Multipole modes within the finite amplitude method and application to the nuclear photo absorption cross section

SSNET 2016 workshop

Markus Kortelainen
University of Jyväskylä

UNIVERSITY OF JYVÄSKYLÄ

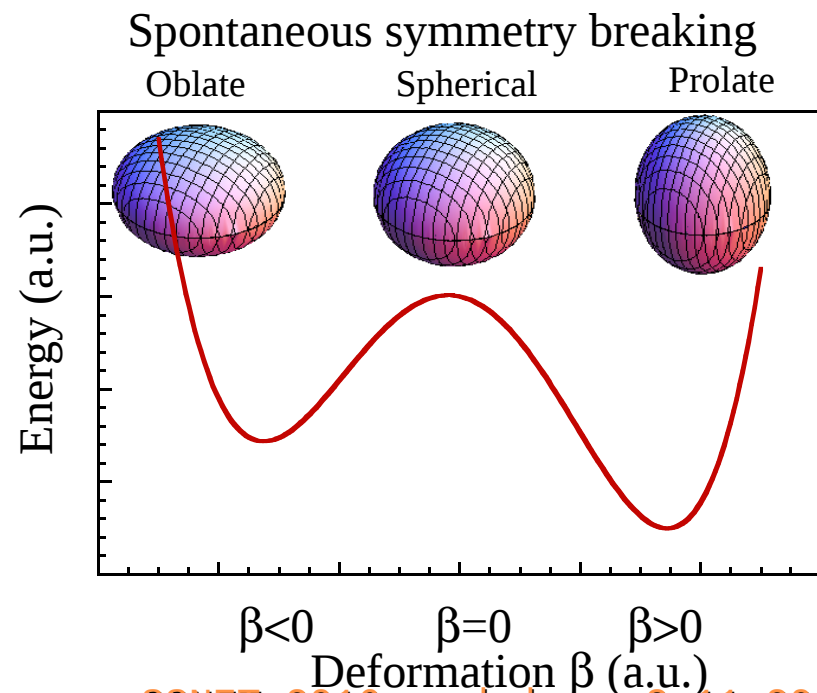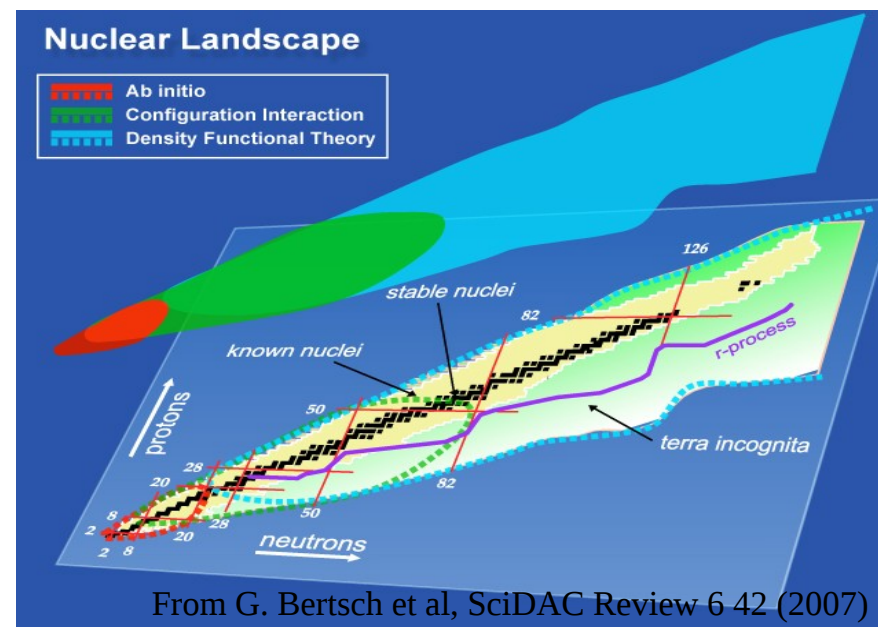HELSINKI INSTITUTE OF PHYSICS

Nuclear DFT

- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart

- Within the superfluid nuclear DFT, one needs to solve the Hartree-Fock-Bogoliubov (HFB) equation:

$$\begin{pmatrix} h-\lambda & -\Delta^{\star} \\ \Delta & -h^{\star}+\lambda \end{pmatrix}\begin{pmatrix} U_n \\ V_n \end{pmatrix} = E_n \begin{pmatrix} U_n \\ V_n \end{pmatrix}$$

- By solving these we obtain the quasiparticle energies E_n and the matrices U and V which determine the generalized Bogoliubov quasiparticle transformation:

$$\hat{b}_\alpha^\dagger = \sum_\beta \left(U_{\beta\alpha}\,\hat{c}_\beta^\dagger + V_{\beta\alpha}\,\hat{c}_\beta \right)$$

- Introduction correlations via spontaneous symmetry breaking

Nuclear Landscape

- Ab initio
- Configuration Interaction
- Density Functional Theory

stable nuclei

known nuclei

r-process

protons

neutrons

terra incognita

From G. Bertsch et al, SciDAC Review 6 42 (2007)

Spontaneous symmetry breaking

Oblate   Spherical   Prolate

Energy (a.u.)

β<0   β=0   β>0

Deformation β (a.u.)

Linear response

- To access the dynamical properties of the superfluid nuclei, in the framework of nuclear DFT, the linear response (that is, the QRPA) is one of the most often employed method

- Essentially, the QRPA corresponds to a small amplitude oscillations around the HFB ground state
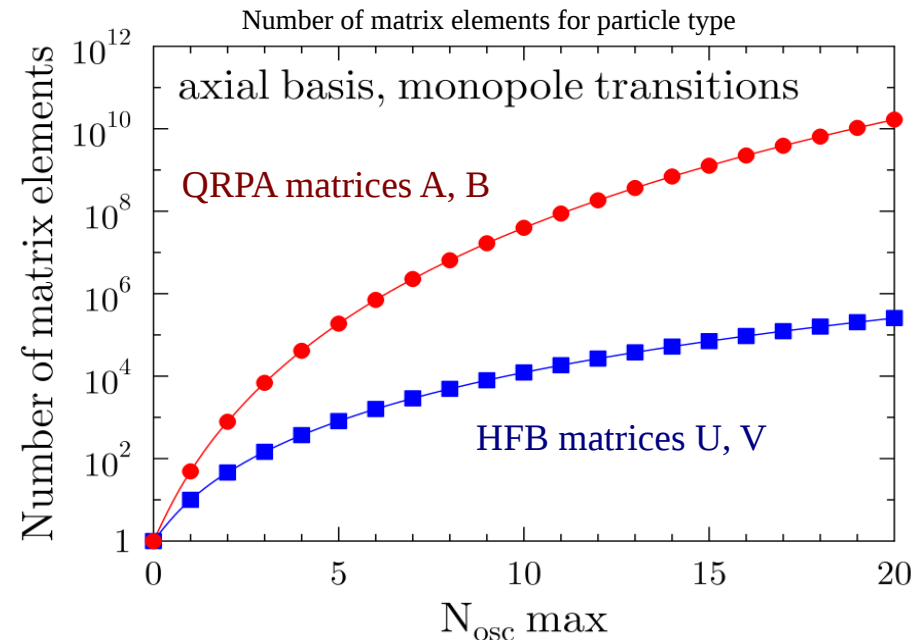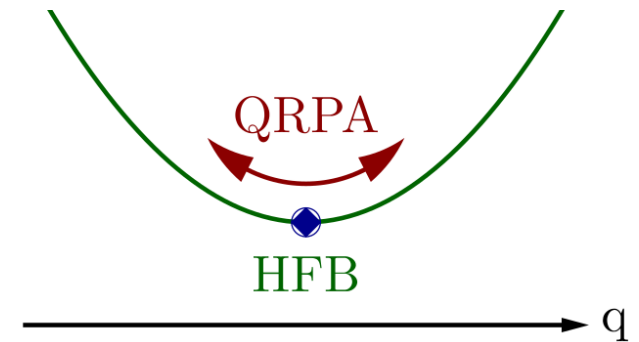
- By diagonalizing the QRPA matrix,

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

one can solve the eigenmodes of the QRPA phonon

- Computational cost of matrix QRPA (MQRPA) becomes huge when spherical symmetry is broken

$\Rightarrow$ Iterative QRPA method required!

QRPA oscillations around the HFB state (schematically)

QRPA

HFB

q

Number of matrix elements for particle type

axial basis, monopole transitions

QRPA matrices A, B

HFB matrices U, V

Number of matrix elements

N_{osc} max

Finite amplitude method QRPA

FAM: T. Nakatsukasa, et. al., PRC 76, 024318 (2007)

1) Perform stationary HFB calculation

2) Introduce time-dependent q.p. operator as

$$\alpha_\mu(t) = (\alpha_\mu + \delta\alpha_\mu(t))e^{iE_\mu t}$$
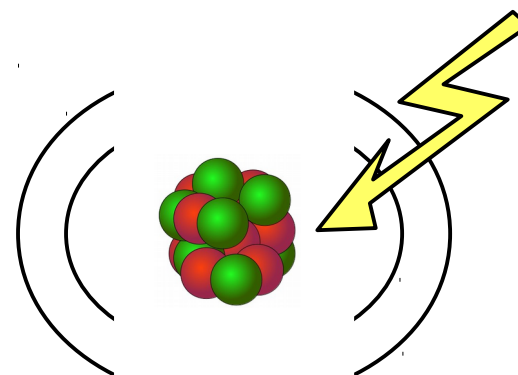
3) Time-dependent HFB equation now reads

$$i\frac{d\,\delta\alpha_\mu(t)}{dt} = [H(t), \alpha_\mu(t)]$$

4) Define oscillating part as

$$\delta\alpha_\mu(t) = \eta\sum_\nu \alpha_\nu^+(X_{\nu\mu}e^{-i\omega t} + Y_{\nu\mu}^* e^{+i\omega t})$$

Here η is small, and hence the amplitude of oscillation is also small
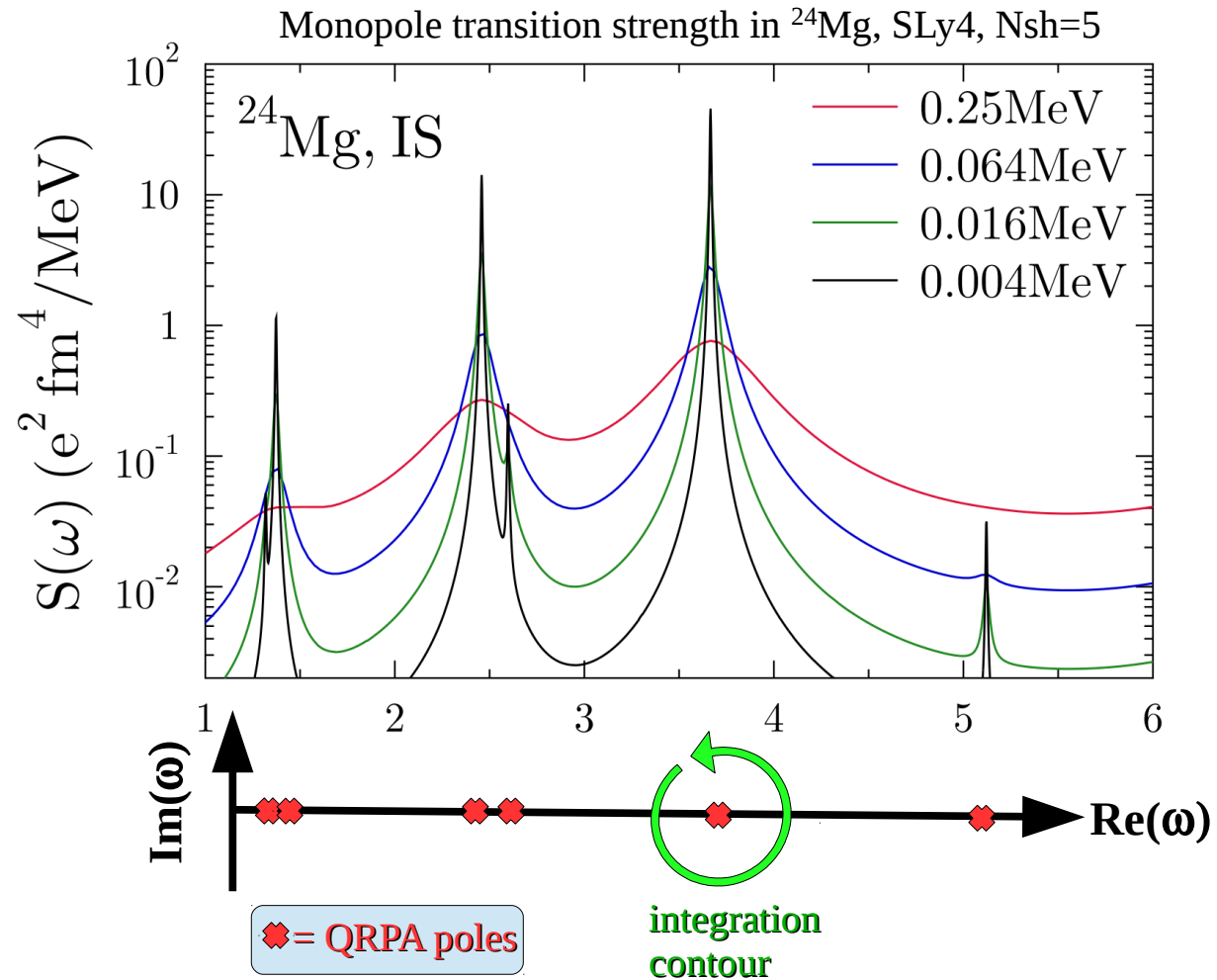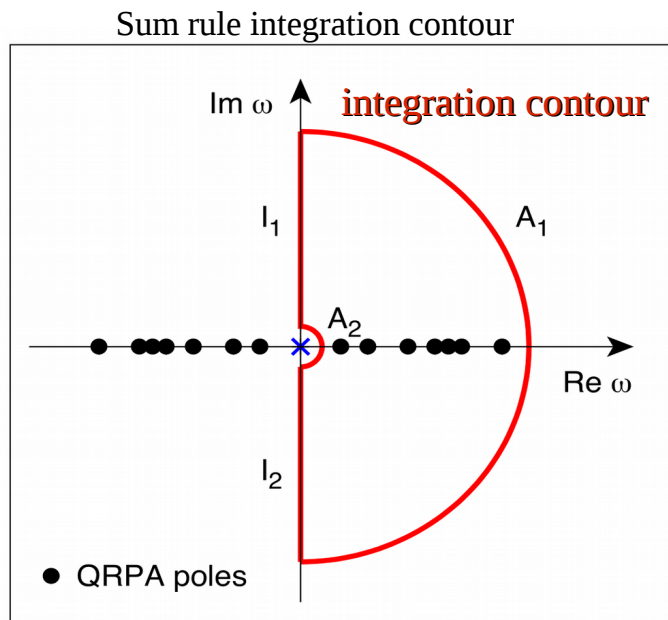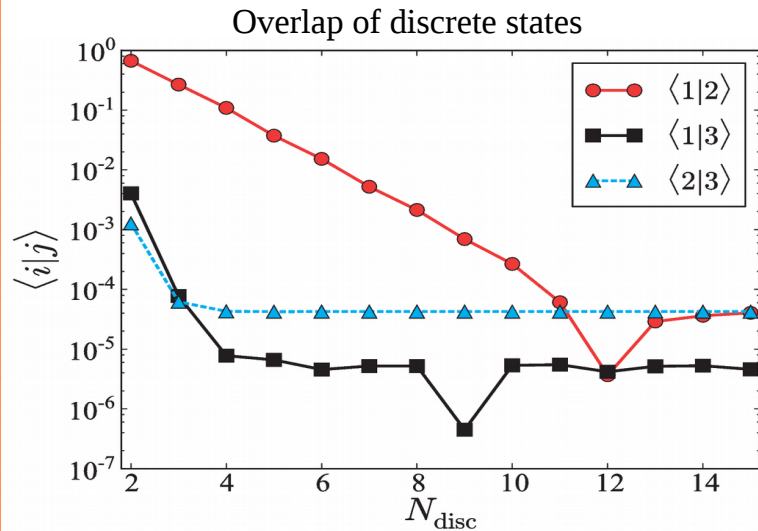
5) Polarize system with an external field F

6) FAM equations then reads

$$(E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{20}(\omega) = F_{\mu\nu}^{20}$$
$$(E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{02}(\omega) = F_{\mu\nu}^{02}$$

7) Introduce a small imaginary width as
$\omega \to \omega + i\gamma$.
Solve FAM eqs. iteratively for each ω.

Discrete low-lying states and sum rules

Overlap of discrete states

Monopole transition strength in ^{24}Mg, SLy4, Nsh=5

Sum rule integration contour

- FAM can be used to access discrete excited states, or to calculate sum rules
- Both methods are based on a contour integral in a complex plane

Discrete states: N. Hinohara, M. K.,
W. Nazarewicz, Phys. Rev. C 87, 064309 (2013)
Sum rules: N. Hinohara, M.K., W. Nazarewicz,
E. Olsen, PRC 91, 044323 (2015)

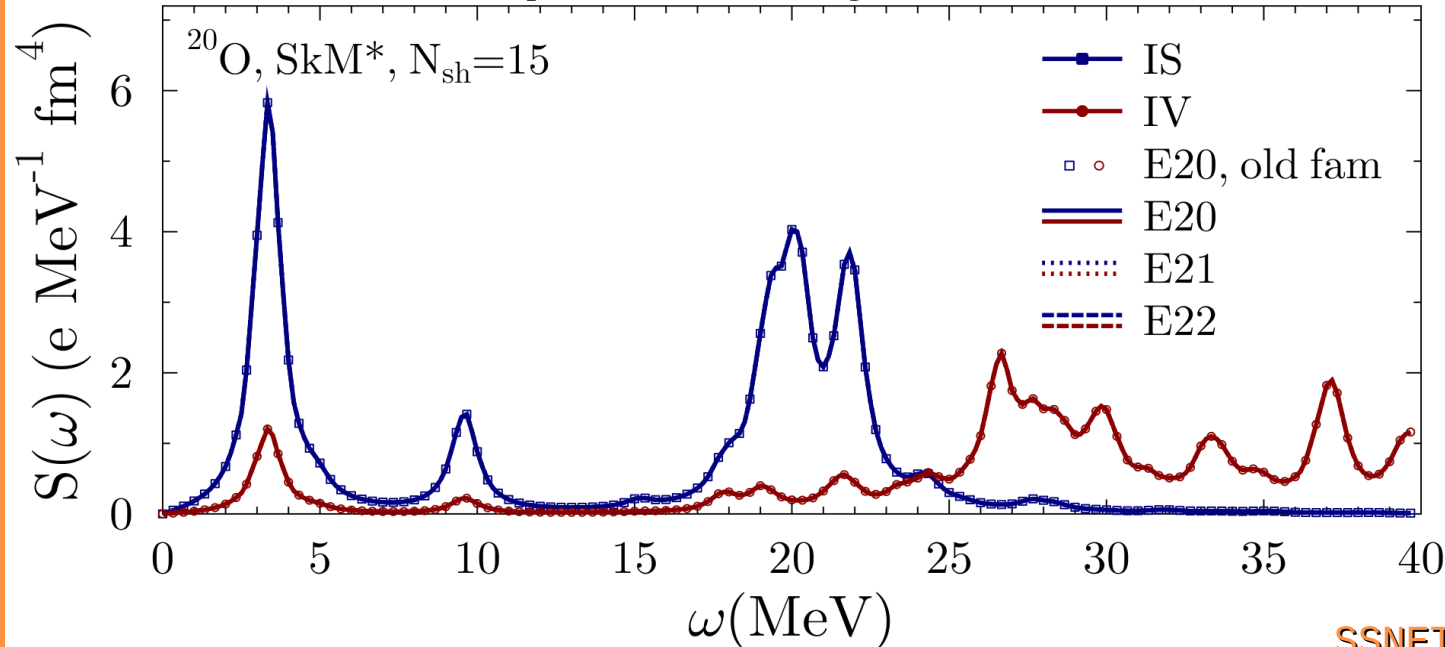# Multipole transitions with axial FAM-QRPA

- For $K \neq 0$ modes, the EM transition operator $r^L Y_{LK}$ has a different block structure than h of HFB when using axial basis
- Need to explicitly linearize density dependent parts (expansion parameter η no longer needed)
- Implemented to HFBTHO
- Wigner-Eckart theorem in spherical nuclei allows to test the implementation
- No truncations in the q.p. space

Matrix structure in axial basis for $K \neq 0$ modes

$$h_{\text{HFB}} = \begin{pmatrix} 1/2 & & & \\ & 3/2 & & \\ & & 5/2 & \\ & & & 7/2 \end{pmatrix}$$
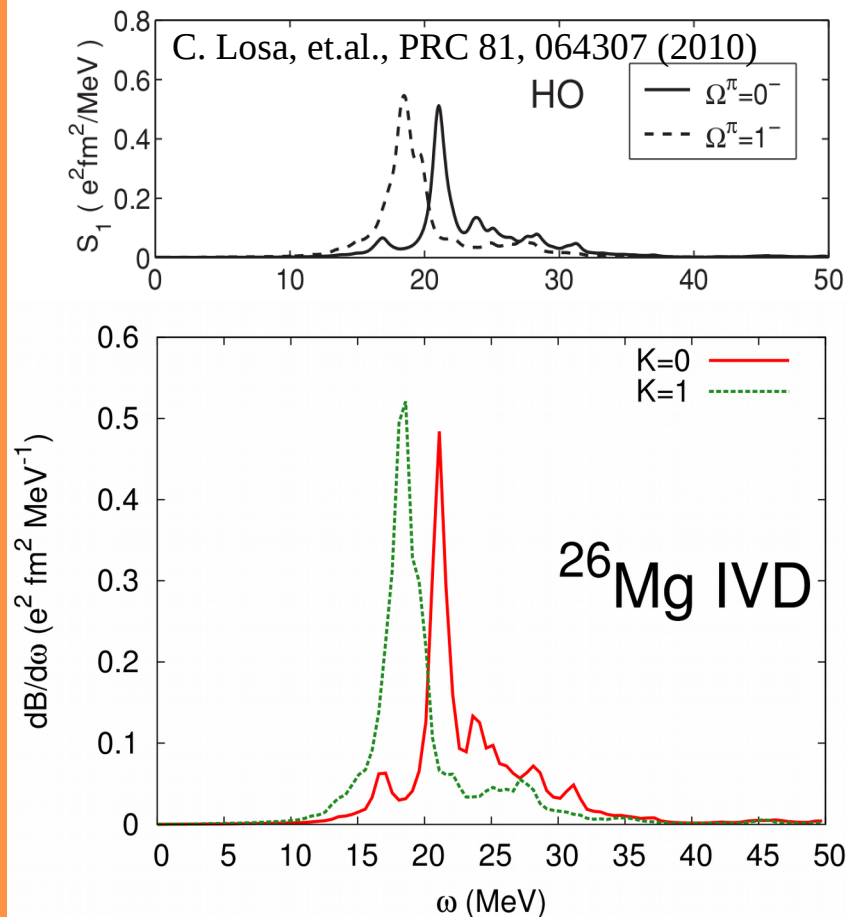
$$F^{20} = \begin{pmatrix} & \blacksquare & & \\ \blacksquare & & \blacksquare & \\ & \blacksquare & & \blacksquare \\ & & \blacksquare & \end{pmatrix}$$

Quadrupole transition strength in ^{20}O

^{20}O, SkM*, $N_{\text{sh}} = 15$

Legend:
- IS
- IV
- E20, old fam
- E20
- E21
- E22

Axes: $S(\omega)$ (e MeV^{-1} fm^4) vs ω(MeV)
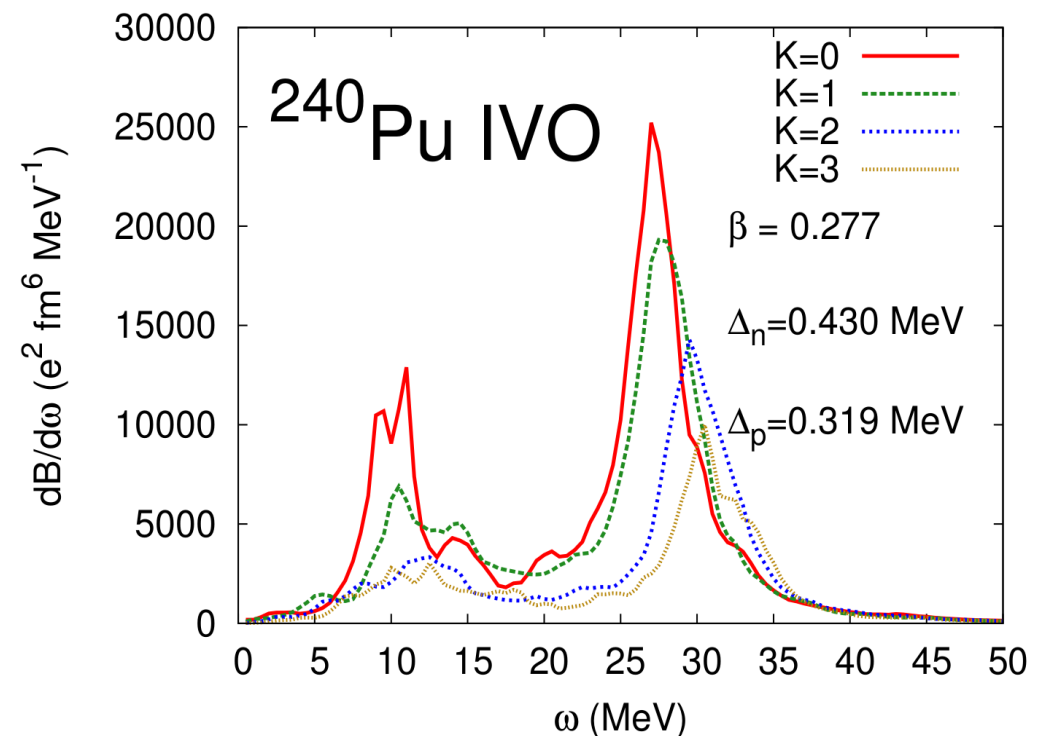
Multipole transitions with axial FAM-QRPA

- Comparison to earlier MQRPA calculation agrees very well (^{26}Mg, N_{sh}=15, SkM*, isovector dipole mode)

C. Losa, et.al., PRC 81, 064307 (2010)

^{26}Mg IVD

- Method feasible for actinide nuclei with N_{sh}=20, without any truncations
- Example of isovector octupole transition strength in ^{240}Pu

^{240}Pu IVO

$\beta = 0.277$

Δ_n=0.430 MeV

Δ_p=0.319 MeV

- Calculation of the strength function is trivially parallelizable

Multipole transitions with axial FAM-QRPA

- The QRPA corresponds to a small amplitude oscillations around the static HFB density ρ_0.
- With isovector octupole operator, the induced transitions densities show a clear octupole-like shapes
- Low-lying iv. octupole modes in ^{240}Pu show collectivity: The induced density covers large portion of the nuclear volume
- The angular dependency of the induced density is

$$\rho(\boldsymbol{r}) = \rho(r,z)\left(e^{+iK\phi} + e^{-iK\phi}\right)/2$$

due to simplex-y symmetry.

Oscillating density ρ_f in ^{240}Pu with isovector octupole operator at $\omega=11$MeV with SLy4 for different K-modes. From M.K, et.al., Phys. Rev. C 92, 051302(R) (2015)

See: M.K, N.Hinohara, W.Nazarewicz, Phys. Rev. C 92, 051302(R) (2015)
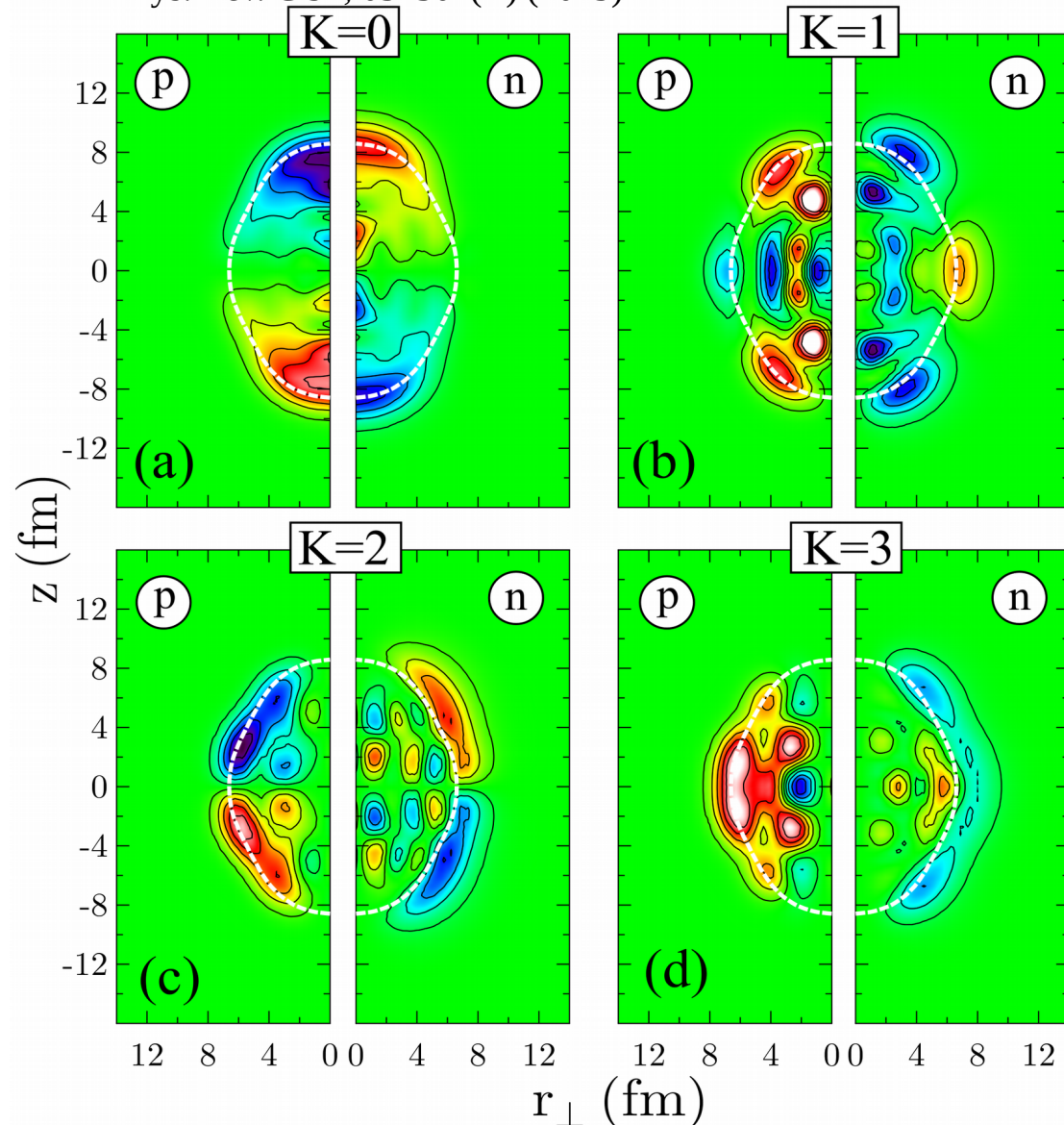
Photo absorption in the heavy rare-earth nuclei

- The nuclear photo-absorption cross-section is connected to the electric isovector dipole transition

$$\sigma_{abs}(\omega) = \frac{4\pi\omega}{\hbar c} \sum_{K=0,\pm 1} \frac{dB(Q_{IVD},\omega)}{d\omega}$$

- The nuclear photo absorption cross section has also impact on the r-process dynamics
- We recently computed photo absorption cross sections in heavy rare-earth nuclei see T. Oishi, M.K., N. Hinohara, PRC 93, 034329 (2016)
- The results show that for heavier rare earths, the experimental cross section can not be reproduced fully, and there is a certain deficiency
- The position of the giant resonance is usually well reproduced

T. Oishi, M.K., N. Hinohara, PRC 93, 034329 (2016)
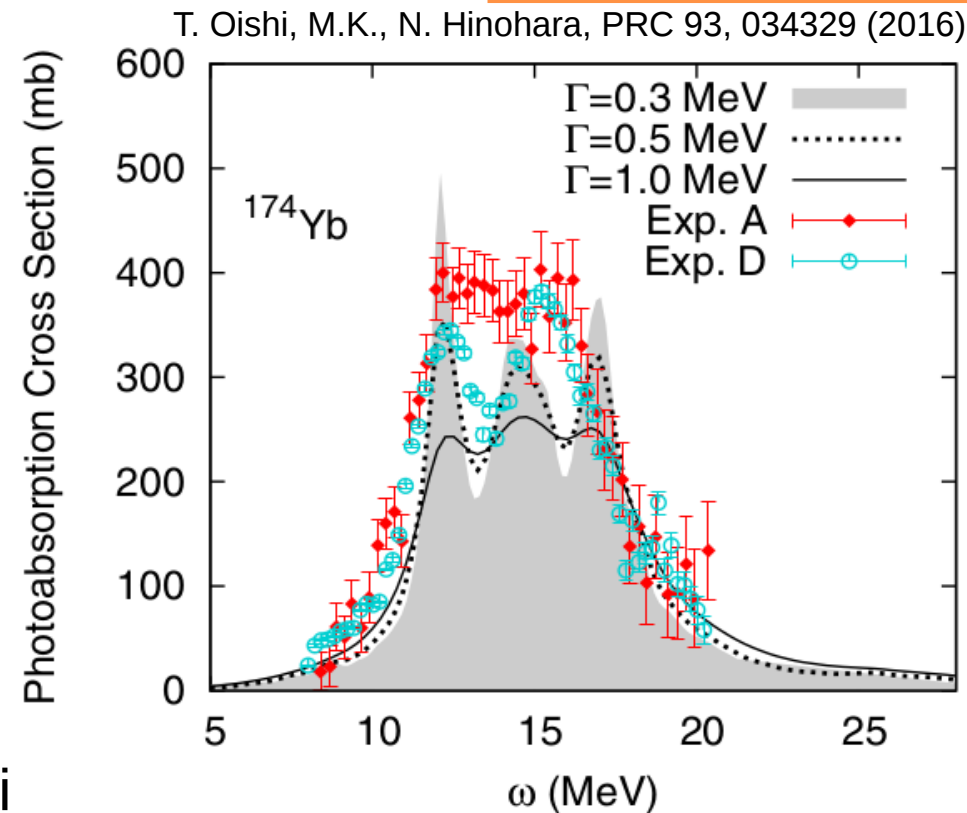
Photo absorption in the heavy rare-earth nuclei

- T. Oishi, M.K., N. Hinohara, PRC 93, 034329 (2016)
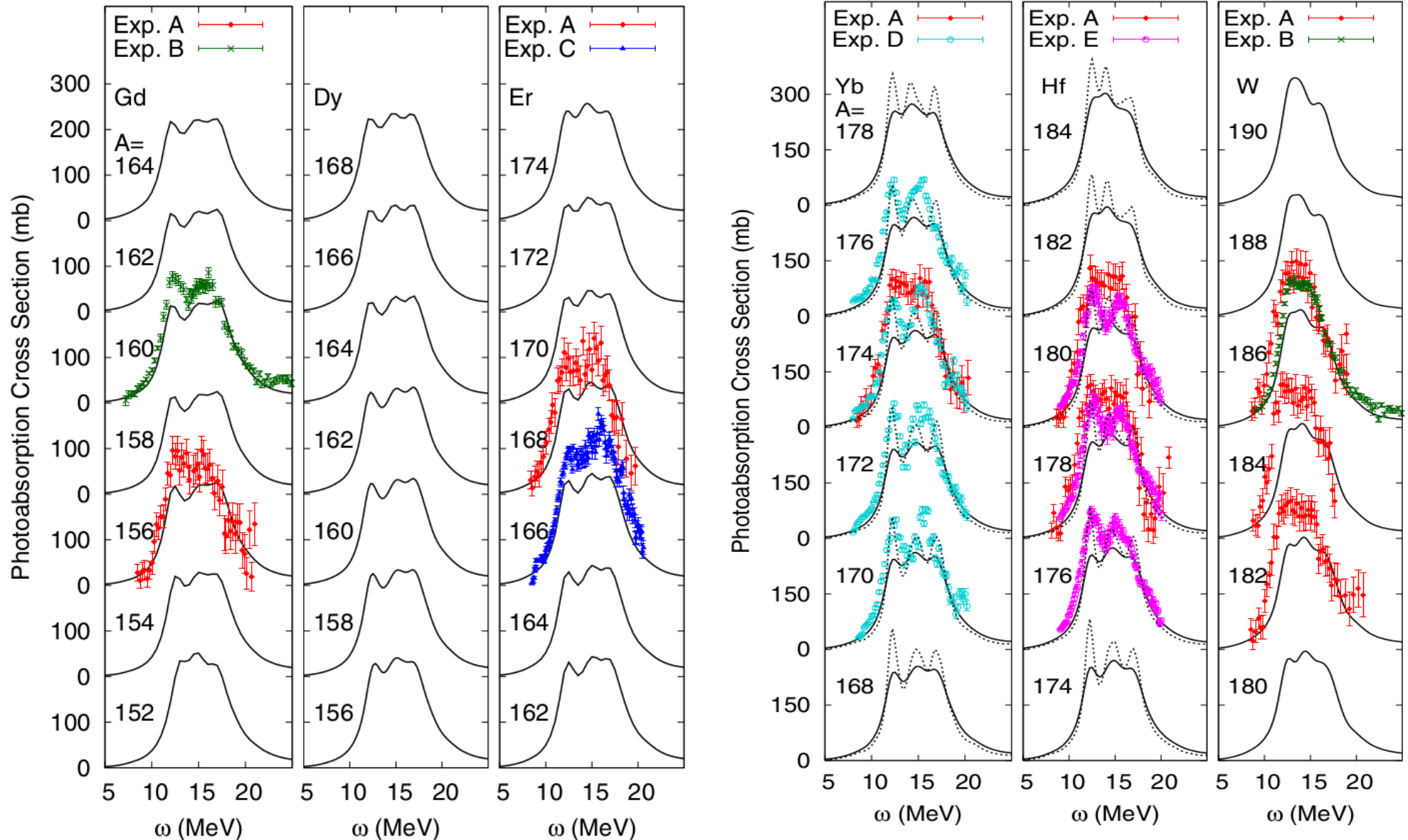
- By systematically varying the Thomas-Reiche-Kuhn (TRK) sum rule enhancement factor, the value of the energy weighted sum rule (EWSR) can be modified
- This, however, does not seem to improve situation when comparing to experimental data. A larger TRK factor just pushes the strength to higher energy, thus increasing the EWSR
- To improve the situation, future EDF parameter optimization schemes should incorporate data on various excitation modes

HFB energy and TRK enhancement factor as a function of deformation

T. Oishi, M.K., N. Hinohara, PRC 93, 034329 (2016)
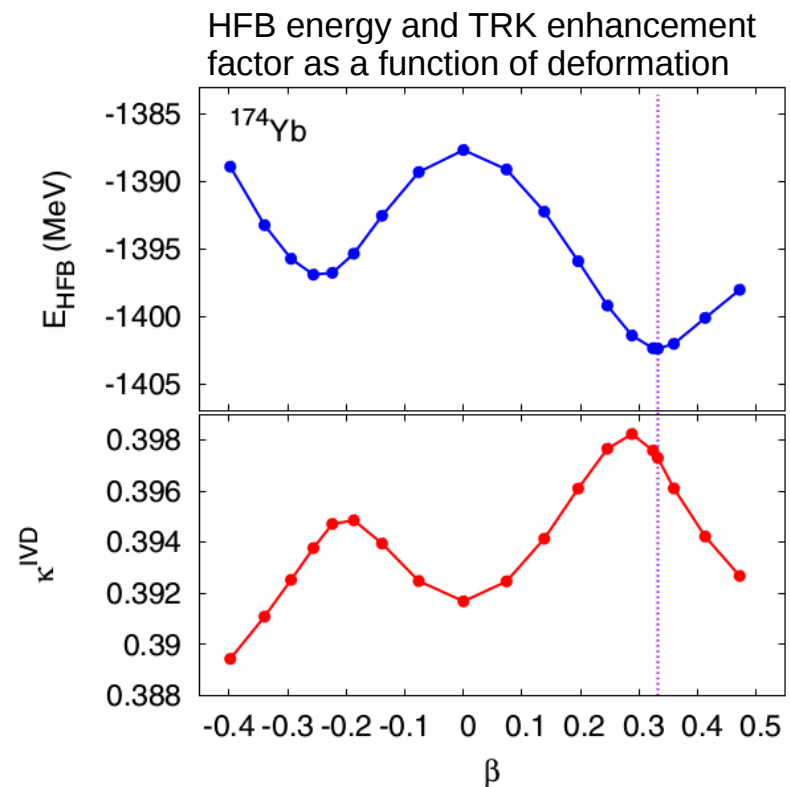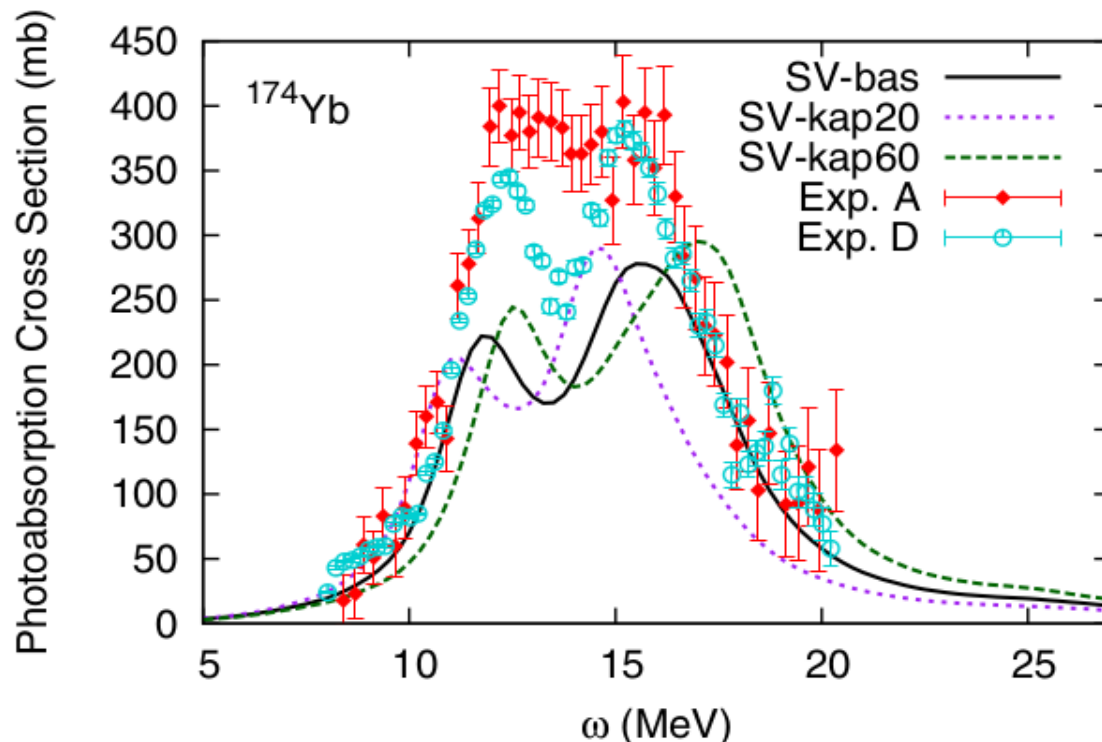
Spurious modes

- If the underlying HFB solution breaks some symmetry, this causes a spurious QRPA mode to appear
- The spurious mode appears at zero energy
- This corresponds to the well-known Nambu-Goldstone mode
- The type of the spurious mode depends on which of the symmetry was broken
- For example, breaking of the rotational symmetry causes a spurious $K^\pi=1^+$ mode to appear. This shows up when calculating isoscalar quadrupole modes
- Work towards removing spurious $K^\pi=1^+$ mode is currently in progress

Mode with mass

Massless Nambu-Goldstone mode
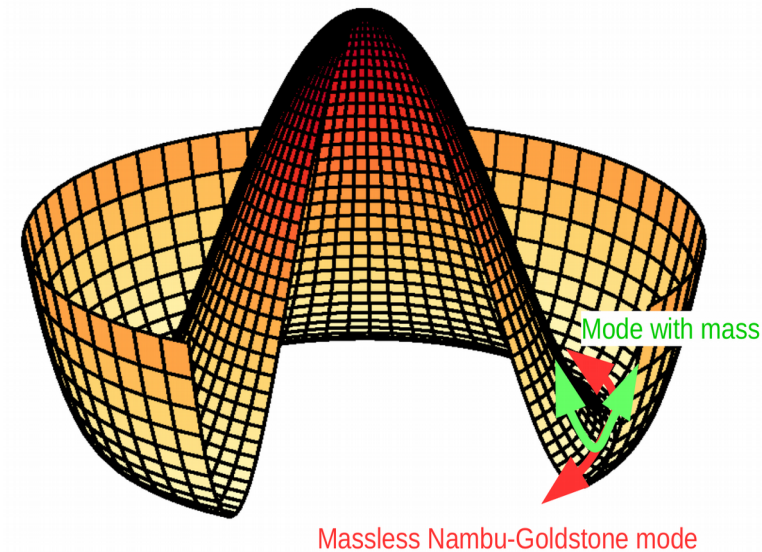
Isoscalar quadrupole transition strength. From M.K, N.Hinohara, W.Nazarewicz, Phys. Rev. C 92, 051302(R) (2015)

^{24}Mg ISQ
K=0
K=1
K=2

$\frac{dB}{d\omega}$ (e^2 fm^4 MeV^{-1})

ω (MeV)
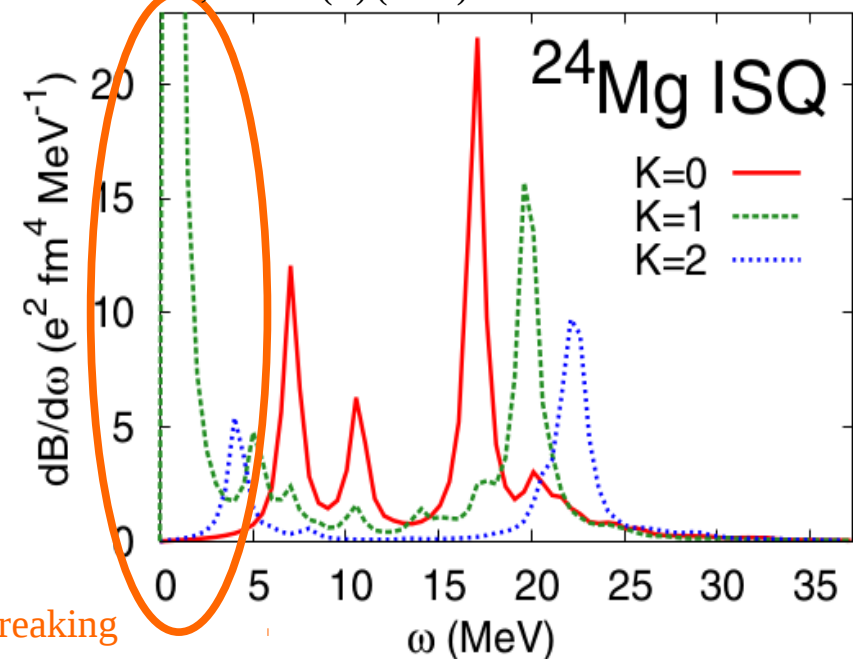
Spurious mode due to breaking of the spherical symmetry

Summary and outlook

- FAM offers an computationally inexpensive way to solve the QRPA problem, by iterative means
- Many new FAM developments have been published recently:
    - Besides transition strength function, FAM can be used to compute discrete states and sum rules
    - New FAM module allows to compute arbitrary multipole mode with an axial code
    - FAM applied to photo absorption calculations in the heavy rare-earth region
- FAM can be trivially parallelized, allowing large scale surveys
- The newly developed FAM module allows systematic studies across significant portion of the nuclear chart (including actinides and superheavy nuclei)

Future plans
- Assessment of the spurious rotational mode
- Implementation of M1 transitions (mostly done)

Backup slides

Induced transition densities
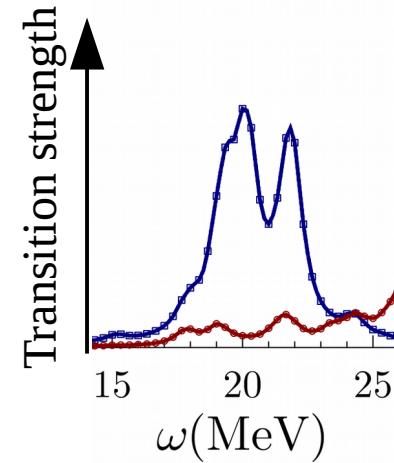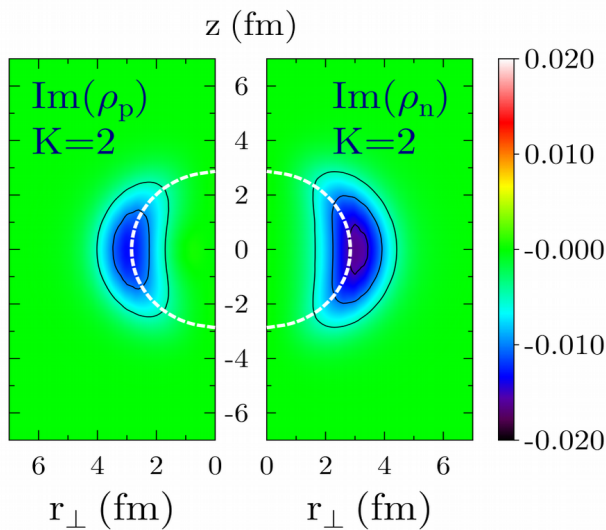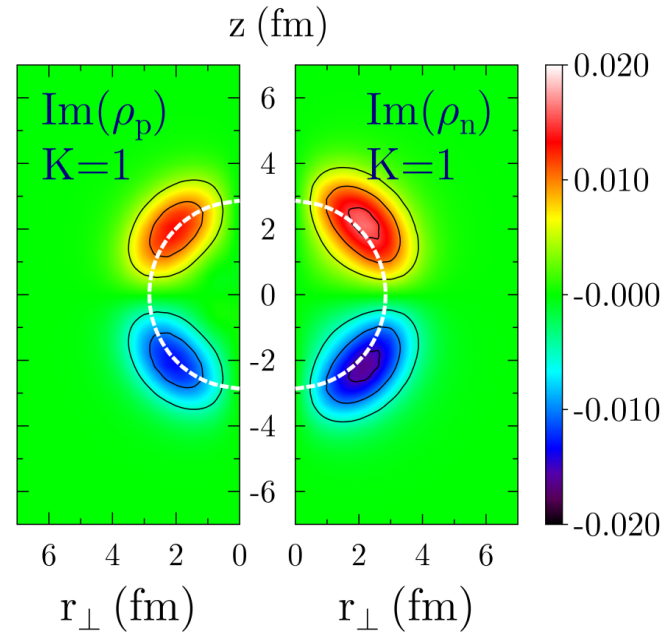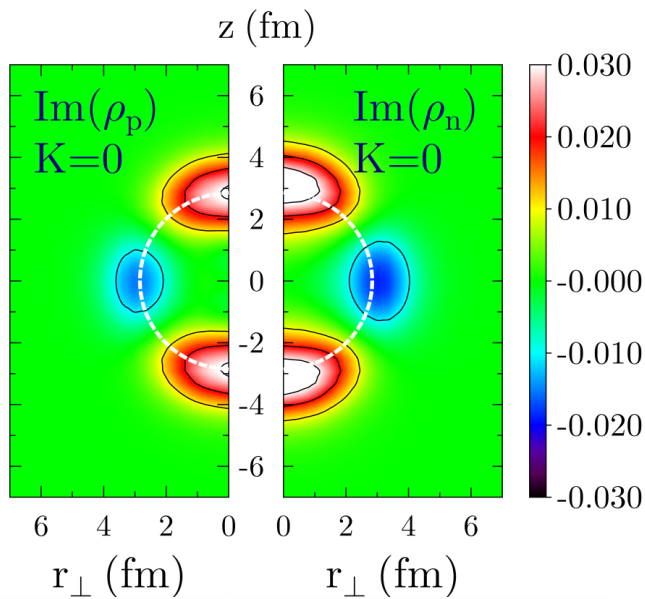
$$\rho(\boldsymbol{r}) = \rho(r,z)\left(e^{+iK\phi} + e^{-iK\phi}\right)/2$$

- The QRPA corresponds to a small amplitude oscillations around the static HFB density ρ_0.
- With FAM equations, we can isolate this oscillating part to induced density ρ_f.
- The shape of this oscillating density depends on the used transition operator, energy ω, and underlying HFB solution
- Figs. show induced proton and neutron transition densities for ^{20}O at energy of 20 MeV for isoscalar quadrupole transition

Deformation and splitting of the giant resonance

- Due to the deformation, the position of the giant resonance is different for different *K*-modes
- This happens for all *L*>0 multipole operators
- Semiclassically this could be explained such that the oscillating frequency is different to each direction. That is, e.g. with dipole operator, the *K*=1 mode corresponds oscillation perpendicular to *z*-axis. With prolate deformation, this leads to higher ω compared to *K*=0 mode case, and conversely, other way around with oblate deformation.
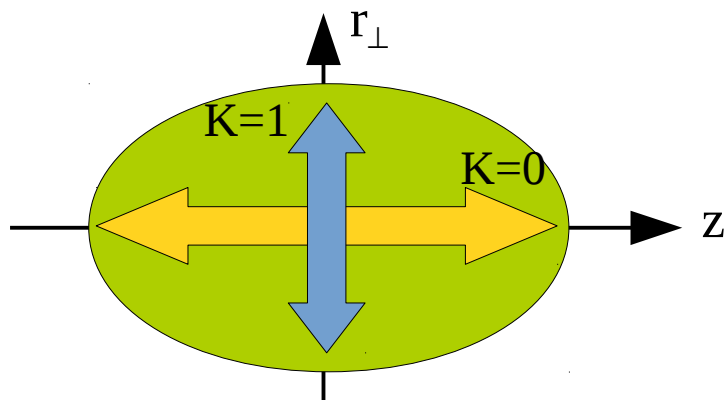
Photoabsorption in Sm isotopes from FAM-QRPA with SkM*. From T. Oishi, et.al, Phys. Rev. C 93, 034329 (2016)
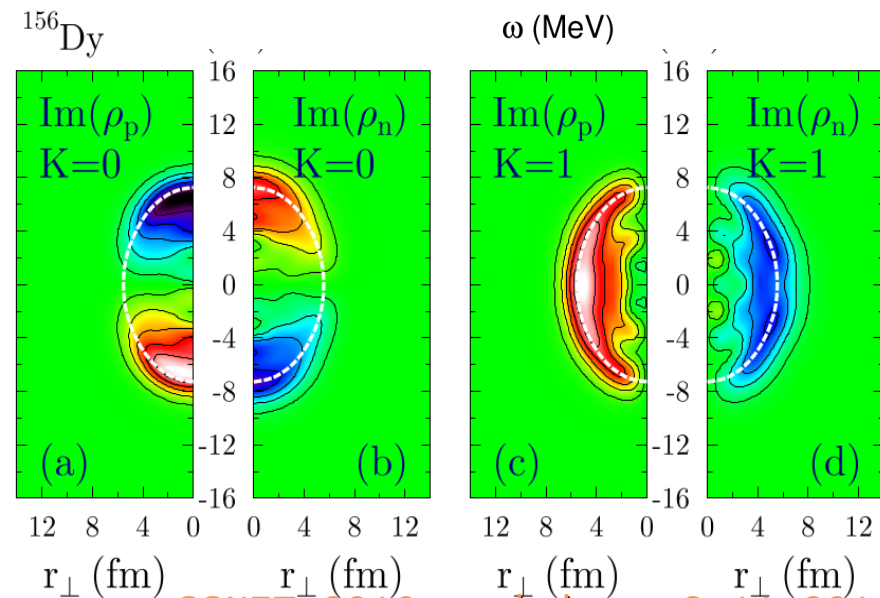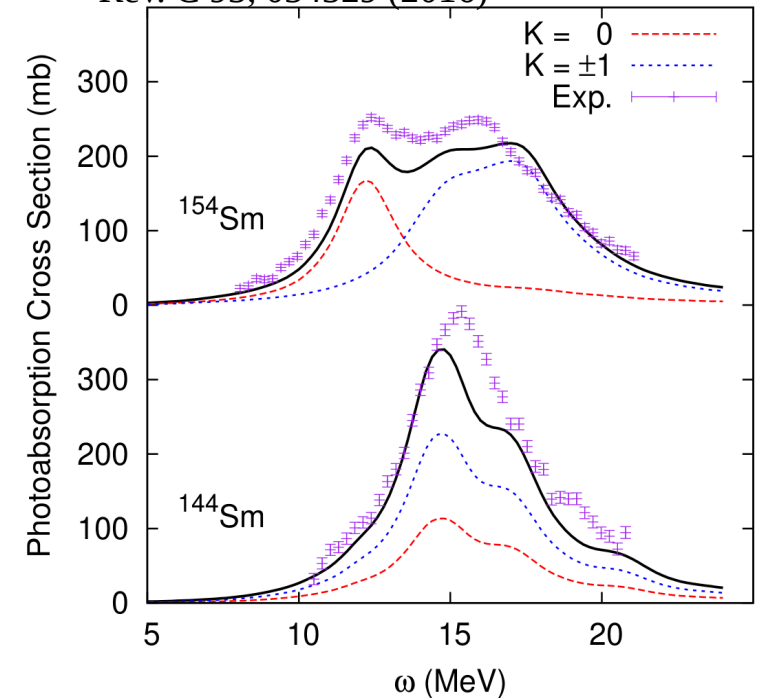
Removal of the spurious modes

- In practice, due to the finite size of the used basis, the spurious mode is usually located slightly above the zero energy
- It is possible to remove this mode within the FAM-QRPA framework. For the spurious center-of-mass mode, see e.g. T. Nakatsukasa, et.al., PRC 76, 024318 (2007) and N. Hinohara, PRC 92, 034321 (2015)
- The idea is to remove spurious contribution from calculated transition density as

FAM-QRPA strength function for the response of the center of mass operator for ^{26}Mg with SLy4. The calculation was done with N_{sh} oscillator shells. From N. Hinohara, Phys. Rev. C 92, 034321 (2015).

$$\delta\rho_{\text{phys}}(\omega) = \delta\rho_{\text{cal}}(\omega) - \lambda_P \delta\rho_P - \lambda_R \delta\rho_R$$

where λ_R and λ_P are determined from canonicity condition $[R,P]=i$
- This technique allows also to access pairing rotational mode, see: N. Hinohara, W. Nazarewicz, Phys Rev. Lett. 116, 152502 (2016)
- Currently we are working with removal of the spurious rotational mode