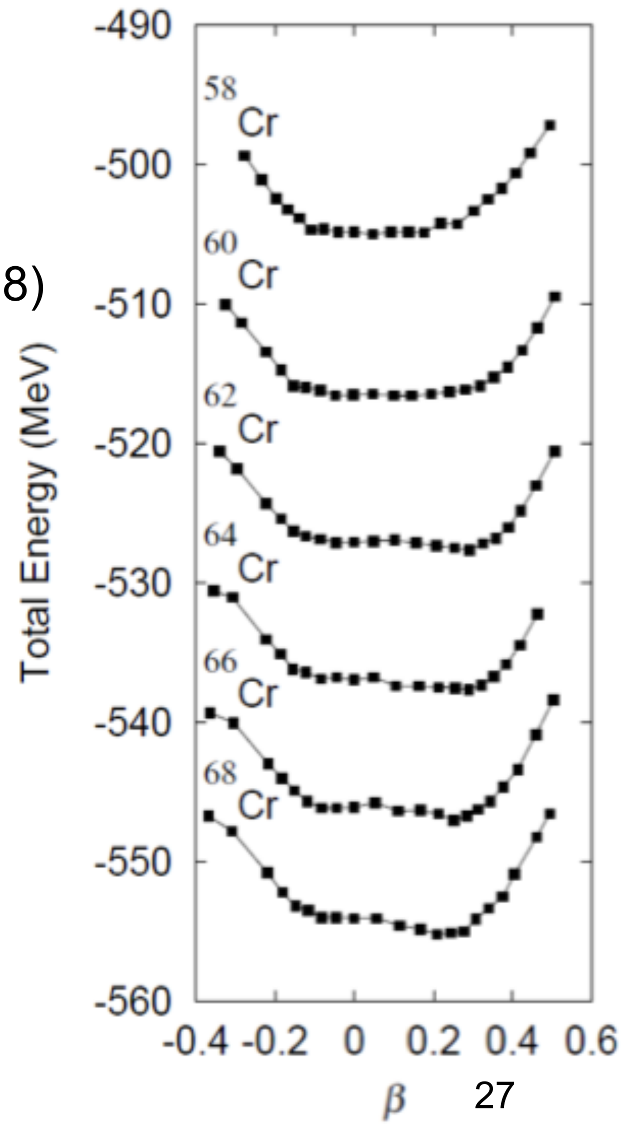
- 2D lattice (axially symmetric)
  - 12.25 fm x 12 fm (0.5 fm mesh)
- Yoshida and Giai, Phys. Rev. **C78**, 064316 (2008)

Collective Hamiltonian for axial deformation (3D)

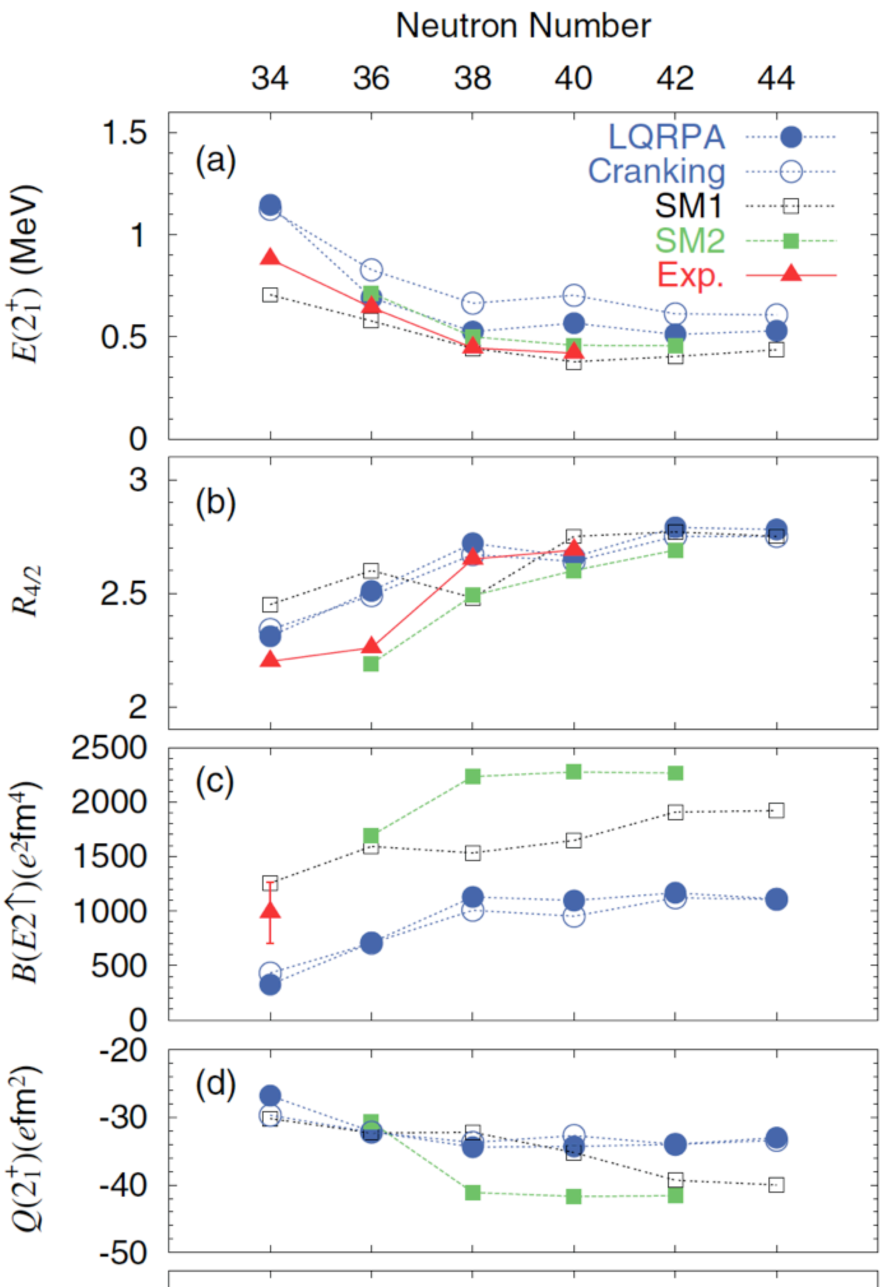
$$\mathcal{H}_{\rm coll} = \frac{1}{2}\boxed{\mathcal{M}_\beta(\beta)}\dot{\beta}^2 + \frac{1}{2}\sum_{i=1}^{2}\boxed{\mathcal{J}_i(\beta)}\omega_i^2 + \boxed{V(\beta)}$$

calculated from Skyrme-CHFB

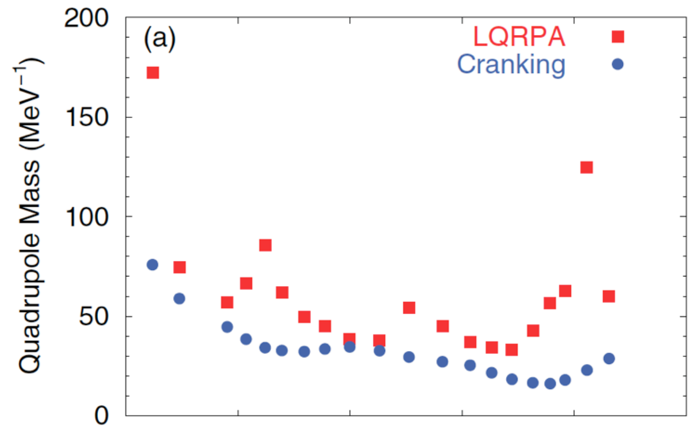
calculated from Skyrme-LQRPA



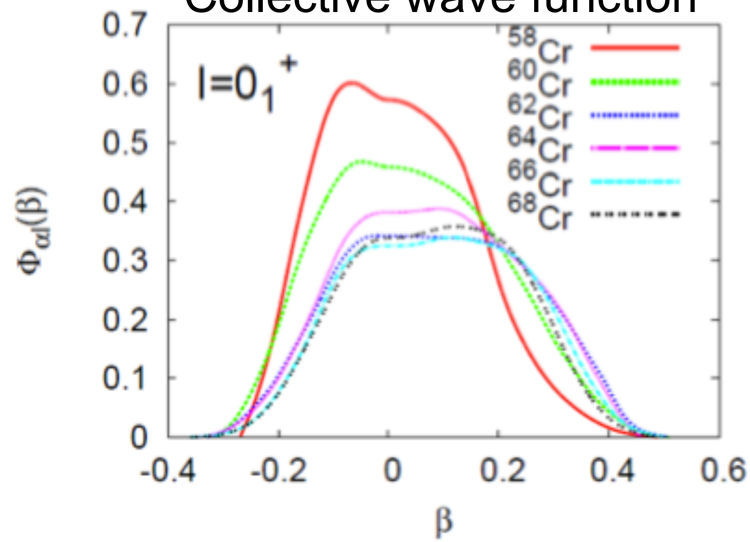
Collectivity of neutron-rich Cr isotopes



vibrational collective mass



Collective wave function



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

Summary

- determination 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 Se and Kr
    shape phase transition around ^{32}Mg and ^{64}Cr
    γ-soft dynamics around ^{26}Mg

  formulation using Skyrme EDF