Finite amplitude method for triaxially deformed superfluid nuclei

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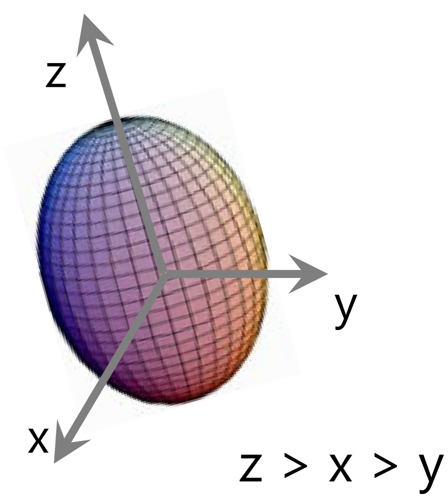
Triaxial → no symmetry axis



Introduction: Shape fluctuation

Goal: 5D collective Hamiltonian, local QRPA

Method: Finite amplitude method in 3D QRPA

Result: Multipole strength, sum rule of triaxial nucleus

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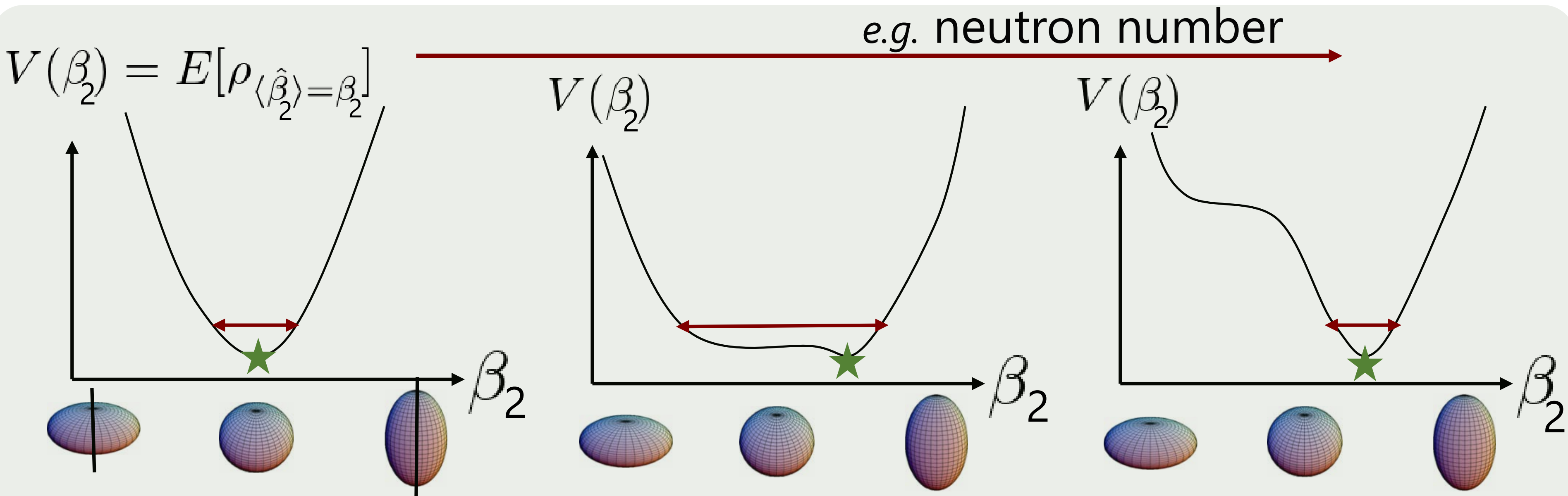
Introduction: Shape fluctuation

Nuclear shape : Quantum object

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



Ground state DFT + (Quasiparticle) Random phase approximation (RPA)

Shape fluctuations

Deformed Ground state + deformed (Q)RPA

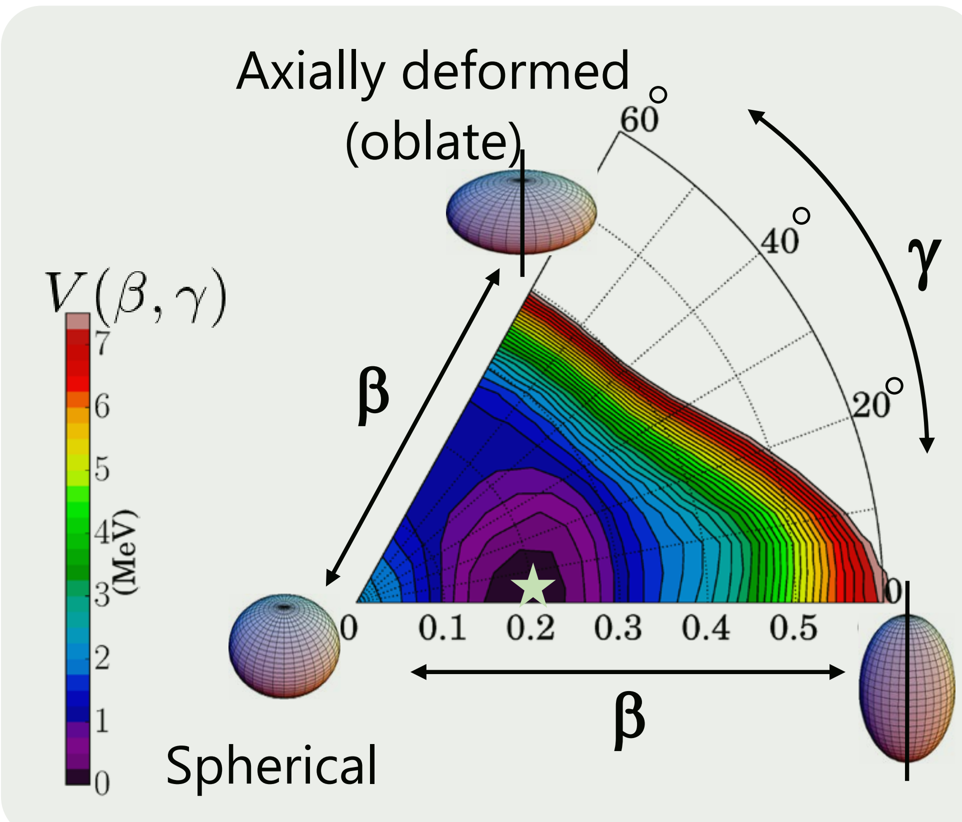
(Q)RPA: Linear response TDDFT
Small amplitude limit of TDDFT

Introduction: Shape fluctuation

Goal: to treat shape fluctuation by an extension of DFT

Quadrupole deformation parameters β, γ

$^{107}_{46}\mathrm{Pd}$



Triaxially deformed
No symmetry axis

Axially deformed
(prolate)

Goal: DFT + more

5D quadrupole collective Hamiltonian

Hinohara et al., PRC82 (2010) 064313

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

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

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

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

$D_{\mu\nu}(\beta,\gamma)$ Inertial mass

$\mathcal{J}_k(\beta,\gamma)$ Moment of inertia

$\longrightarrow$ Normal modes from QRPA at each β, γ

3D QRPA with Skyrme DFT at each β, γ

HFB: HF Bogoliubov, Bogoliubov-de Gennes, for superfluidity

Skyrme DFT: Local functional, ~10 parameters

Aim of this talk

To construct an efficient framework to solve
3D QRPA with self-consistent Skyrme EDF
as a first step

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

Objective in this talk: Linear response around the ground state

Finite amplitude method (FAM)

Linear response TDDFT

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

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

$F_{\mu\nu}$: External perturbation field

(Isoscalar quadrupole moment in this talk)

$$\hat{F} \propto \sum_{i=1}^{A} r_i^2 Y_{2K}(\theta_i, \phi_i)$$

Isoscalar: protons and neutrons in phase

Traditional QRPA---Matrix diagonalization

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

$$A_{\alpha\beta\mu\nu} = E_\mu + E_\nu + \frac{\partial H_{\mu\nu}}{\partial \mathcal{R}_{\alpha\beta}}$$

- Time-consuming computation of $\frac{\partial H_{\mu\nu}}{\partial \mathcal{R}_{\alpha\beta}}$ in A B matrix
- Diagonalization of A B matrix (~$10^{5\text{-}6}$) for deformed nuclei

Finite amplitude method (FAM)

Linear response TDDFT

Nakatsukasa et al., PRC76 (2007) 024318
Avogadro & Nakatsukasa, PRC84(2011)014314
Stoitsov et al., PRC84 (2011) 041305
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$F_{\mu\nu}$: External perturbation field

(Isoscalar quadrupole moment in this talk)

$$\hat{F} \propto \sum_{i=1}^{A} r_i^2 Y_{2K}(\theta_i, \phi_i)$$

Isoscalar: protons and neutrons in phase

Original QRPA matrix

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}$$ N^2 x N^2

FAM matrix

$$\delta H^{20}_{\mu\nu}$$ N x N

Finite amplitude method (FAM)

$$\delta H_{\mu\nu} = \frac{\partial H_{\mu\nu}}{\partial \mathcal{R}_{\alpha\beta}} \partial \mathcal{R}_{\alpha\beta}$$

$$\rightarrow \delta H_{\mu\nu} = \frac{1}{\eta}\{H_{\mu\nu}[\mathcal{R}_0 + \eta\delta\mathcal{R}] - H_{\mu\nu}[\mathcal{R}_0]\}$$

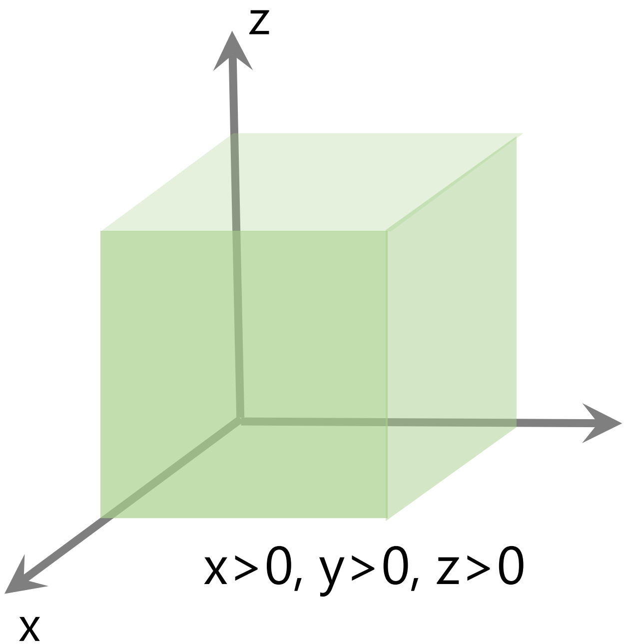
Residual part → finite difference form

$\mathcal{R}_0$: Ground state density

$\delta\mathcal{R}$: Fluctuating density

η : Small parameter

Setup: Coordinate, symmetry, basis



- Parity
- Modified Broyden method for iteration
- Smearing width of γ = 0.5 MeV $\omega \to \omega + i\gamma$
- Strength function

$$S(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(\sum_{\mu<\nu} F^{20*}_{\mu\nu} X_{\mu\nu} + F^{02*}_{\mu\nu} Y_{\mu\nu}\right)$$

Hartree-Fock basis & Quasi-particle basis

Mesh: 15 x 15 x 15 – 17 x 17 x 17 with Δx = 0.8 fm

Δω = 0.5 MeV

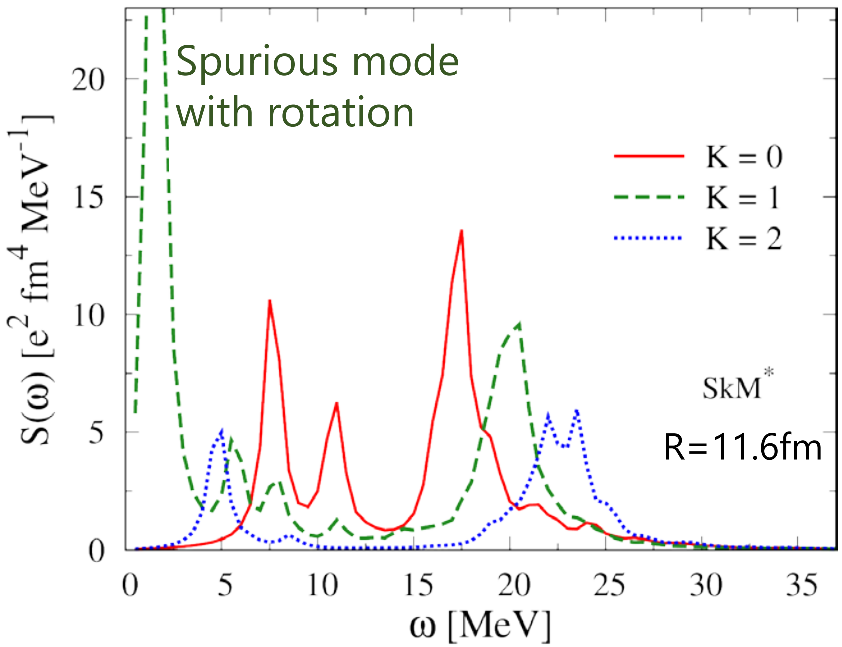
Boundary condition for continuum HF states

Cubic box ⟶ Spherical box

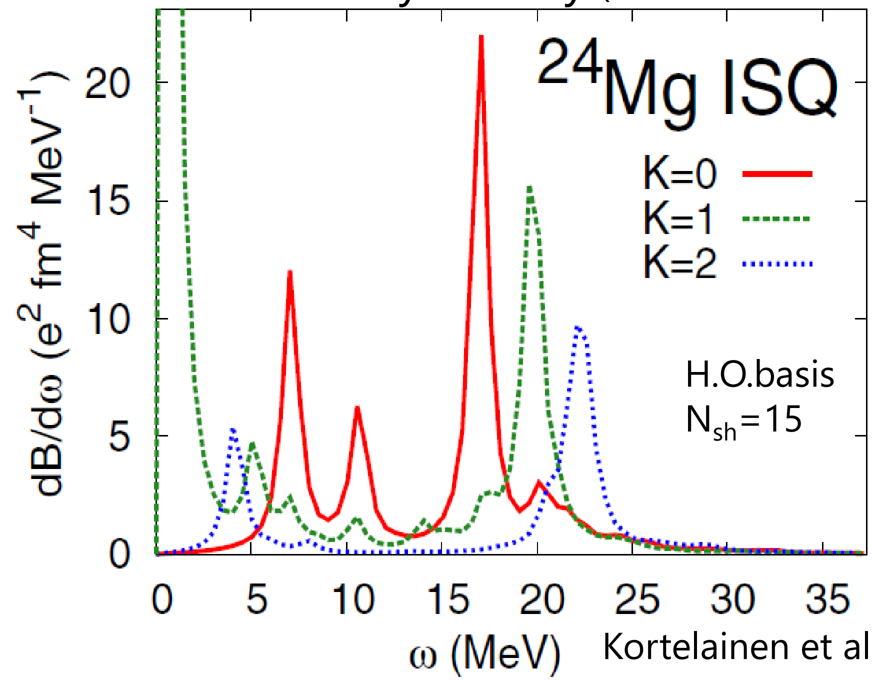
Benchmark: Axially deformed nucleus ^{24}Mg

Isoscalar quadrupole response $\hat{F} = \sum f(\boldsymbol{r}_i) \propto \sum r_i^2 Y_{2K}(\theta_i, \phi_i)$

Our result



Result with axial symmetry (based on HFBTHO)



Kortelainen et al., PRC92(2015)051302

Energy-weighted sum rule (EWSR)

$$\int_0^\infty \omega S(\omega) d\omega = \frac{1}{2}\langle[\hat{F}, [\hat{H}, \hat{F}]]\rangle$$
$$= \frac{\hbar^2}{2m}\int d^3r |\nabla f(\boldsymbol{r})|^2 \rho(\boldsymbol{r})$$

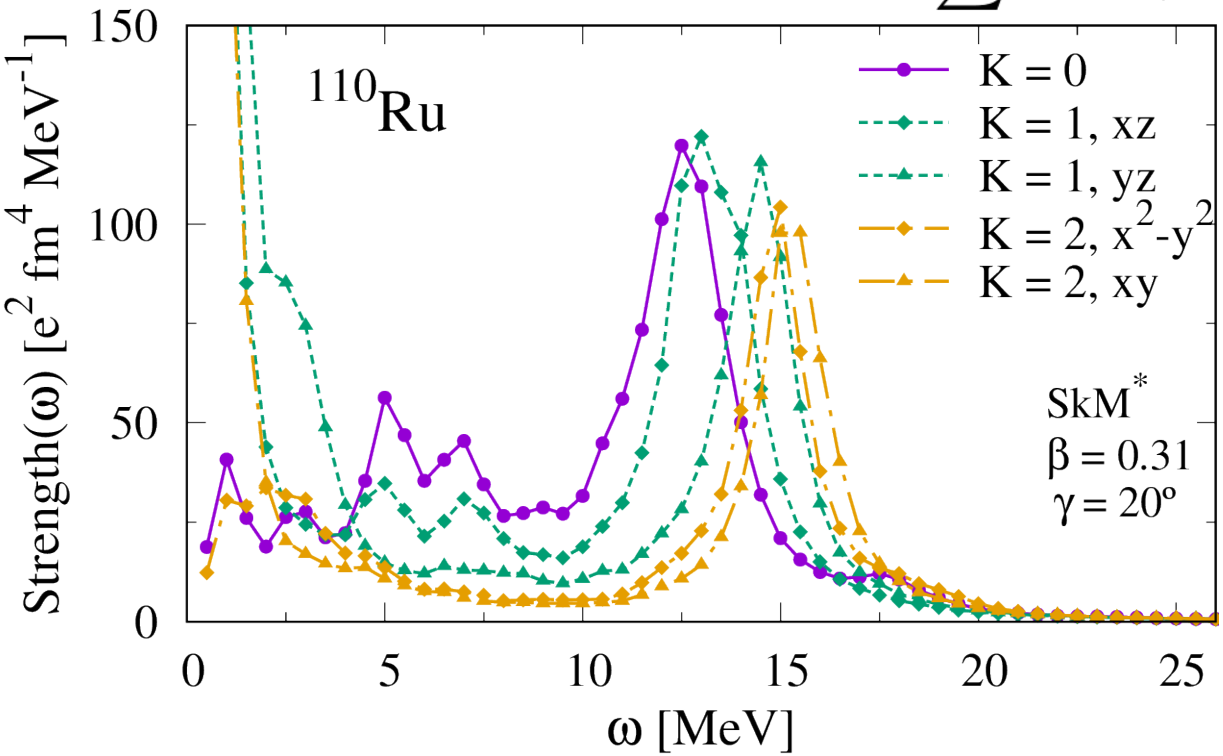
EWSR (ω < 50 MeV)

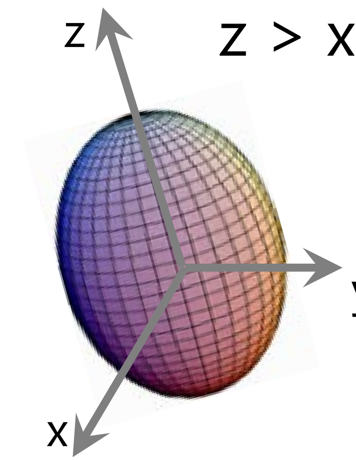
98.4 % (K = 0)

98.4 % (K = 2)

Strength of triaxial superfluid nucleus $^{110}_{44}$Ru

Isoscalar quadrupole response $\hat{F} \propto \sum r_i^2 Y_{2K}(\theta_i, \phi_i)$





~140CPUh for 100ω

~2-2.5GB memory

Five strength functions (K=0, ±1, ±2)

Three spurious rotations around x, y, z axes

⟶ Only appear in triaxial nuclei

EWSR (ω < 50 MeV)

97.8 % (K=0)

99.9 % (K=2, x^2-y^2)

Summary

Shape fluctuation → Bohr Hamiltonian

3D FAM+QRPA with Skyrme EDF is ready

Benchmark: Axially deformed nucleus ^{24}Mg

Triaxially deformed superfluid nucleus ^{110}Ru

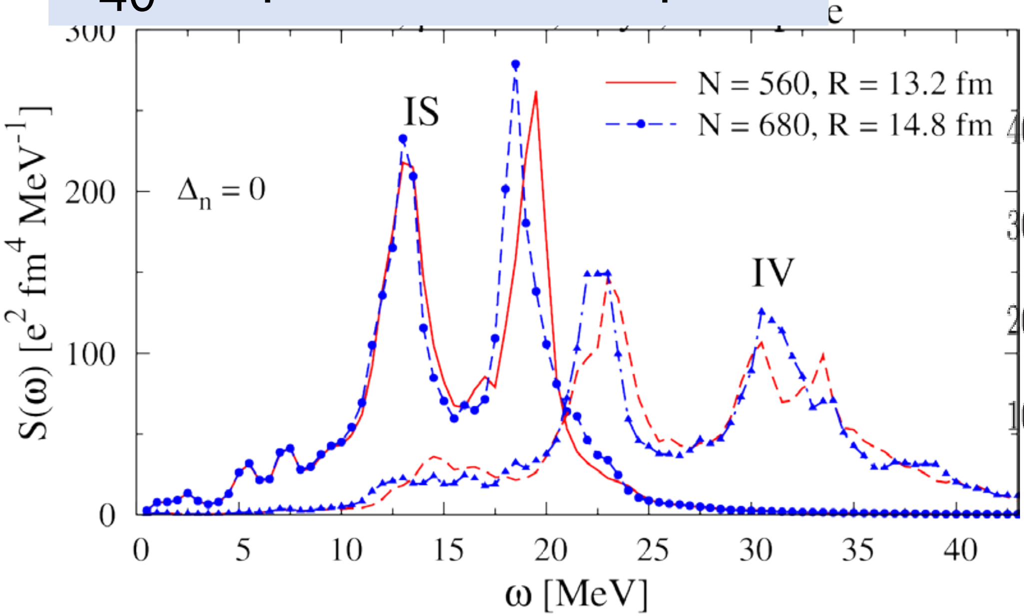
Future plan

FAM+Local QRPA → Mass inertial functions

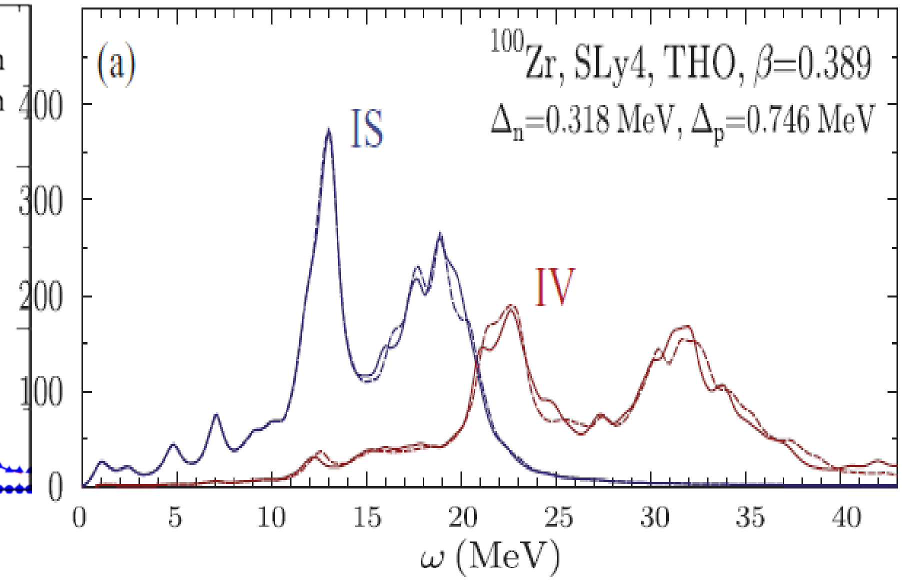
Bohr Hamiltonian

Benchmark: Deformed superfluid nucleus

$^{100}_{40}$Zr, prolate, monopole



Result with axial symmetry (based on HFBTHO)
Stoitsov et al., PRC84(2011)041305



Energy weighted sum rule (EWSR)

$$\int_0^\infty \omega S(\omega) d\omega = \frac{1}{2}\langle[\hat{F},[\hat{H},\hat{F}]]\rangle$$
$$= \frac{\hbar^2}{2m}\int d^3r |\nabla f(\boldsymbol{r})|^2 \rho(\boldsymbol{r})$$
$$f(\boldsymbol{r}) \propto r^2$$

EWSR

98.2 % (R=13.2fm)

98.3 % (R=14.8fm)

Goal: 5D Bohr Hamiltonian

5D quadrupole collective Hamiltonian

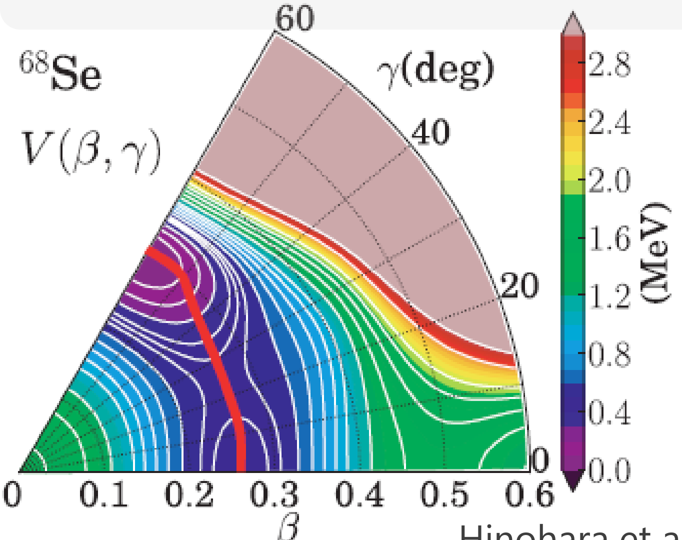
$$\mathcal{H} = T_{\text{vib}} + T_{\text{rot}} + V(\beta,\gamma)$$

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

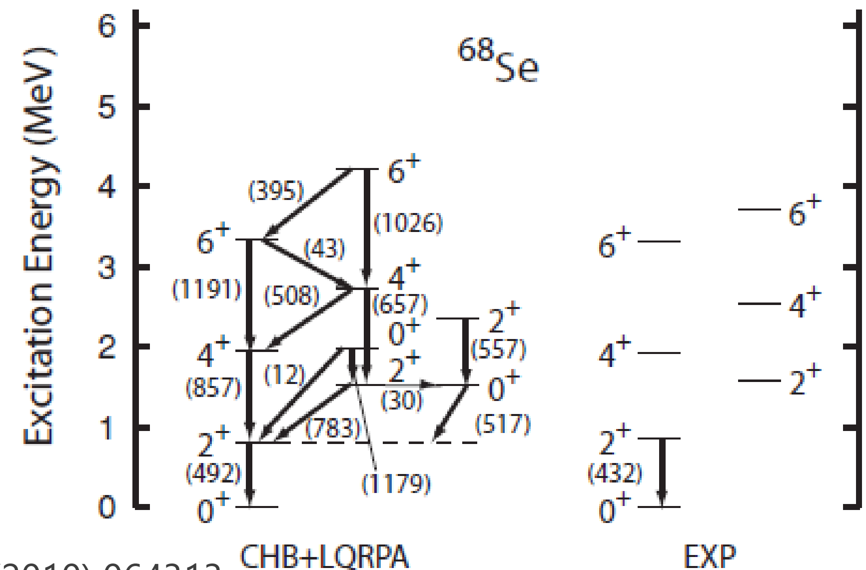
$$T_{\text{rot}} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{J}_k(\beta,\gamma)\omega_k^2$$

Quantization

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



Energy spectra

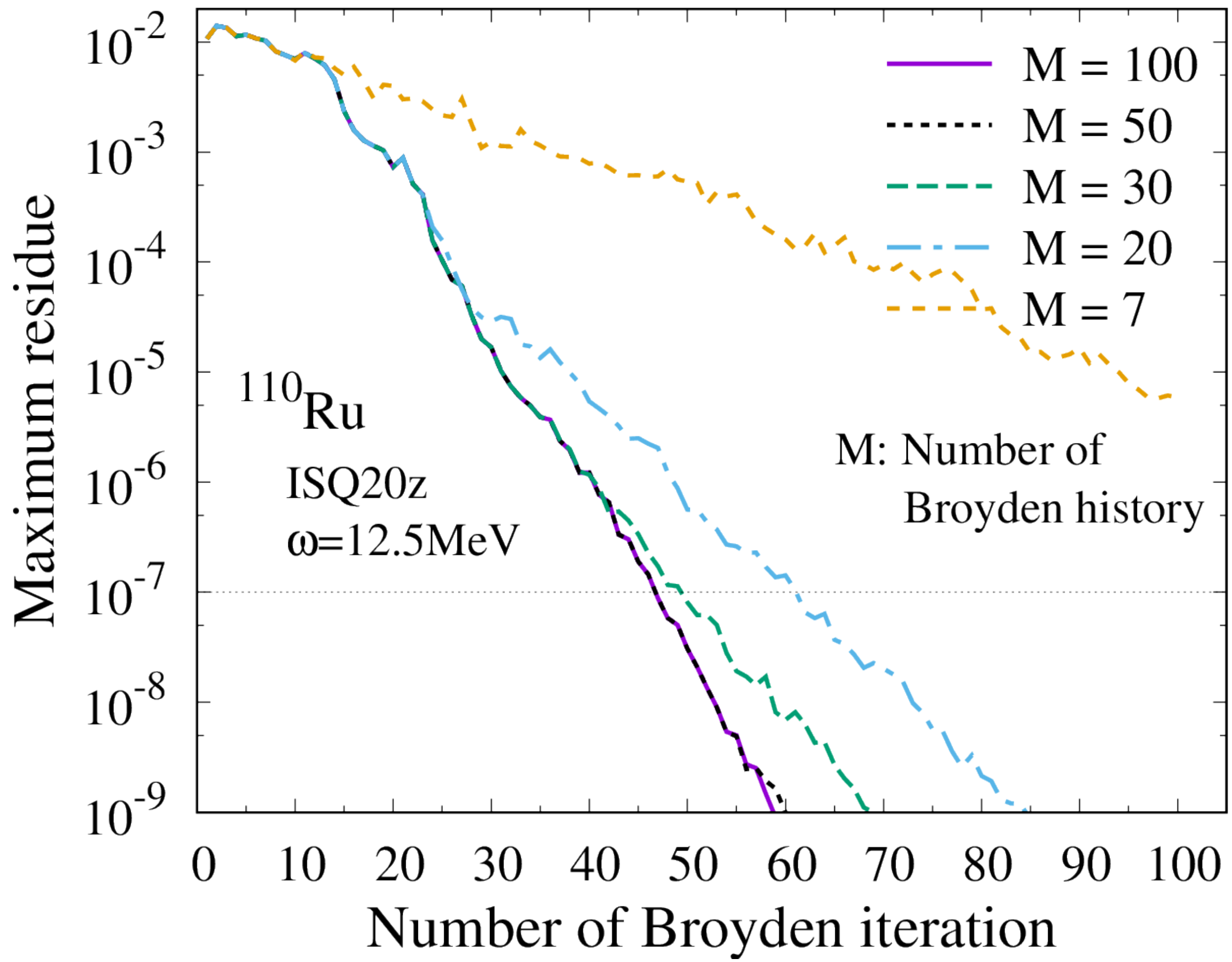


Hinohara et al., PRC82 (2010) 064313

Result: Convergence on iteration

Modified Broyden method

$\mathrm{Maxval}(X_{i+1}-X_i, Y_{i+1}-Y_i)$



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

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

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 (~$10^{5\text{-}6}$)

Energy density functional

- Skyrme energy density functional

$$\mathcal{E}_{\rm Sk} \equiv \int d^3r \sum_{t=0,1} \mathcal{H}_t(\boldsymbol{r}) \qquad \begin{aligned} \rho_{t=0} &= \rho_n + \rho_p \\ \rho_{t=1} &= \rho_n - \rho_p \end{aligned}$$

$$\mathcal{H}_t = C_t^\rho \rho_t^2 + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^\tau \rho_t \tau_t + C_t^{\nabla\cdot J} \rho_t \nabla\cdot\boldsymbol{J}_t - C_t^T \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\mu\nu} \cdots$$
$$+ C_t^s \boldsymbol{s}_t^2 + C_t^{\Delta s} \boldsymbol{s}_t \cdot \Delta\boldsymbol{s}_t - C_t^\tau \boldsymbol{j}_t^2 + C_t^{\nabla\cdot J} \boldsymbol{s}_t \cdot \nabla\times\boldsymbol{j}_t + C_t^T \boldsymbol{s}_t \cdot \boldsymbol{T}_t + \cdots$$

$$\rho_q(\boldsymbol{r}) = \rho_q(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \tau_q(\boldsymbol{r}) = \nabla\cdot\nabla'\rho_q(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad J_{q,\mu\nu}(\boldsymbol{r}) = -\frac{i}{2}(\nabla_\mu - \nabla'_\mu) s_{q,\nu}(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$
$$\boldsymbol{s}_q(\boldsymbol{r}) = \boldsymbol{s}_q(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \boldsymbol{T}_q(\boldsymbol{r}) = \nabla\cdot\nabla'\boldsymbol{s}_q(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}, \quad \boldsymbol{j}_q(\boldsymbol{r}) = -\frac{i}{2}(\nabla - \nabla')\rho_q(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$\rho_q(\boldsymbol{r},\boldsymbol{r}') = \sum_{\sigma=\pm1} \rho_q(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma) = \sum_{\sigma=\pm1}\sum_k n_k \phi_k(\boldsymbol{r}\sigma q)\phi_k^*(\boldsymbol{r}'\sigma q)$$
$$\boldsymbol{s}_q(\boldsymbol{r},\boldsymbol{r}') = \sum_{\sigma,\sigma'=\pm1} \rho_q(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')\langle\sigma'|\hat{\boldsymbol{\sigma}}|\sigma\rangle$$

Bender, Heenen, Reinhard, Rev. Mod. Phys. 75 (2003) 121

Method: Finite amplitude method (FAM)

QRPA equation

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

Modified Broyden method
→ 40-60 iterations at most

<u>At each ω</u>

$$X_{\mu\nu}, Y_{\mu\nu} \longleftarrow \begin{aligned} \delta H^{20} &= U^\dagger \delta h V^* - V^\dagger \delta h^T U^* - V^\dagger \overline{\delta\Delta}^* V^* + U^\dagger \delta\Delta U^* \\ \delta H^{02} &= U^T \delta h^T V - V^T \delta h U - V^T \delta\Delta V + U^T \overline{\delta\Delta}^* U. \end{aligned}$$

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

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

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

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

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

Method: Constrained HFB + Local QRPA

Hinohara et al., PRC82 (2010) 064313

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

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

$$\delta\langle\phi(\beta,\gamma)|[\hat{H}_{\rm CHFB}(\beta,\gamma),\frac{1}{i}\hat{P}^i(\beta,\gamma)] - C_i(\beta,\gamma)\hat{Q}^i(\beta,\gamma)|\phi(\beta,\gamma)\rangle = 0 \quad i = 1,2$$

$$\longrightarrow \hat{Q}^i(\beta,\gamma), \hat{P}^i(\beta,\gamma) \longrightarrow D_{\mu\nu}(\beta,\gamma)$$

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

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

$$\langle\phi(\beta,\gamma)|[\hat{\Psi}_k(\beta,\gamma),\hat{I}_{k'}]|\phi(\beta,\gamma)\rangle = i\delta_{kk'} \qquad k = 1,2,3$$

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

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)

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

$$\Psi_{i\hat{j}}(\mathbf{r}) = \sum_{\sigma=\pm1} (-1)^{1-\sigma}\psi_i(\mathbf{r},\sigma)\psi_{\hat{j}}(\mathbf{r},-\sigma)$$

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 $\rho(\mathbf{r}) = \sum_a n_a |\phi_a(\mathbf{r})|^2$, $\quad h[\rho(\mathbf{r})]$, $\quad \Delta(\mathbf{r}) = V_P(\mathbf{r}) \sum_{k\hat{l}} \kappa_{k\hat{l}} \Psi_{k\hat{l}}(\mathbf{r})$
5. Imaginary-time evolution $\psi_i(\mathbf{r}, t+\Delta t) = \exp\left(\frac{-\Delta t}{\hbar} h(\rho)\right)\psi_i(\mathbf{r},t)$