
Finite amplitude method and Canonical-Basis TDHFB

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Finite amplitude Method

- Calculations of the (Q)RPA matrix are very expensive.
- An alternative way to reach the full (Q)RPA
 - Cheap programming task
 - Computationally efficient

Linearized TDDFT

$$i \frac{\partial}{\partial t} \rho(t) = [\rho(t), h(t)]$$

- Small-amplitude TDDFT eq. in the time rep.

$$i \frac{\partial}{\partial t} \delta\rho(t) = [\delta\rho(t), h_0] + [\rho_0, \delta h(t)]$$

$$\delta\rho(t) = \sum_{i:\text{occ}} \left\{ |\delta\psi_i(t)\rangle\langle\phi_i| + |\phi_i\rangle\langle\delta\psi_i(t)| \right\}$$

- Linear response equation in the freq. rep.

$$\omega\delta\rho(\omega) = [\delta\rho(\omega), h_0] + [\rho_0, \delta h(\omega)]$$

$$\delta\rho(\omega) = \sum_{i:\text{occ}} \left\{ |X_i(\omega)\rangle\langle\phi_i| + |\phi_i\rangle\langle Y_i(\omega)| \right\}$$

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

Linear response equation

$$\hat{Q} = 1 - \sum_j |\phi_j\rangle\langle\phi_j|$$

$$\omega |X_i(\omega)\rangle = (h_0 - \epsilon_i) |X_i(\omega)\rangle + \hat{Q} \{V_{\text{ext}}(\omega) + \delta h(\omega)\} |\phi_i\rangle$$

$$\omega \langle Y_i(\omega)| = -\langle Y_i(\omega)| (h_0 - \epsilon_i) - \langle\phi_i| \{V_{\text{ext}}(\omega) + \delta h(\omega)\} \hat{Q}$$

Single-particle Hamiltonian as a functional of independent bra and ket

$$h[\langle\psi|, |\psi\rangle]$$

$$h_0 = h[\langle\phi|, |\phi\rangle]$$

Then, the residual (induced) field can be numerically estimated as

$$h_0 + \eta \delta h(\omega) \approx h[\langle\phi| + \eta \langle Y(\omega)|, |\phi\rangle + \eta |X(\omega)\rangle]$$

$$h_0 + \eta \delta h^\dagger(\omega) \approx h[\langle\phi| + \eta \langle X(\omega)|, |\phi\rangle + \eta |Y(\omega)\rangle]$$

Numerical Algorithm

T.N., Inakura, Yabana, PRC76 (2007) 024318.

We want to solve the following linear-response equations:

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = - \begin{pmatrix} (V_{\text{ext}})_{mi} \\ (V_{\text{ext}})_{im} \end{pmatrix}$$

This is the linear algebraic equation of the form:

$$\mathbf{A}\vec{x} = \vec{b}$$

Starting from an initial vector $\vec{x}^{(0)}$, one can use an iterative method to solve the equations.

In the iterative algorithm, we do not need an explicit matrix of \mathbf{A} , but only need to calculate $\mathbf{A}\vec{x}^{(n)}$

For non-hermitian matrix \mathbf{A} , Bi-Conjugate Gradient Method, Generalized Conjugate Gradient Method, etc.

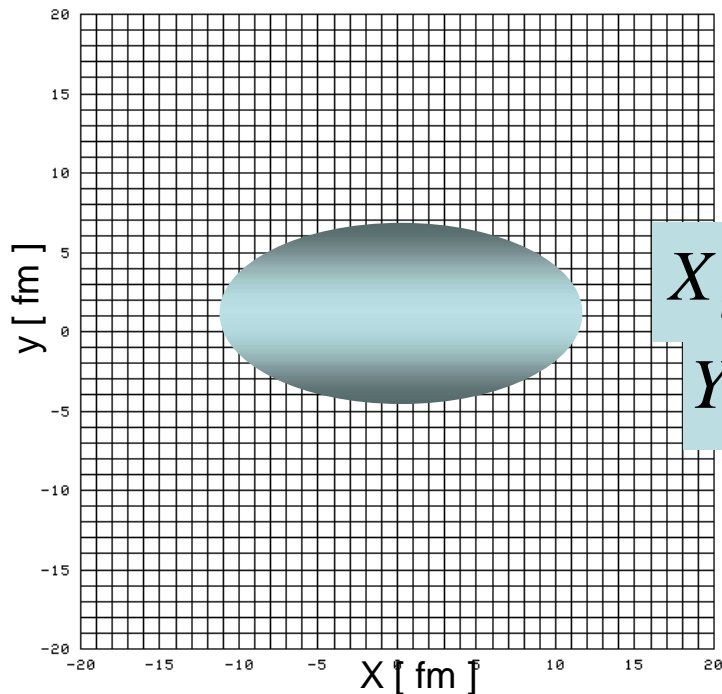
Skyrme-FAM in 3D mesh space

Hartree-Fock Hamiltonian

$$h_{\text{HF}}[\rho, \tau, \mathbf{j}, \mathbf{s}, \vec{\mathbf{J}}] \Rightarrow h_{\text{HF}}[\langle \psi |, | \psi \rangle']$$

$$\rho(\mathbf{r}) = \sum \psi_i'(\mathbf{r}) \psi_i^*(\mathbf{r}) \quad \tau(\mathbf{r}) = \sum (\nabla \psi_i'(\mathbf{r})) \cdot (\nabla \psi_i(\mathbf{r}))^*$$

$$\mathbf{j}(\mathbf{r}) = \sum \psi_i'(\mathbf{r}) (\nabla \psi_i(\mathbf{r}))^* - (\nabla \psi_i'(\mathbf{r})) \psi_i^*(\mathbf{r})$$



3D space is discretized in lattice

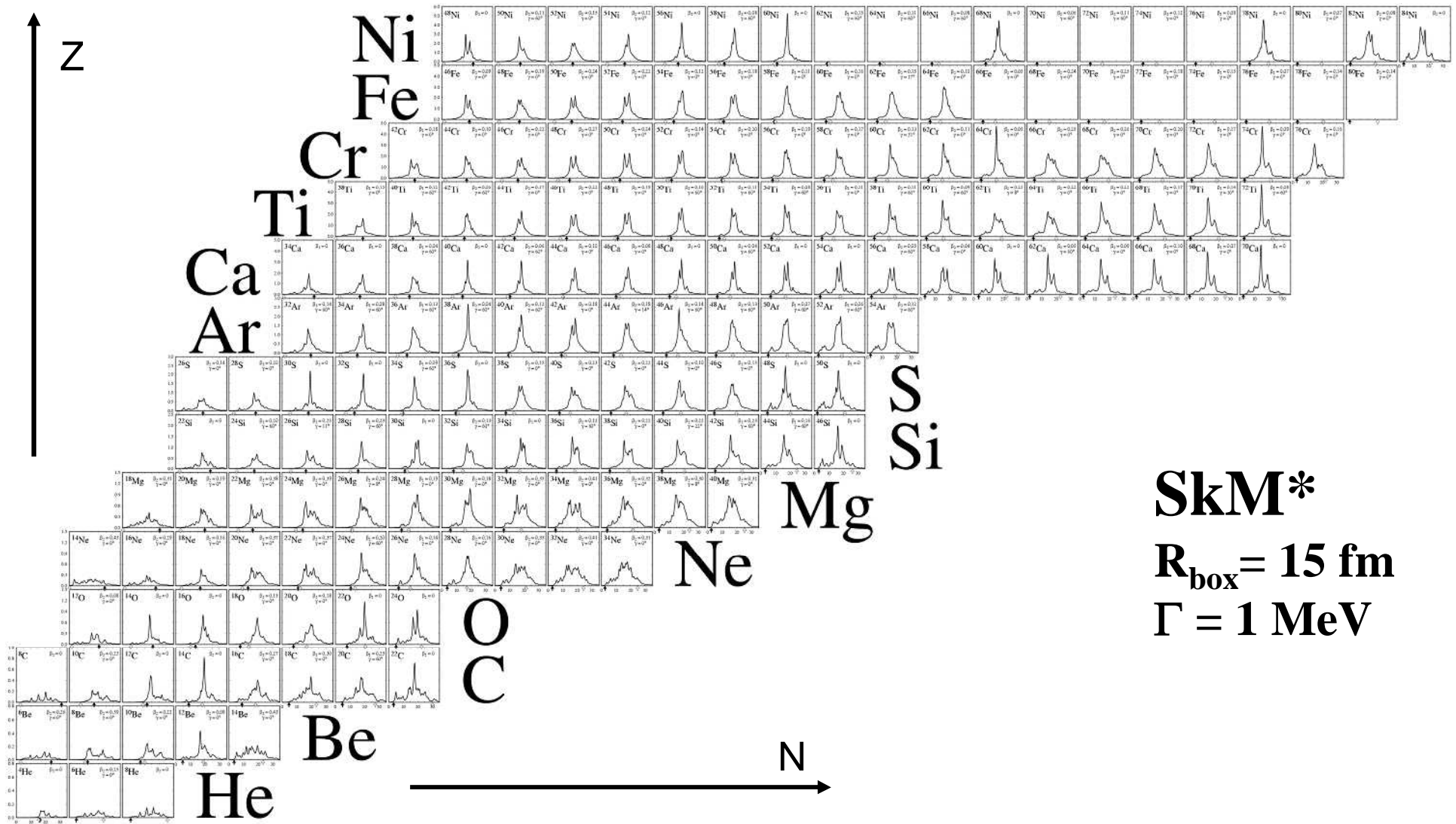
Forward & backward amplitudes

$$X_i(\mathbf{r}; \omega) = \{ X_i(\mathbf{r}_k, \omega_n) \}_{k=1, \dots, Mr}^{n=1, \dots, M\omega}, \quad i = 1, \dots, A$$

$$Y_i(\mathbf{r}; \omega) = \{ Y_i(\mathbf{r}_k, \omega_n) \}_{k=1, \dots, Mr}^{n=1, \dots, M\omega}, \quad i = 1, \dots, A$$

Fully self-consistent calculation of E1 strength distribution

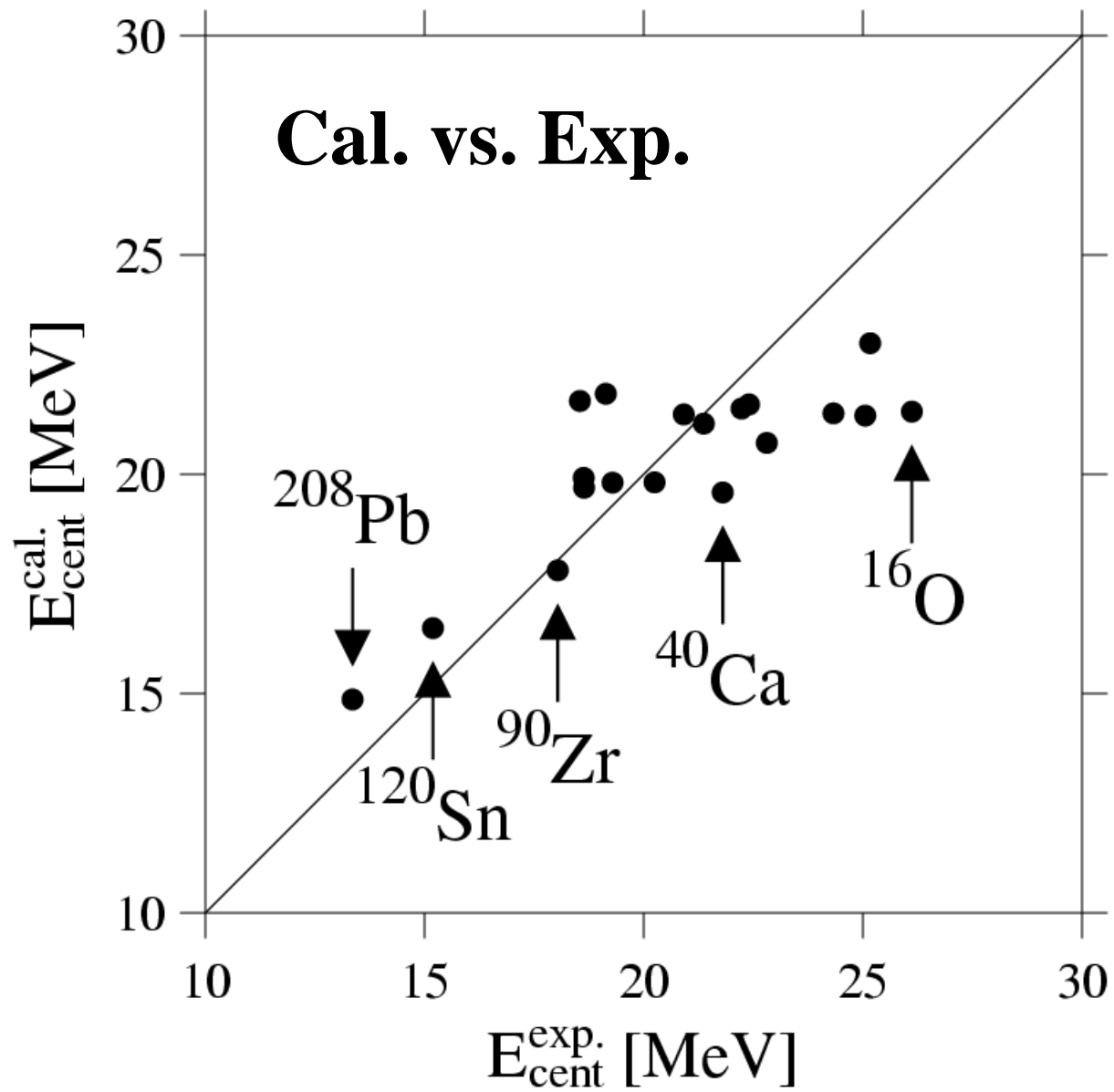
Inakura, Nakatsukasa, Yabana, in preparation



SkM*

$R_{\text{box}} = 15 \text{ fm}$

$\Gamma = 1 \text{ MeV}$



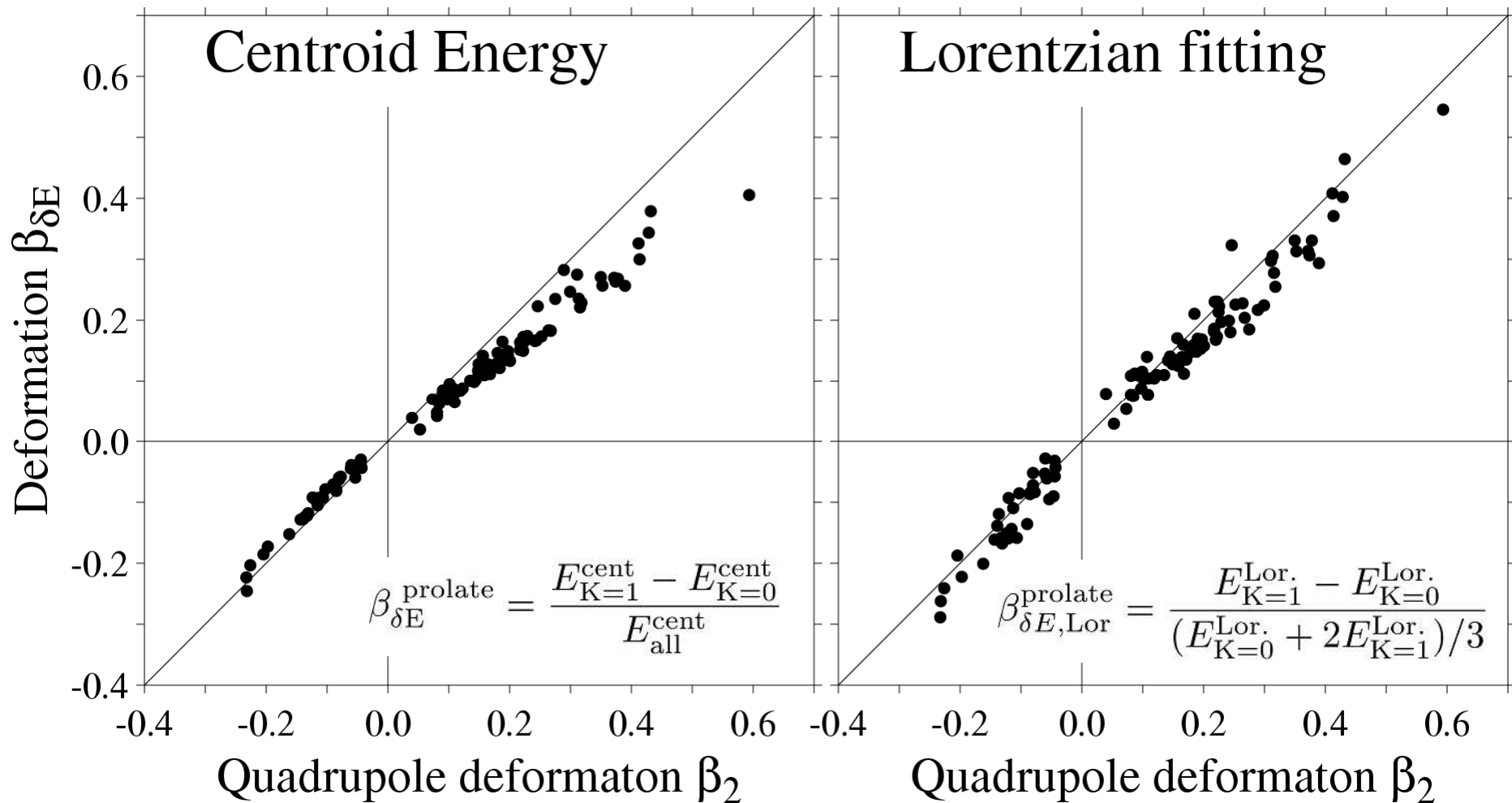
Peak splitting by deformation

3D H.O. model

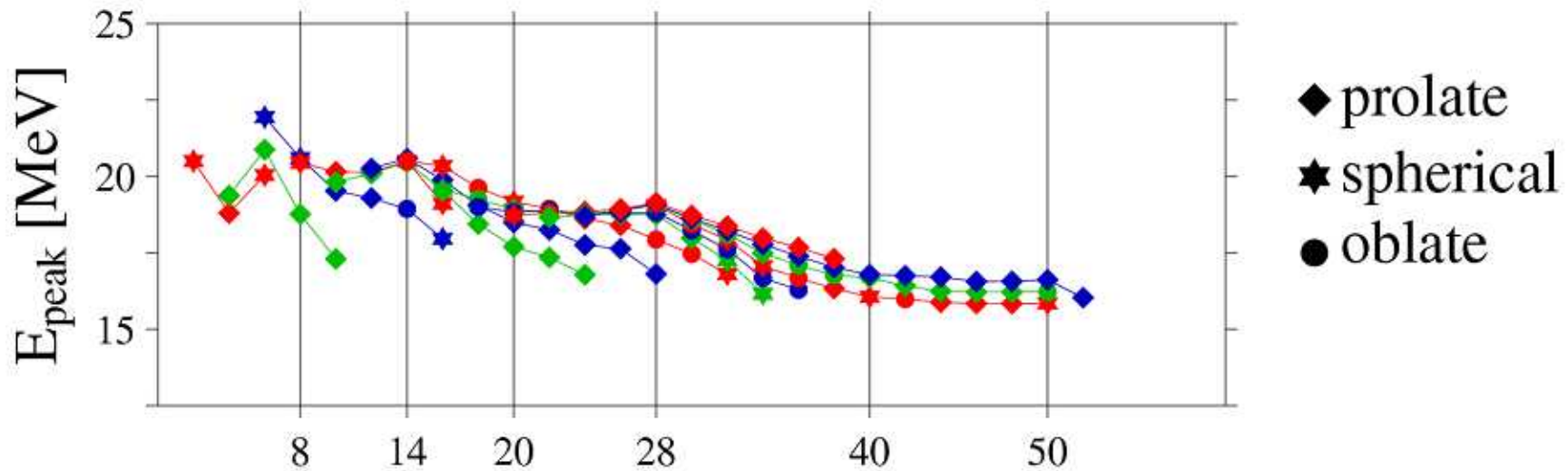
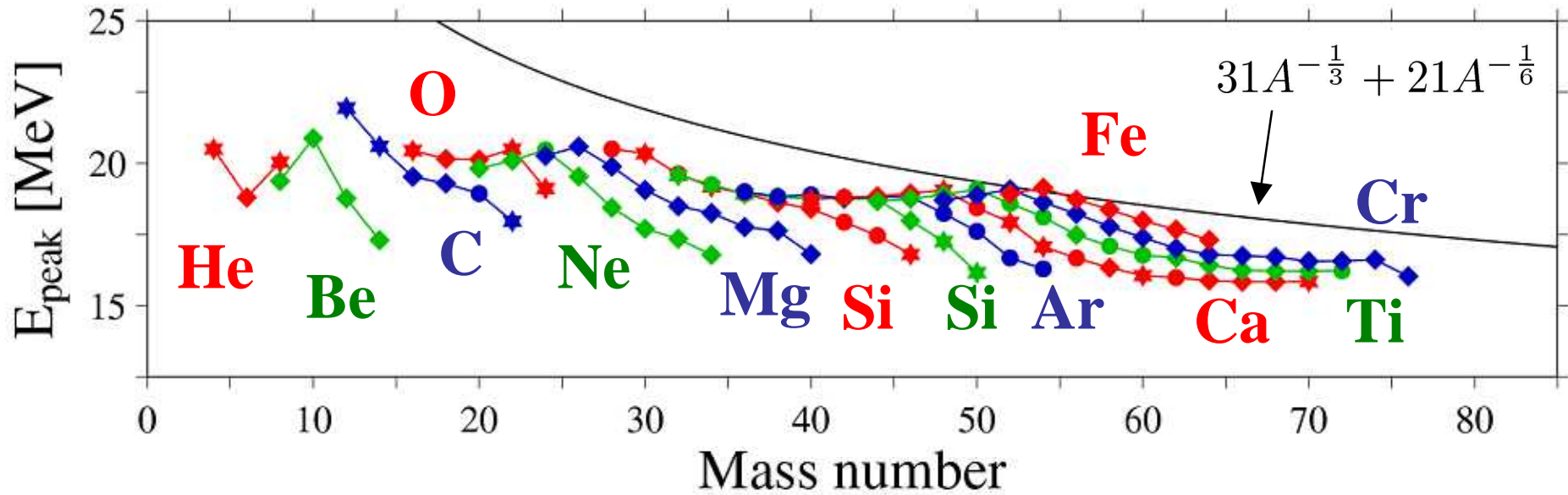
$$\beta_{\delta E} \sim \beta_2$$

Bohr-Mottelson, text book.

$$\beta_{2m} = \frac{4\pi}{3} \frac{\langle r^2 Y_{2m} \rangle}{\frac{5}{3} \langle r^2 \rangle}$$



Centroid energy of IVGDR



FAM for QRPA

HFB equation for quasi-particles

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}$$

QRPA equations for normal modes

$$(E_\mu + E_\nu)X_{\mu\nu} + \delta H_{\mu\nu} = \omega X_{\mu\nu}$$

$$(E_\mu + E_\nu)Y_{\mu\nu} + \delta \tilde{H}_{\mu\nu}^* = -\omega Y_{\mu\nu}$$

$$\begin{pmatrix} * & \delta H \\ \delta \tilde{H} & * \end{pmatrix} = W^+ \begin{pmatrix} \delta h & \delta \Delta \\ -\delta \tilde{\Delta}^+ & -\delta h^T \end{pmatrix} W$$

FAM for QRPA

Residual fields can be calculated by the following finite differences:

$$\delta h = \frac{1}{\eta} (h[v^*, v'] - h_0)$$

$$\delta \Delta = \frac{1}{\eta} (\Delta[v^*, u'] - \Delta_0)$$

where

$$v^* \equiv V^* + \eta UX, \quad v' \equiv V + \eta U^* Y$$

$$u^* \equiv U^* + \eta VX, \quad u' \equiv U + \eta V^* Y$$

Canonical-basis TDHFB

The time-dependent HFB calculation is very expensive.

A “cheaper” way to include the pairing in the time-dependent framework?

For instance, time-dependent equation in the canonical form?

$$|\Psi(t)\rangle = \prod_{i>0} \left(u_i(t) + v_i(t) c_i^+(t) c_{\bar{i}}^+(t) \right) |0\rangle$$

$$\left\{ c_i^+(t), c_{\bar{i}}^+(t), u_i(t), v_i(t) \right\} \quad i = 1, \dots, M/2$$

However, TDVP leads to an inconsistent set of equations, even if we restrict the case with the monopole pairing.

CB-TDHFB with “monopole” pairing

Blocki, Floard, NPA273 (1976) 45.

If the pairing functional has the following form

$$E_{\text{pair}}[u, v] = -G \left| \sum_{i>0} u_i(t) v_i(t) \right|$$

and the Lagrangian has an additional term

$$L_{\text{add}} = - \sum_k \lambda_k(t) \langle k(t) | k(t) \rangle, \quad |k(t)\rangle \equiv c_k^+(t) |0\rangle$$
$$\lambda_k(t) = \rho_k(t) \langle k(t) | h(t) | k(t) \rangle = \rho_k(t) \varepsilon_k(t)$$
$$\rho_k(t) \equiv |v_k(t)|^2$$

then, we may reach something “consistent”.

Properties of CB-TDHFB

$$i \frac{\partial}{\partial t} |k(t)\rangle = (h(t) - \varepsilon_k(t)) |k(t)\rangle$$

$$i \frac{\partial}{\partial t} \rho_k(t) = \Delta^*(t) K_k(t) - \text{c.c.}$$

$$i \frac{\partial}{\partial t} K_k(t) = (\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)) K_k(t) + \Delta(t) (2\rho_k(t) - 1)$$

$$\rho_k(t) \equiv |v_k(t)|^2, \quad K_k(t) \equiv u_k(t)v_k(t)$$

- Conserve the particle number and the total energy
- Conserve the orthonormality of orbitals
- Normal-phase limit is identical to TDHF
- Static limit coincides with the HF+BCS with the monopole pairing

$$\frac{d}{dt} \langle N \rangle = \frac{d}{dt} E_{\text{tot}} = 0$$

$$\frac{d}{dt} \langle k(t) | k'(t) \rangle = 0$$

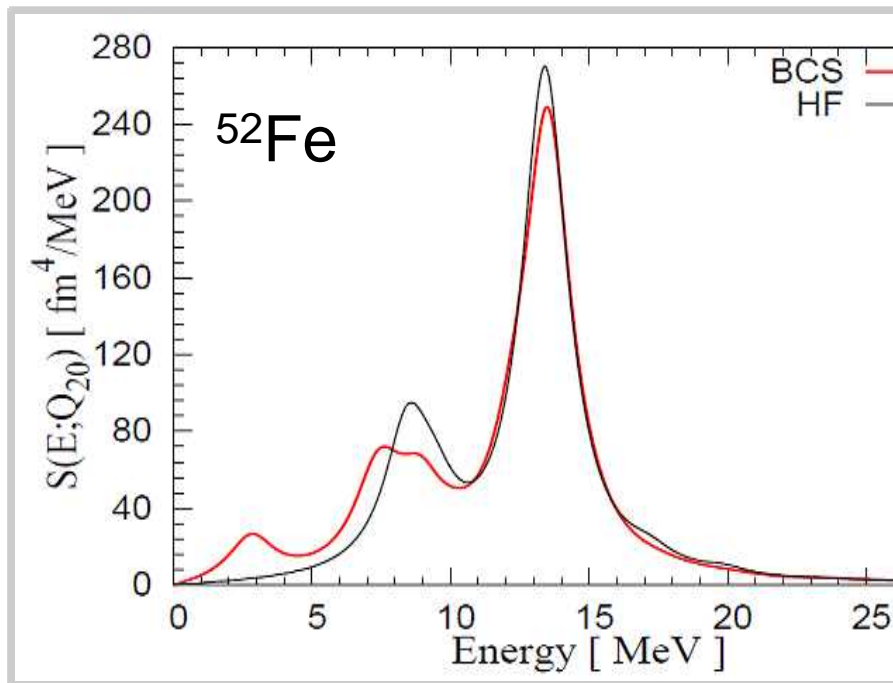
In the small-amplitude limit,

- Nambu-Goldstone modes appear as the zero-energy modes.
- The pairing vibrations in the normal phase coincide with the pp- and hh-RPA

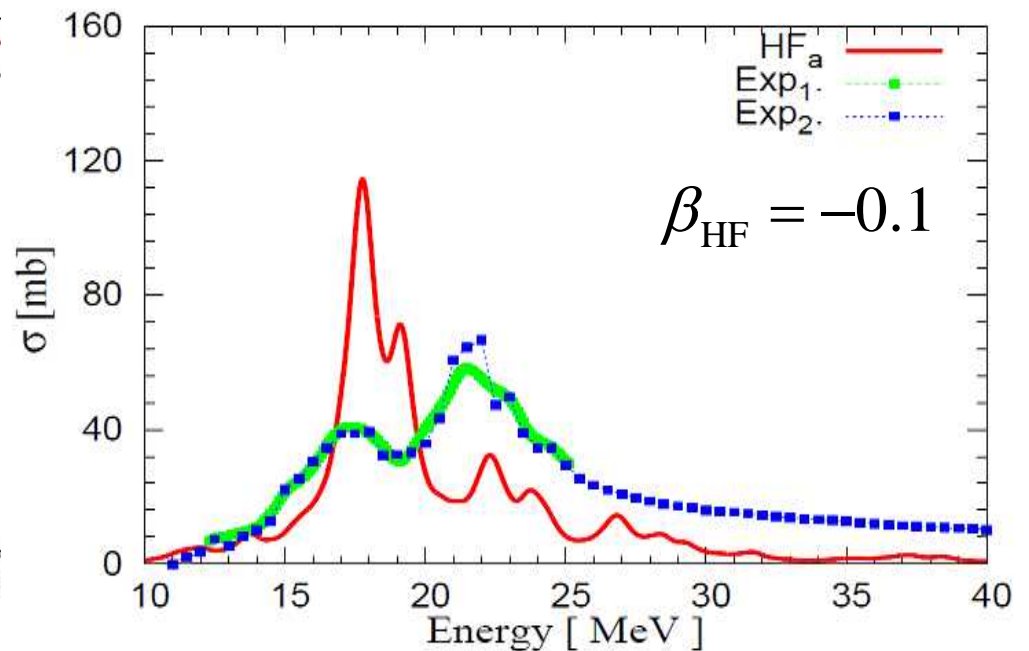
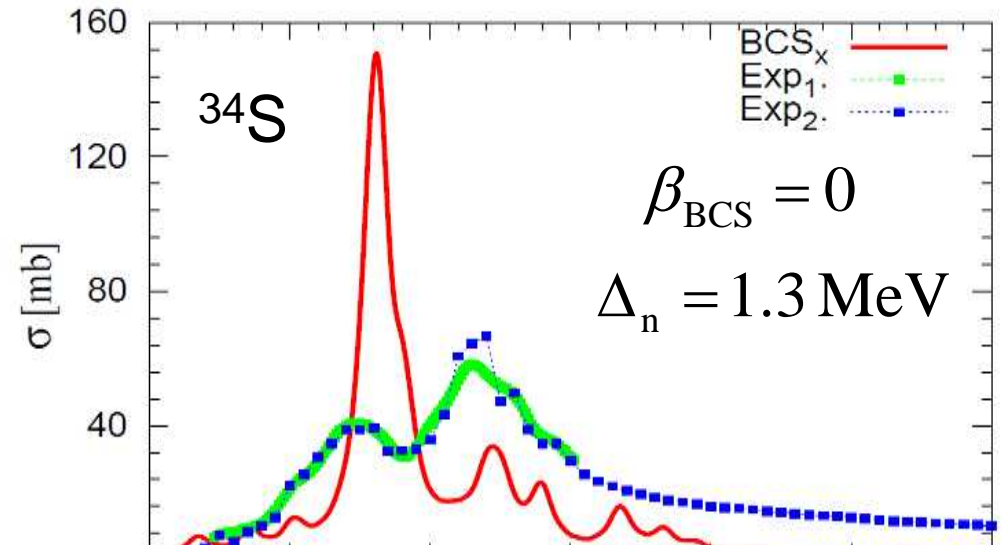
Numerical results

IS quadrupole (K=0) (BKN)

$$\beta_{\text{HF(BCS)}} = 0.49(0.45)$$



IV dipole (SkM*)



Summary

- **Skyrme-TDDFT Calculations with the finite amplitude method (FAM)**

Systematic calculations of nuclear response

-- Collaborators: T. Inakura, K. Yabana (Univ. Tsukuba)

Extension to QRPA-FAM

-- Collaborators: P. Avogadro (RIKEN)

- **Canonical-Basis TDHFB**

Possible formulation with specific choice of pairing functional and phase of single-particle states

-- Collaborators: S. Ebata, K. Yabana (Univ. Tsukuba)

Short-term plan

- **FAM**

 - IS and spin response

 - QRPA codes for Skyrme, Gogny, RMF?

- **CB-TDHFB**

 - Systematic calculation for IV dipole modes

 - Parallelization