Finite amplitude method for QRPA in three-dimensional coordinate

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Introduction: Shape fluctuation

Goal: Bohr Hamiltonian, Constrained HFB + Local QRPA

Method: Finite amplitude method in 3D QRPA

Result: Multipole strength, sum rule

Result: Triaxial nucleus

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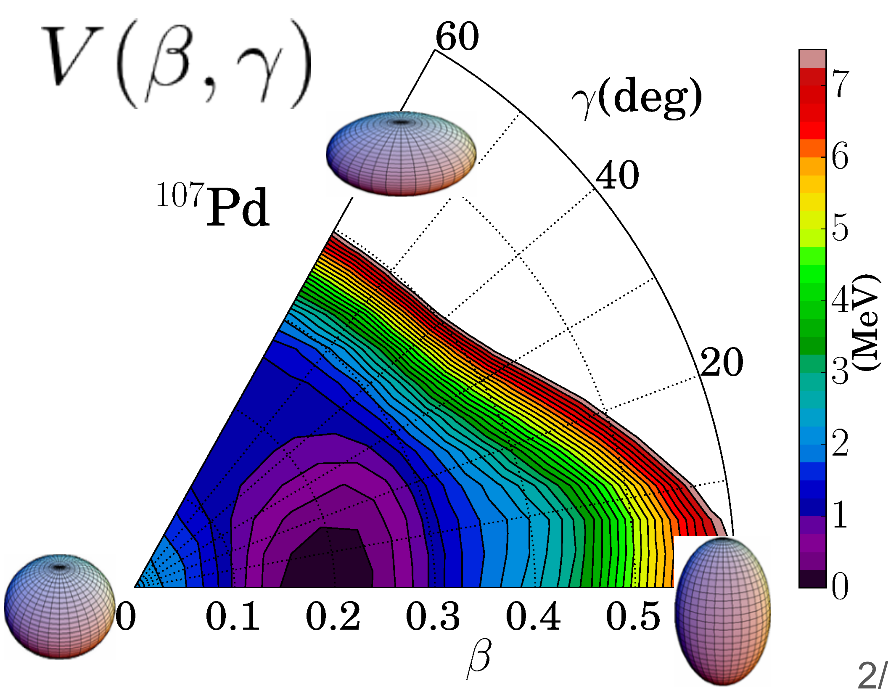
Introduction: Shape fluctuation

A~100 nuclei

- Spherical → deformed, soft, transitional
- Excited states

Shape fluctuations



Goal: 5D Bohr Hamiltonian

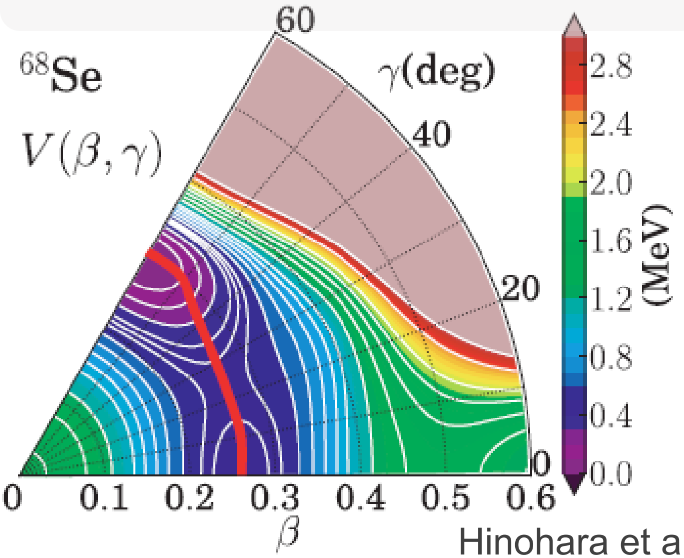
5D quadrupole collective Hamiltonian

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

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

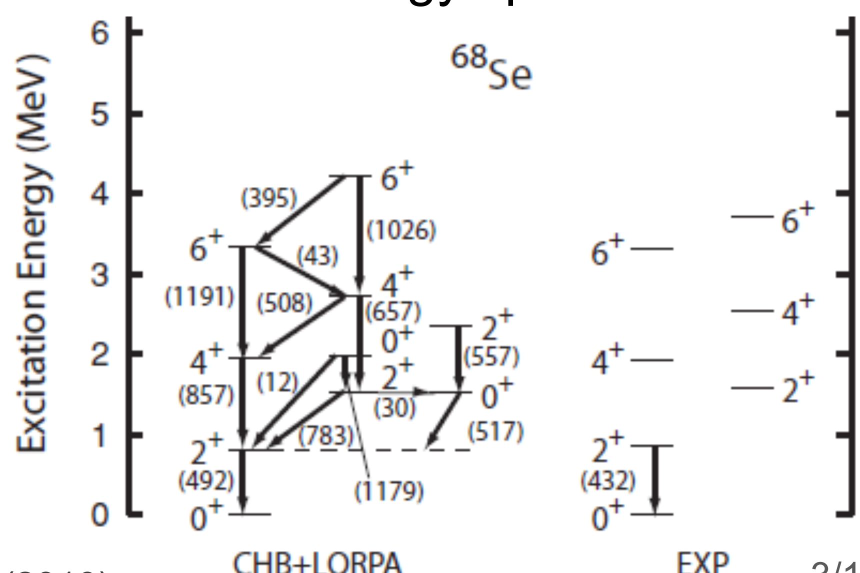
$$T_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{J}_k(\beta,\gamma)\omega_k^2$$

$V(\beta,\gamma),\ D_{\mu\nu}(\beta,\gamma),\ \mathcal{J}_k(\beta,\gamma)$



Quantization

Energy spectra



Hinohara et al., PRC82 (2010) 064313

Goal: Constrained HFB + Local QRPA

5D quadrupole collective Hamiltonian

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

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

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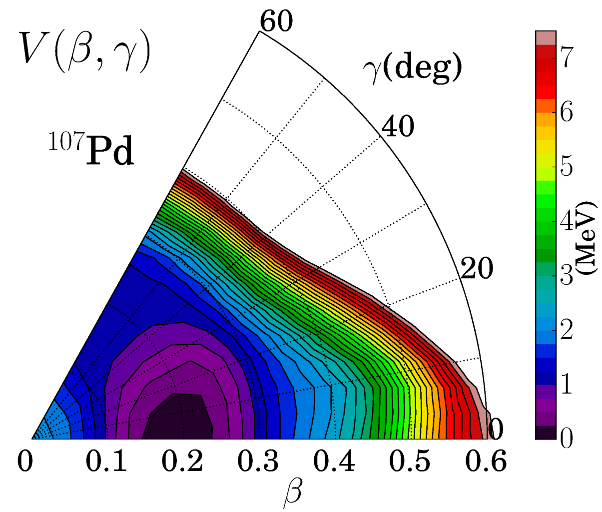

$V(\beta,\gamma)$ Constrained HFB with Skyrme energy density functional

Three-dimension in β-γ plane

$D_{\mu\nu}(\beta,\gamma)$ $\mathcal{J}_k(\beta,\gamma)$ Local QRPA with Skyrme energy density functional

3D QRPA is necessary for β-γ dynamics

Aim of this talk

To construct a finite amplitude method (FAM) for 3D QRPA with self-consistent Skyrme EDF as a first step

Finite amplitude method: Efficient method to solve QRPA with a reasonable computational cost

Method: Quasi-particle RPA (QRPA)

QRPA equation

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

1. Construct A and B matrix

$$A_{minj} = (\varepsilon_m - \varepsilon_i)\delta_{mn}\delta_{ij} + \frac{\partial h_{mi}}{\partial \rho_{nj}} \qquad B_{minj} = \frac{\partial h_{mi}}{\partial \rho_{jn}}$$ (for RPA)

2. Diagonalize A B matrix to obtain ω and (X,Y) amplitude

- Time-consuming computation $\frac{\delta h}{\delta \rho}$ (residual interaction)
- Diagonalization of big matrix A B (~$10^{5\text{-}6}$)

Method: 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
Pei et al., PRC90 (2014) 051304

QRPA equation

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

Finite amplitude method (FAM)

$$\delta h = \frac{\delta h}{\delta\rho}\delta\rho \longrightarrow \delta h \approx \frac{h[\rho_0 + \eta\delta\rho] - h[\rho_0]}{\eta}$$
$$\approx h[\delta\rho]$$

Explicit linearization
Kortelainen et al., PRC92(2015)051302

Advantages:

- Avoid computing $\frac{\delta h}{\delta\rho}$
- δh can be computed by static HFB codes with slight change
- Avoid diagonalizing A, B: Iterative method

Method: Finite amplitude method (FAM)

QRPA equation

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

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Kortelainen et al., PRC92(2015)051302

<u>At each ω</u>

$$X_{\mu\nu}, Y_{\mu\nu} \leftarrow$$

$$\delta H^{20} = U^\dagger \delta h V^* - V^\dagger \delta h^T U^* - V^\dagger \overline{\delta\Delta}^* V^* + U^\dagger \delta\Delta U^*$$
$$\delta H^{02} = U^T \delta h^T V - V^T \delta h U - V^T \delta\Delta V + U^T \overline{\delta\Delta}^* U.$$

$$\delta\rho = UXV^T + V^*Y^TU^\dagger$$
$$\delta\kappa = UXU^T + V^*Y^TV^\dagger$$
$$\overline{\delta\kappa} = V^*X^\dagger V^\dagger + UY^*U^T$$

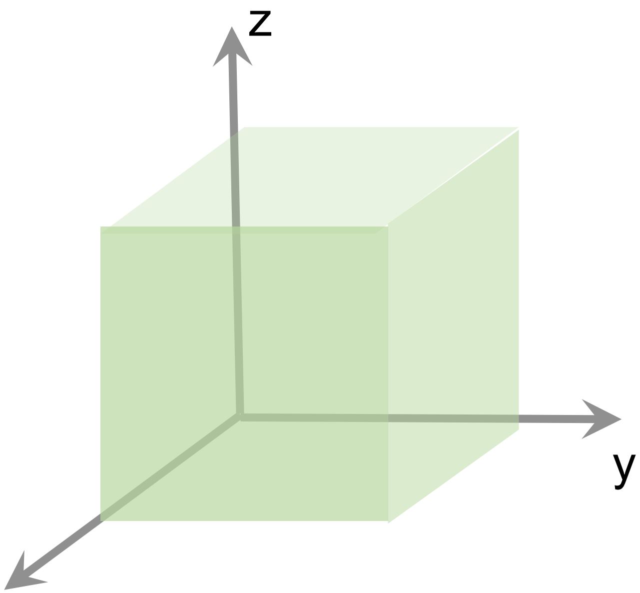
$$\delta h(\omega) = h[\delta\rho]$$
$$\delta\Delta(\omega) = \Delta[\delta\kappa]$$
$$\overline{\delta\Delta}(\omega) = \Delta[\delta\bar\kappa]$$

$$\delta\rho(\boldsymbol{r}) = \sum_{ij,\sigma} \phi_i(\boldsymbol{r},\sigma)\ \delta\rho_{ij}\ \phi_j^*(\boldsymbol{r},\sigma) \qquad \delta\kappa(\boldsymbol{r}) = \sum_{i\hat{j},\sigma=\pm1} \sigma\ \phi_i(\boldsymbol{r},\sigma)\ \delta\kappa_{i\hat{j}}\ \phi_{\hat{j}}(\boldsymbol{r},-\sigma)$$

$X, Y, \delta H^{20}, \delta H^{02}, F^{20}, F^{02}, E$: Quasiparticle basis

$\delta\rho, \delta\kappa, \overline{\delta\kappa}, h, \delta\Delta, \overline{\delta\Delta}$: Hartree-Fock basis

Setup: Coordinate, symmetry, base



x>0, y>0, z>0

Computer code for 3D-FAM is constructed from evb8 code (similar to ev8)

HF basis and quasi-particle basis are used

Parity, isospin, and z-signature blocks

Skyrme EDF (SkM*, SLy4) (no tensor terms)

Contact volume pairing

Δx = 0.8 fm

Mesh: 13 x 13 x 13 – 18 x 18 x 18

Modified Broyden method for iteration

$\omega \to \omega + i\gamma$

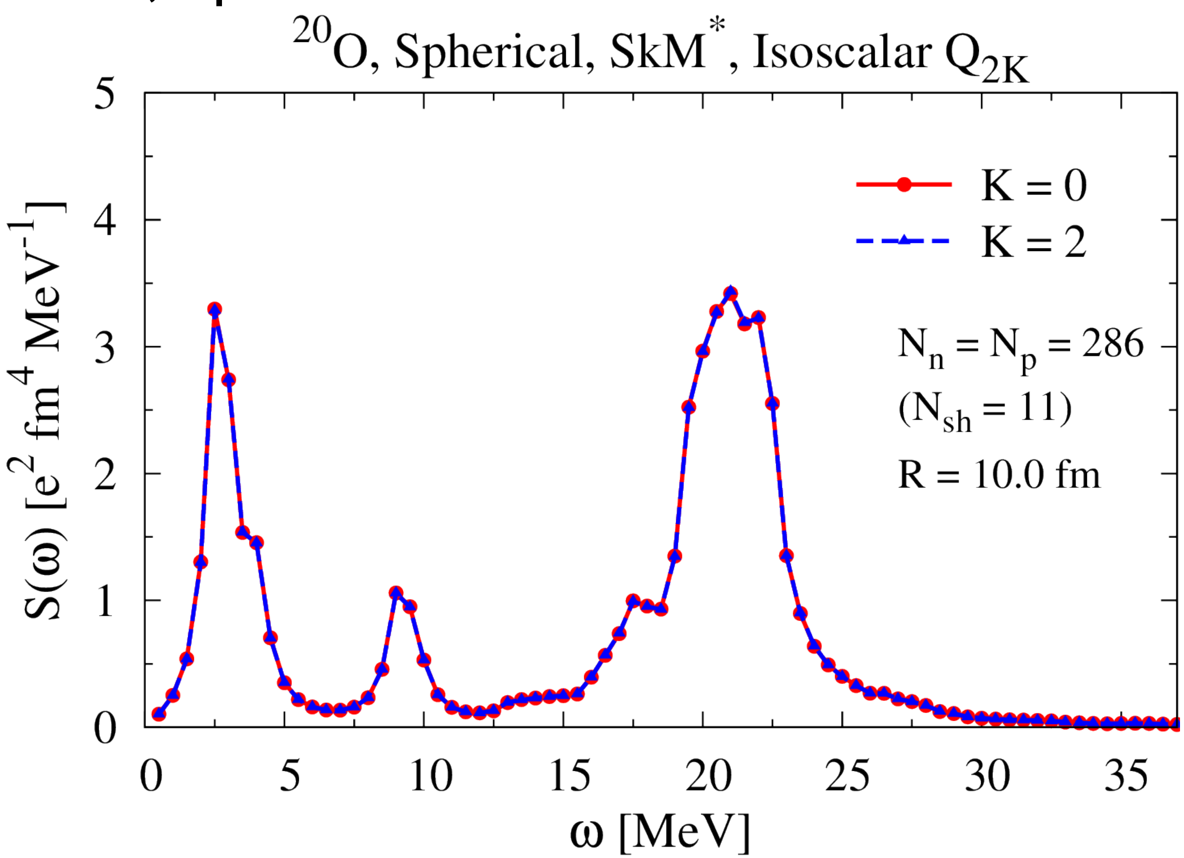
0.5MeV smearing width

Benchmark: Spherical nucleus

Isoscalar quadrupole mode

$$f_{LK}^{IS} = \frac{eZ}{A} \sum_i^A r_i^L Y_{LK}(\hat{\boldsymbol{r}}_i)$$

^{20}O, spherical → all K are identical

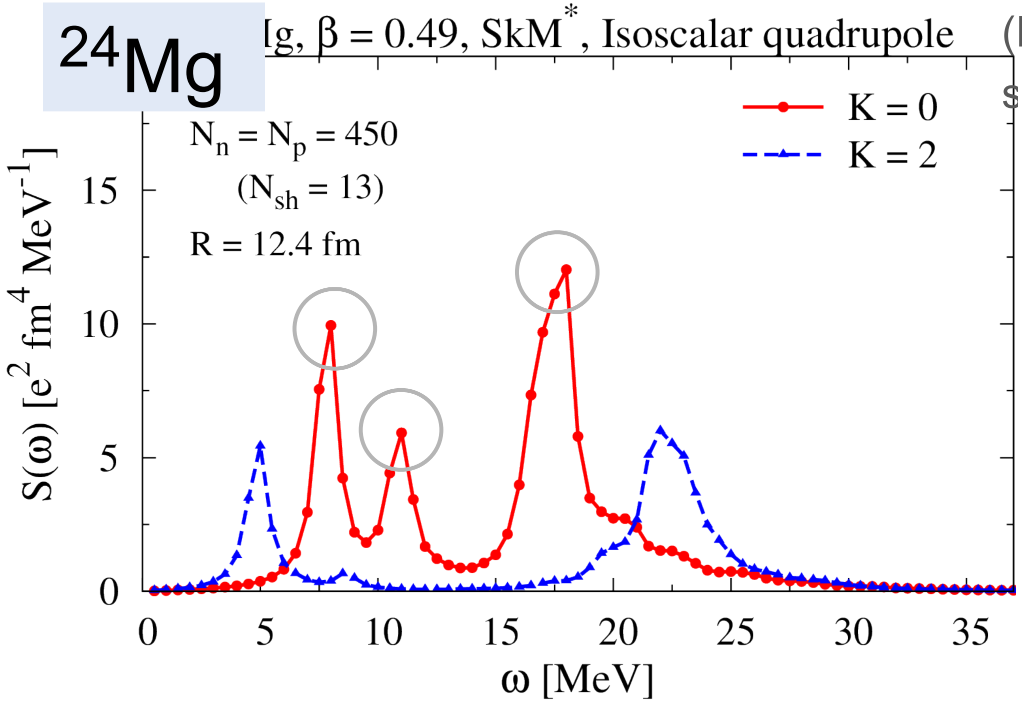


K=0 & K=2: identical

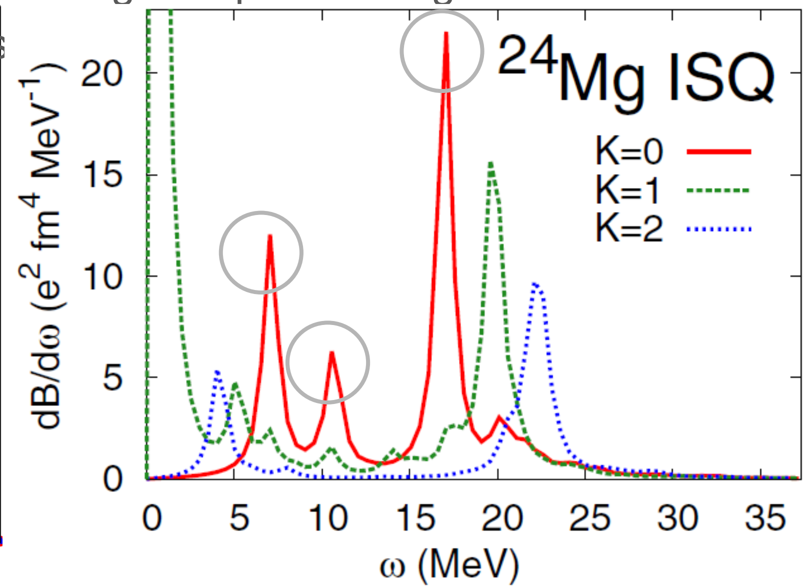
K=1: different signature block (Not shown)

Smearing width = 0.5 MeV

Benchmark: Isoscalar quadrupole strength



(Pairing collapse in the ground



FAM of HFBTHO, N_{sh} = 15

Kortelainen et al.,

PRC92(2015)051302

Energy weighted sum rule value(E < 50MeV)

98% (K=0), 96% (K=2)

70 CPU hours, 2GB memory for 100 ω points

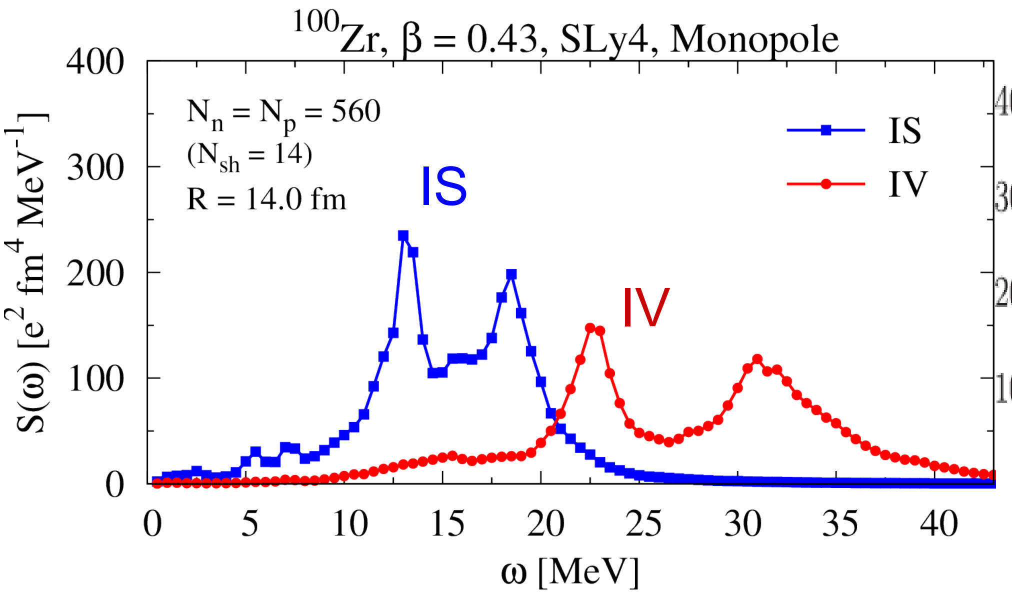
40-50 iterations at most

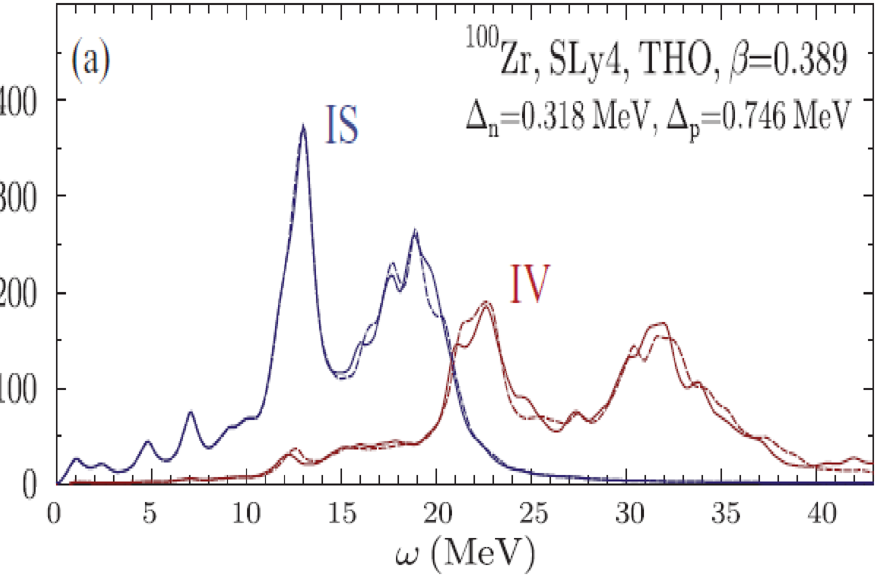
$$\int_0^\infty \omega S(\omega) d\omega = \frac{1}{2}\langle[\hat{F},[\hat{H},\hat{F}]]\rangle$$

$$= \frac{\hbar^2}{2m}\int d^3r|\nabla f(\boldsymbol{r})|^2\rho(\boldsymbol{r})$$

Benchmark: Deformed superfluid nucleus

^{100}Zr, prolate, monopole





Stoitsov et al., PRC84(2011)041305

Two-peak structure

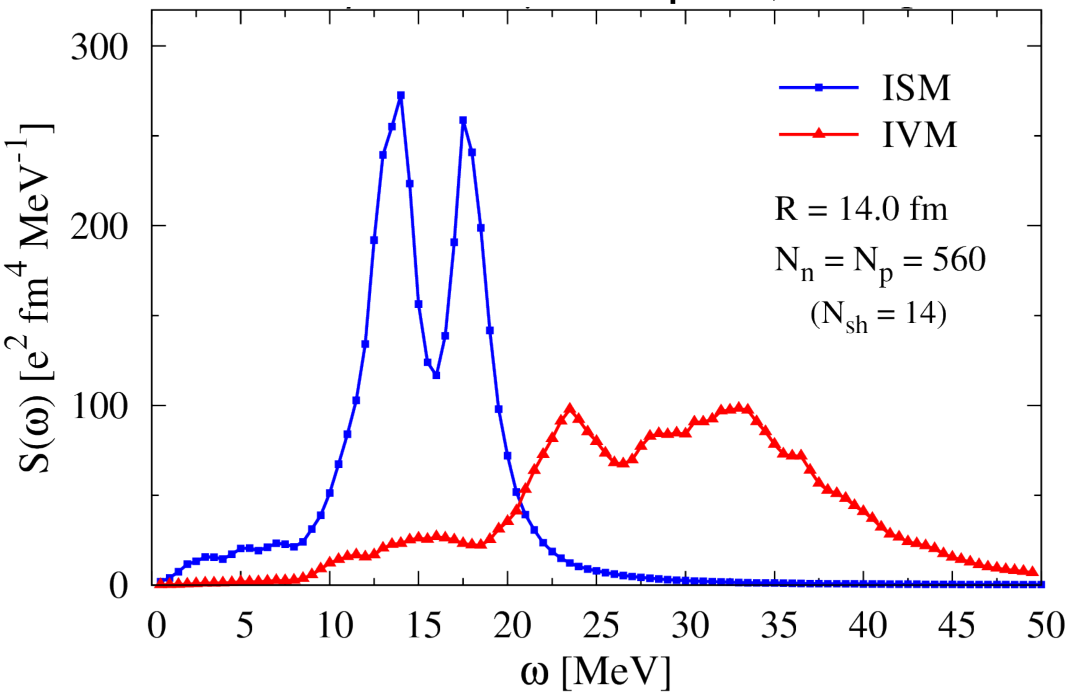
Difference in height of the peaks

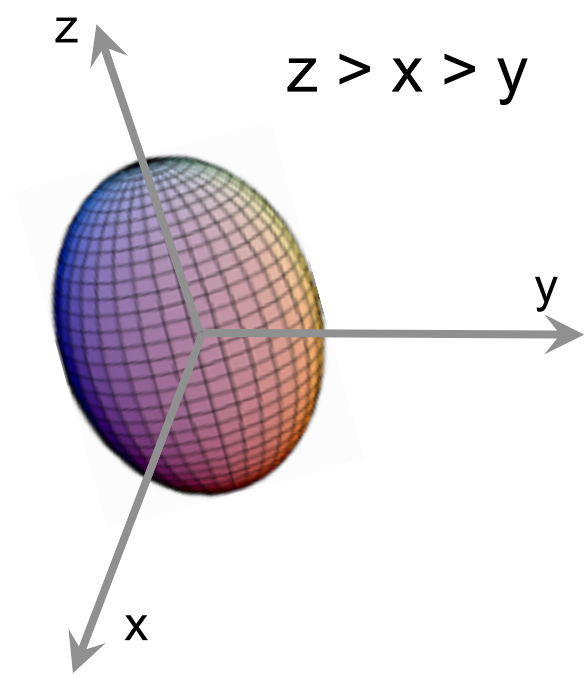
EWSR: 97% (IS)

Result: Triaxial nucleus

^{110}Ru, β = 0.31, γ = 20^o

Isoscalar & isovector monopole, SkM*





Finite pairing in the ground state
Smearing width = 0.5 MeV

Summary

3D FAM+QRPA with Skyrme EDF is ready

Benchmark

Spherical: ^{20}O

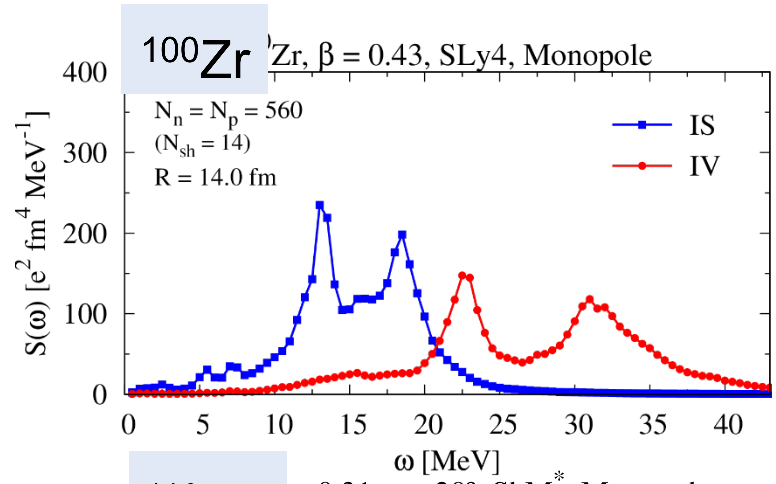
Deformed: ^{24}Mg, ^{100}Zr

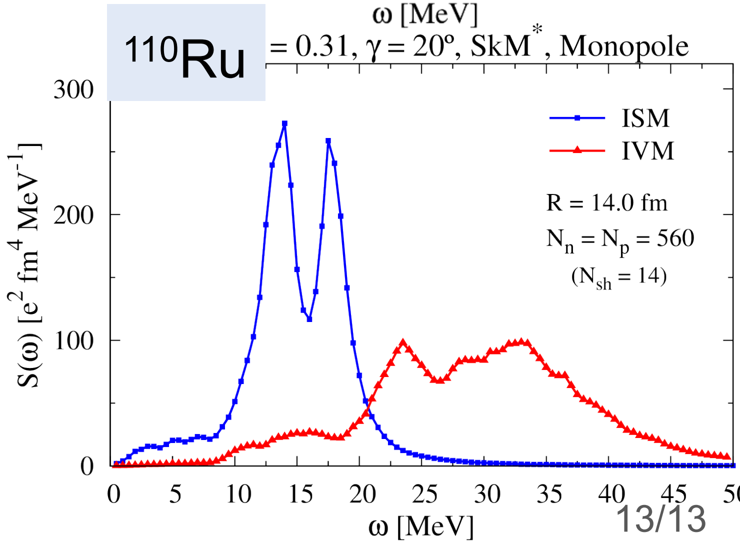
Triaxial nucleus: ^{110}Ru

Future plan

FAM+Local QRPA $\rightarrow$ Mass inertia

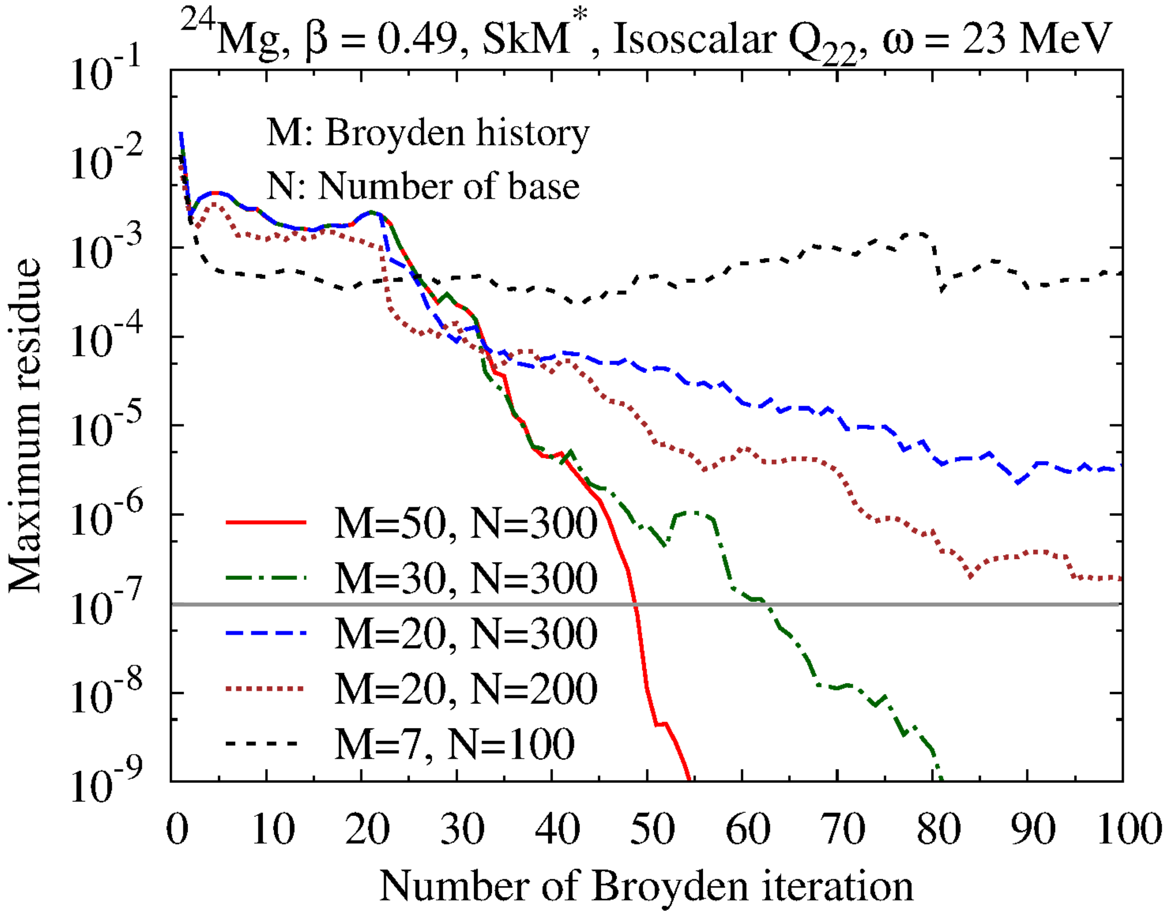
Bohr Hamiltonian





Result: Convergence on iteration

Modified Broyden method



Two-basis method for constrained HFB

Gall et al., Z.Phys.A348 (1994) 183
Terasaki et al., NPA593 (1995) 1

- Hartree-Fock basis $\psi_i(\mathbf{r},\sigma)$, canonical basis $\phi_a(\mathbf{r},\sigma)$
- Imaginary-time method
- Three-dimensional space (Parity imposed)

$$\Delta_{i\hat{j}} = \int d^3r \Psi^*_{i\hat{j}}(\mathbf{r})\Delta(\mathbf{r})$$

$$\Psi_{i\hat{j}}(\mathbf{r}) = \sum_{\sigma=\pm 1} (-1)^{1-\sigma}\psi_i(\mathbf{r},\sigma)\psi_{\hat{j}}(\mathbf{r},-\sigma)$$

1. Construct HFB matrix in HF basis

$$H = \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}$$

2. Diagonalize $H \longrightarrow U, V \longrightarrow \rho, \kappa$

Internal iteration to fix the Fermi energy

3. Diagonalize $\rho \longrightarrow n_a, W_{ia}$ $\quad \phi_a(\mathbf{r}) = \sum_i \psi_i(\mathbf{r}) W_{ia}$

4. Construct $\rho(\mathbf{r}) = \sum_a n_a |\phi_a(\mathbf{r})|^2$, $h[\rho(\mathbf{r})]$, $\Delta(\mathbf{r}) = V_P(\mathbf{r}) \sum_{k\hat{l}} \kappa_{k\hat{l}} \Psi_{k\hat{l}}(\mathbf{r})$

5. Imaginary-time evolution $\psi_i(\mathbf{r}, t+\Delta t) = \exp\left(\frac{-\Delta t}{\hbar} h(\rho)\right) \psi_i(\mathbf{r}, t)$