Recent developments with the finite amplitude method

The future of multireference Density Functional Theory workshop
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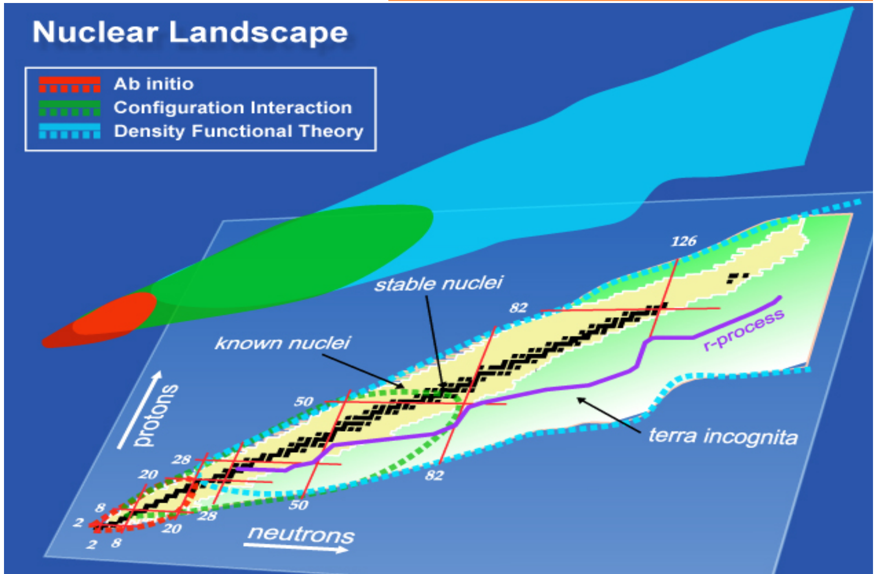
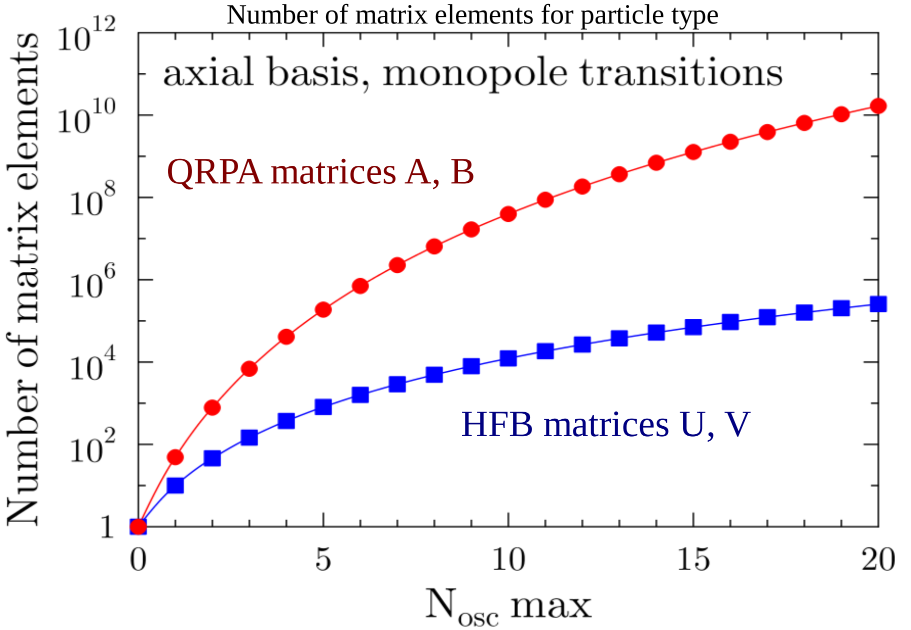
Linear response

- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart
- To access the dynamical properties of the superfluid nuclei, in framework of nuclear DFT, the linear response (that is, QRPA) on one of the most often employed method
- Computational cost of matrix QRPA (MQRPA) becomes huge when spherical symmetry is broken
- To circumvent large numerical cost of MQRPA, finite amplitude method (FAM) solves the QRPA problem as an iterative problem
- Initially FAM could be applied to computation of the transition strength function



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



⇒Iterative QRPA method required!

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

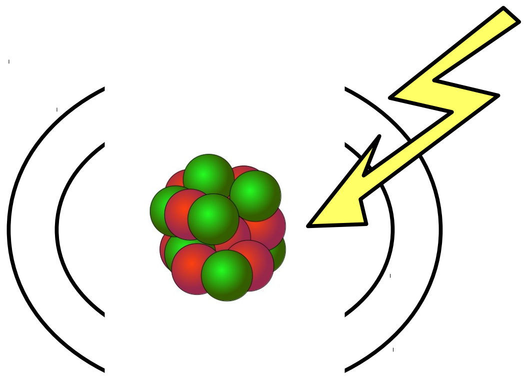
$$i\frac{d\,\delta\alpha_\mu(t)}{dt} = [H(t), \alpha_\mu(t)]$$

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 the amplitude of oscillation is also small

5) Polarize system with an external field F



6) FAM equations then reads

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

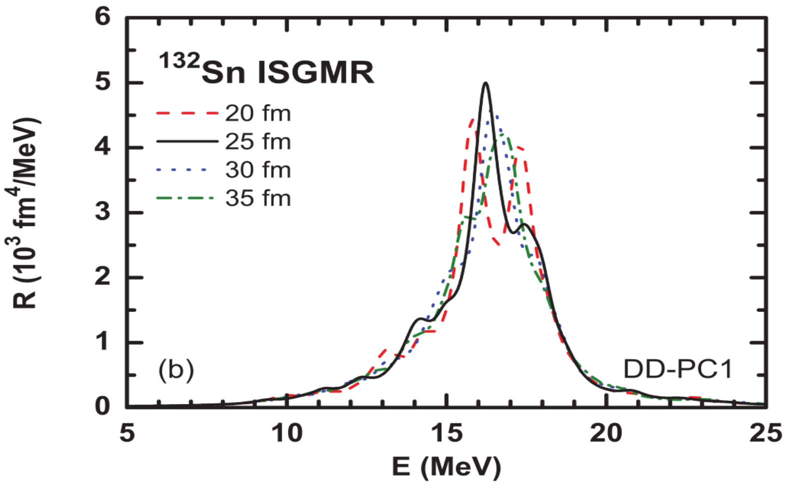
7) Introduce a small imaginary width as

$\omega \rightarrow \omega + i\gamma$.

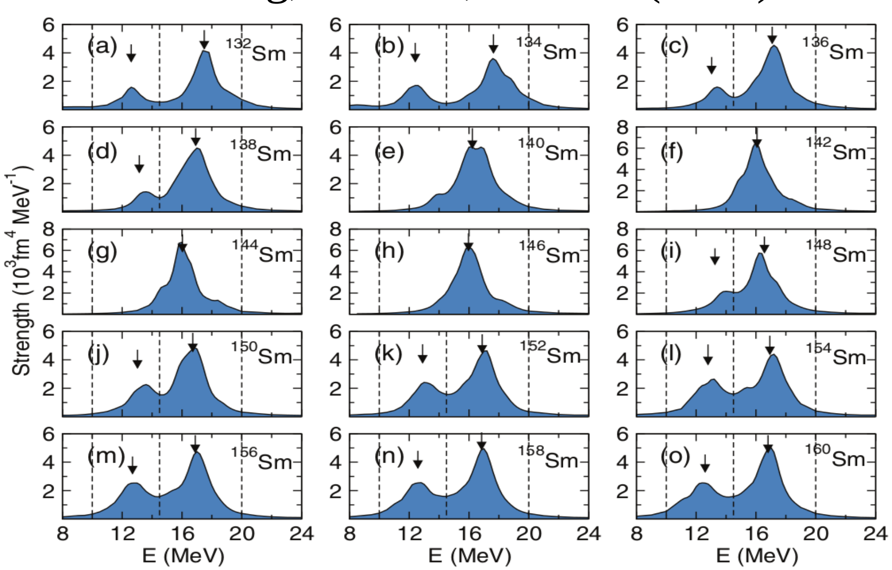
Solve FAM eqs. iteratively for each ω.

Recent FAM developments by other groups

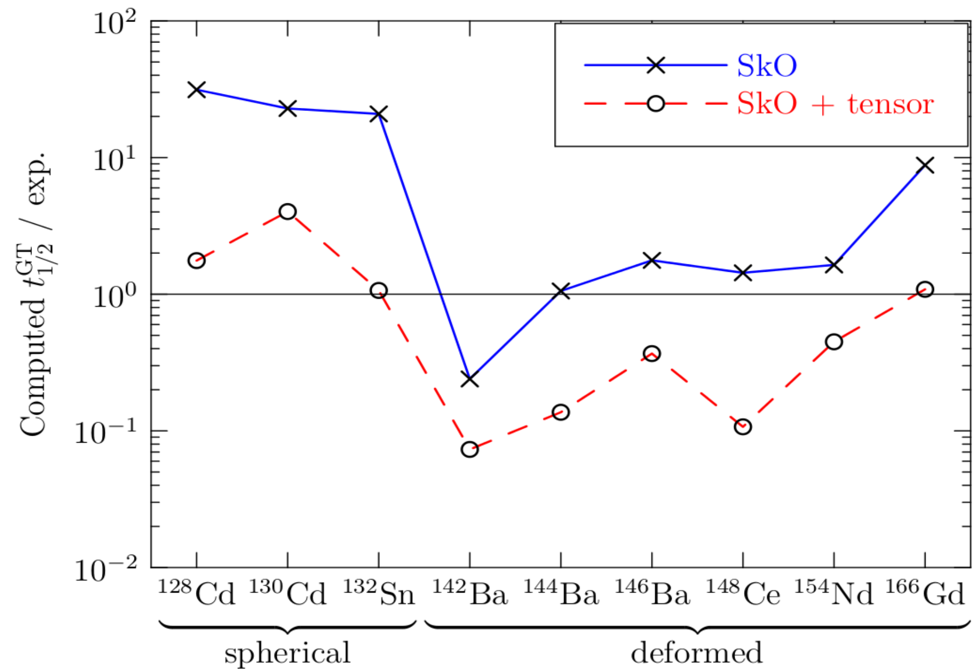
- Feasibility of FAM in the RMF framework: H. Liang, T. Nakatsukasa, Z. Niu, and J. Meng, PRC 87, 054310 (2013)



- FAM in the axial RMF framework: T. Nikšić, N. Kralj, T. Tutiš, D. Vretenar, and P. Ring, PRC 88, 044327 (2013)

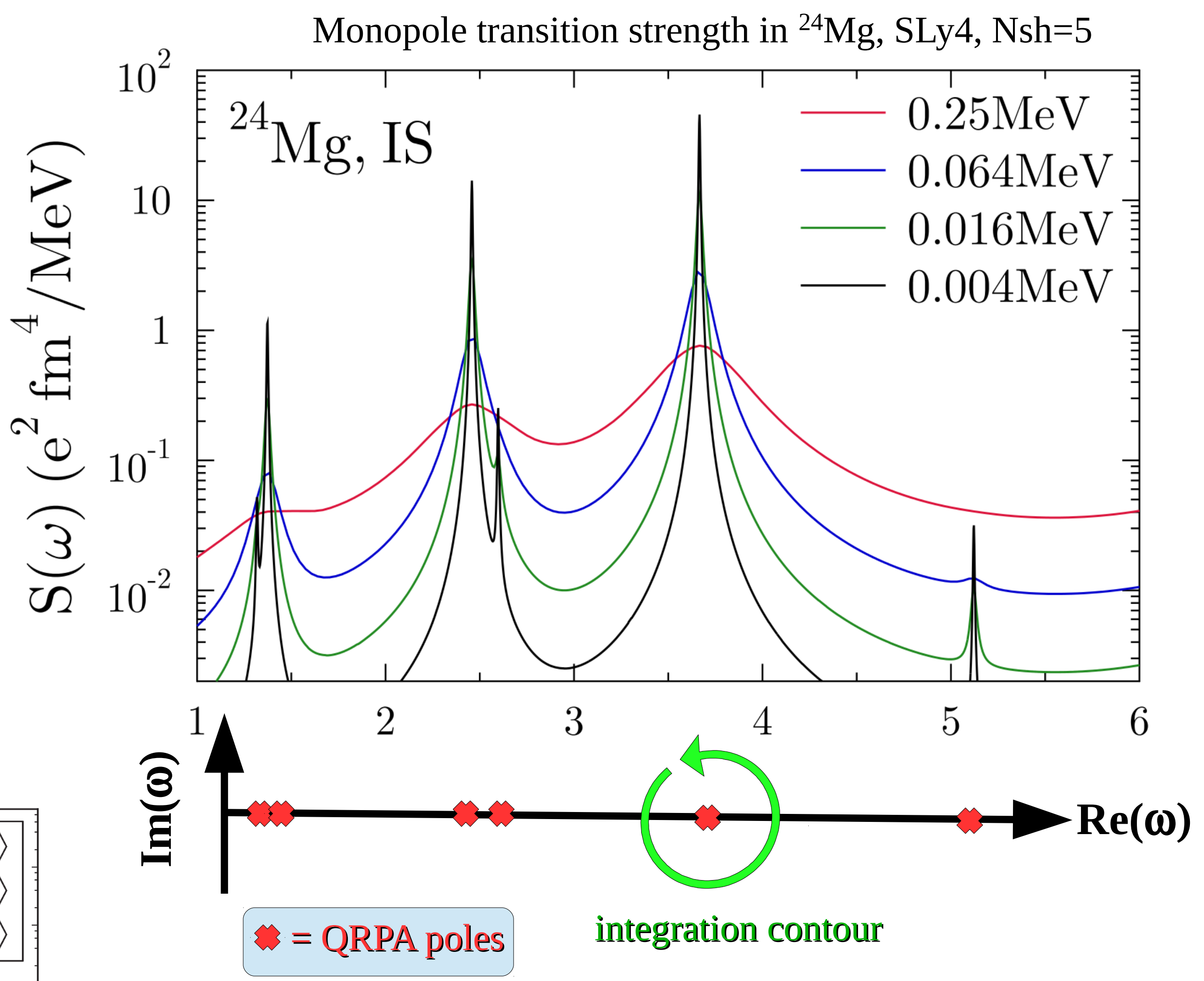


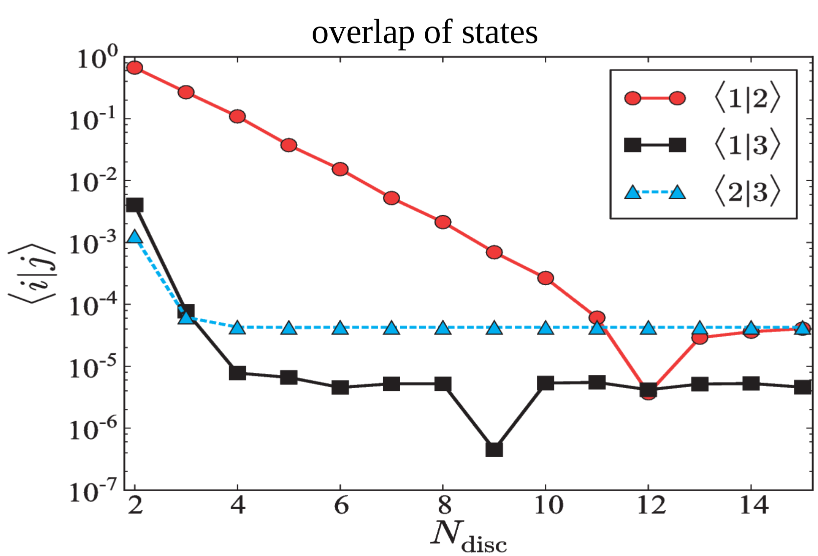
- pnFAM for calculation of beta-decays: M. T. Mustonen, T. Shafer, Z. Zenginerler, and J. Engel, PRC 90, 024308 (2014)



FAM and discrete low-lying states

- FAM can be used to access discrete excited states
- The method is based on a contour integral in a complex place, around the QRPA pole
- Contour integration converges with a relatively small amount of integration points

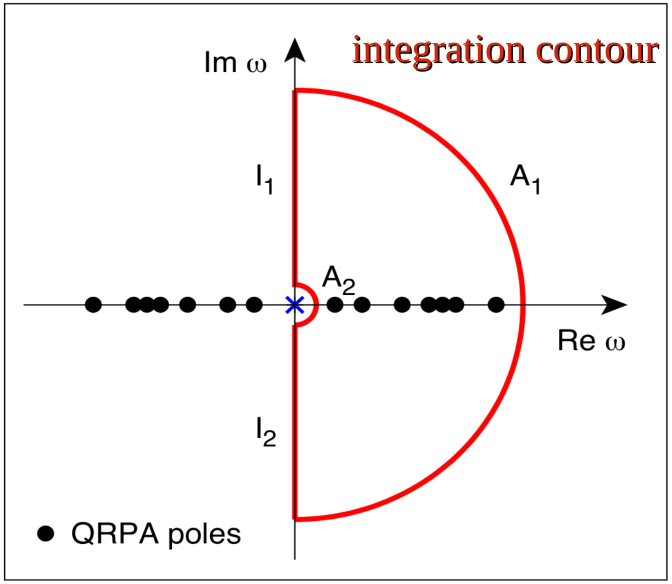




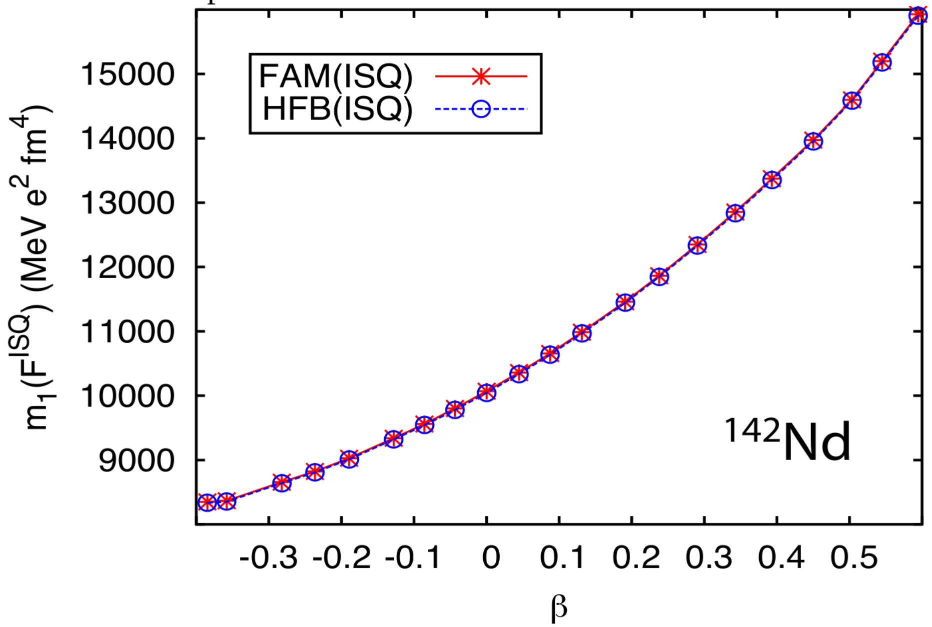
- Published at: N. Hinohara, M. Kortelainen, W. Nazarewicz, Phys. Rev. C 87, 064309 (2013)

FAM and sum rules

- Sum rules within the FAM framework can be calculated by a complex integration technique
- A path circulating all QRPA poles gives the sum rule of associated operator
- Method works for any power of energy or inverse energy weight
- Converges fast as a number of integration points
- Comparison of energy weighted sum rule to Thouless theorem and inverse energy weighted sum rule to dielectric theorem shows excellent correspondence
- N. Hinohara, M. Kortelainen, W. Nazarewicz, and E. Olsen, PRC 91, 044323 (2015)



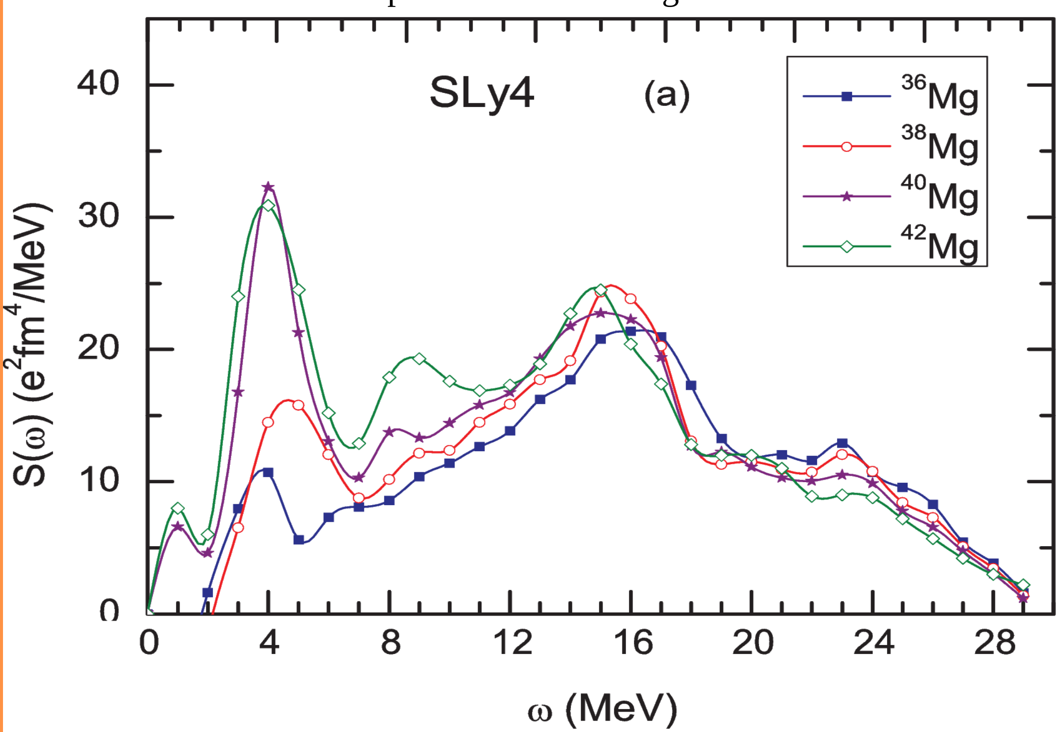
Energy-weighted sum rule of the isoscalar quadrupole operator as a function of deformation



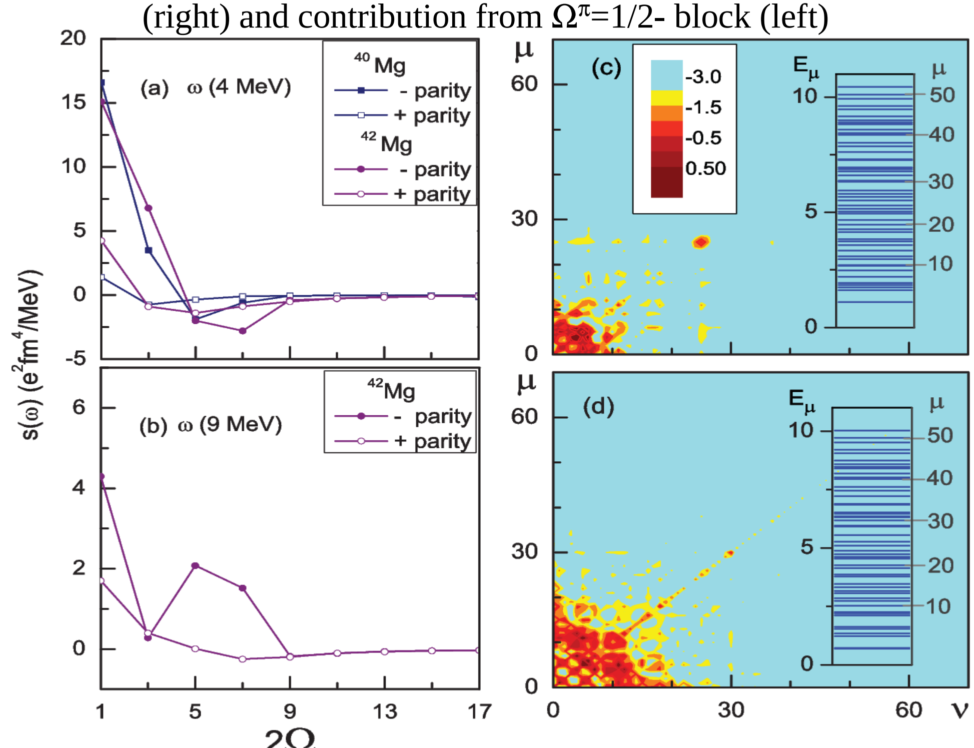
FAM in axially symmetric coordinate space

- For very neutron rich nuclei, close to a drip line, a coordinate based approach is more suitable than harmonic oscillator basis
- FAM has been implemented on a coordinate based HFBAX code (solves HFB eqs. in presence of axial symmetry)
- Results show an emergence of a collective low energy monopole mode due to near-threshold effects
- J. C. Pei, M. Kortelainen, Y. N. Zhang, and F. R. Xu, PRC 90, 051304(R) (2014)

Monopole transition strength function



Monopole transition strength from different Ω^π blocks (right) and contribution from Ω^π=1/2- block (left)



Multipole transitions with axial FAM-QRPA

- For purpose of linear response, axial basis offers a good compromise: Most of the nuclei at single-reference HFB level are axial, with only a few tri-axial ones
- For $K \neq 0$ modes, the electric transition operator

$$r^L \mathcal{Y}_{LK}(\Omega)$$

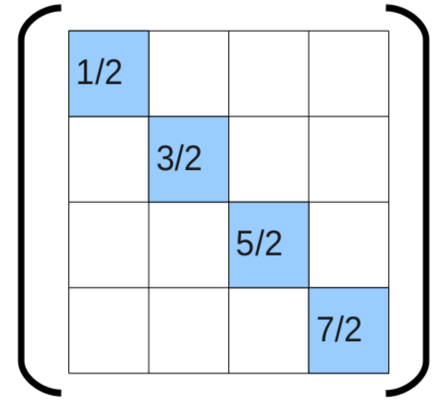
has a different block structure than *h* of HFB

- Need to explicitly linearize density dependent parts in order not to mix different *K*-modes (expansion parameter η no longer needed)
- Simplex-*y* point-symmetry imposed: Electric operator does not connect basis states and their conjugate states
- Oscillating transition density is now of the form of

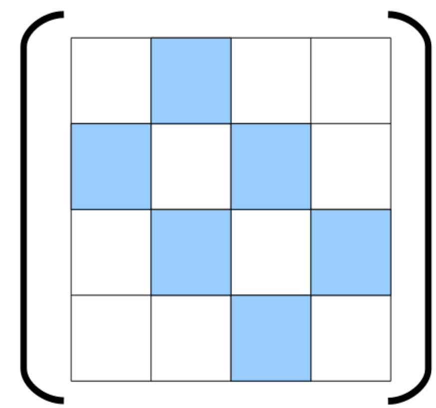
$$\rho_{\mathrm{ind}}(r_p, \varphi, z) = \rho_{\mathrm{ind}}(r_p, z)\left(e^{+iK\varphi} + e^{-iK\varphi}\right)/2$$

Schematic matrix structure in axial basis for $K \neq 0$ modes

$h_{\mathrm{HFB}} =$



$F^{20} =$

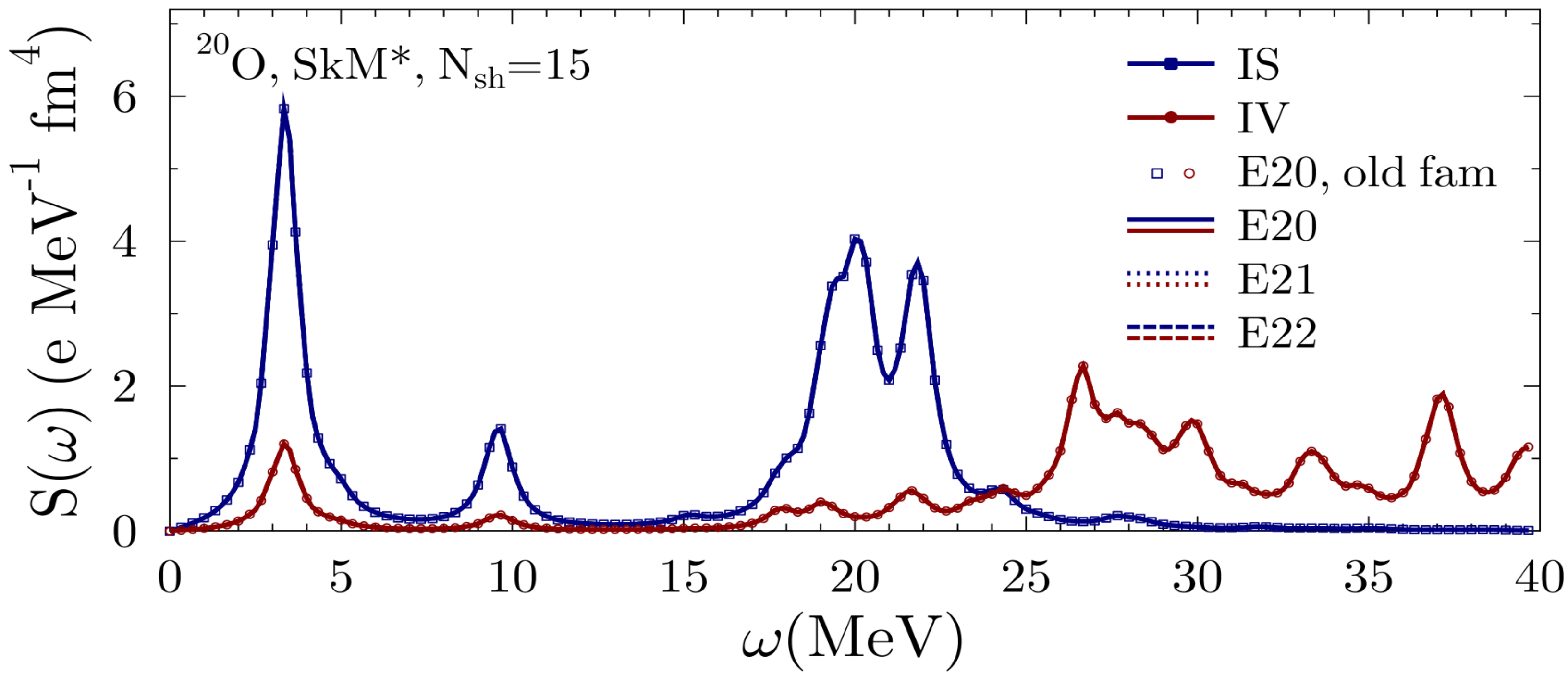


In collaboration with N. Hinohara and W. Nazarewicz

Multipole transitions with axial FAM-QRPA

- Implemented atop of HFBTHO
- Wigner-Eckart theorem in spherical nuclei allows to test the implementation: The same transition strength for all *K* modes
- No truncations in q.p. space, in order to keep self-consistency with respect of the underlying HFB
- Relatively fast computation of the strength function (~1000 CPU h with 20 oscillator shells)

Quadrupole transition strength in ^{20}O



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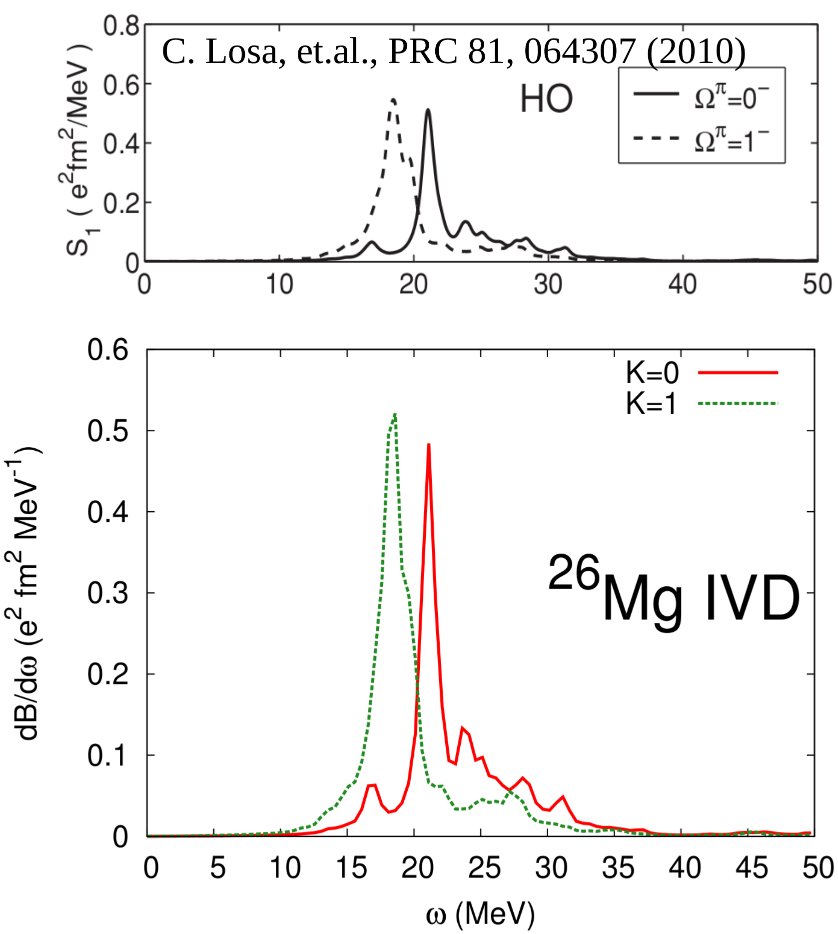
Multipole transitions with axial FAM-QRPA

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



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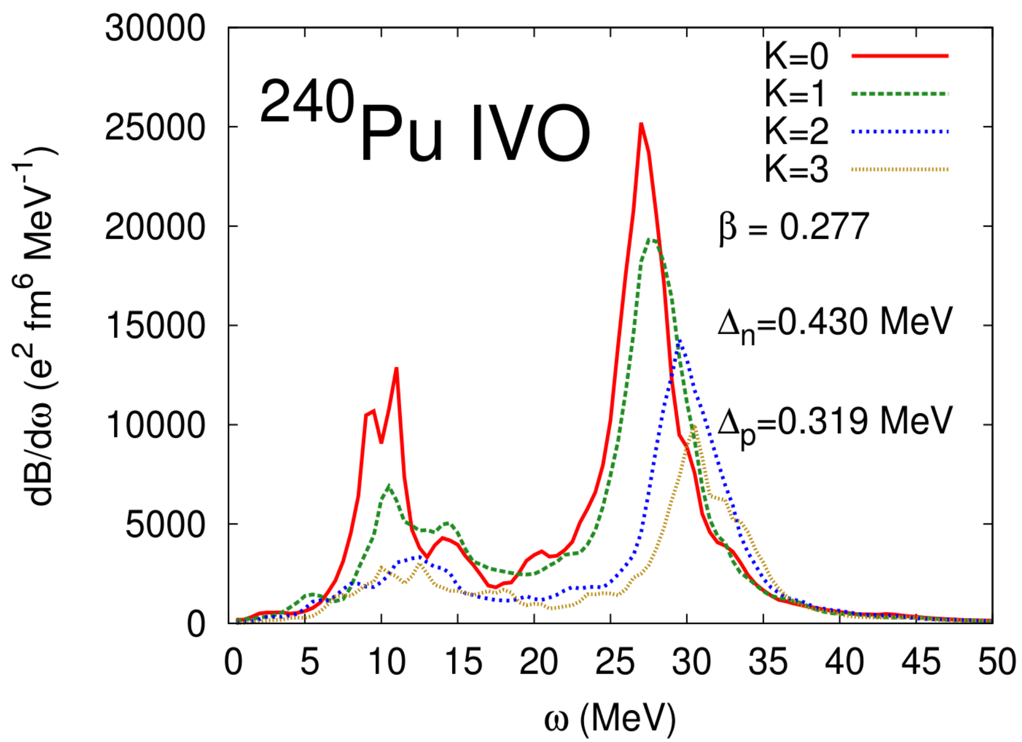
- Method feasible for actinide nuclei with N_{sh}=20, without any truncations
- Example of isovector octupole transition strength in ^{240}Pu

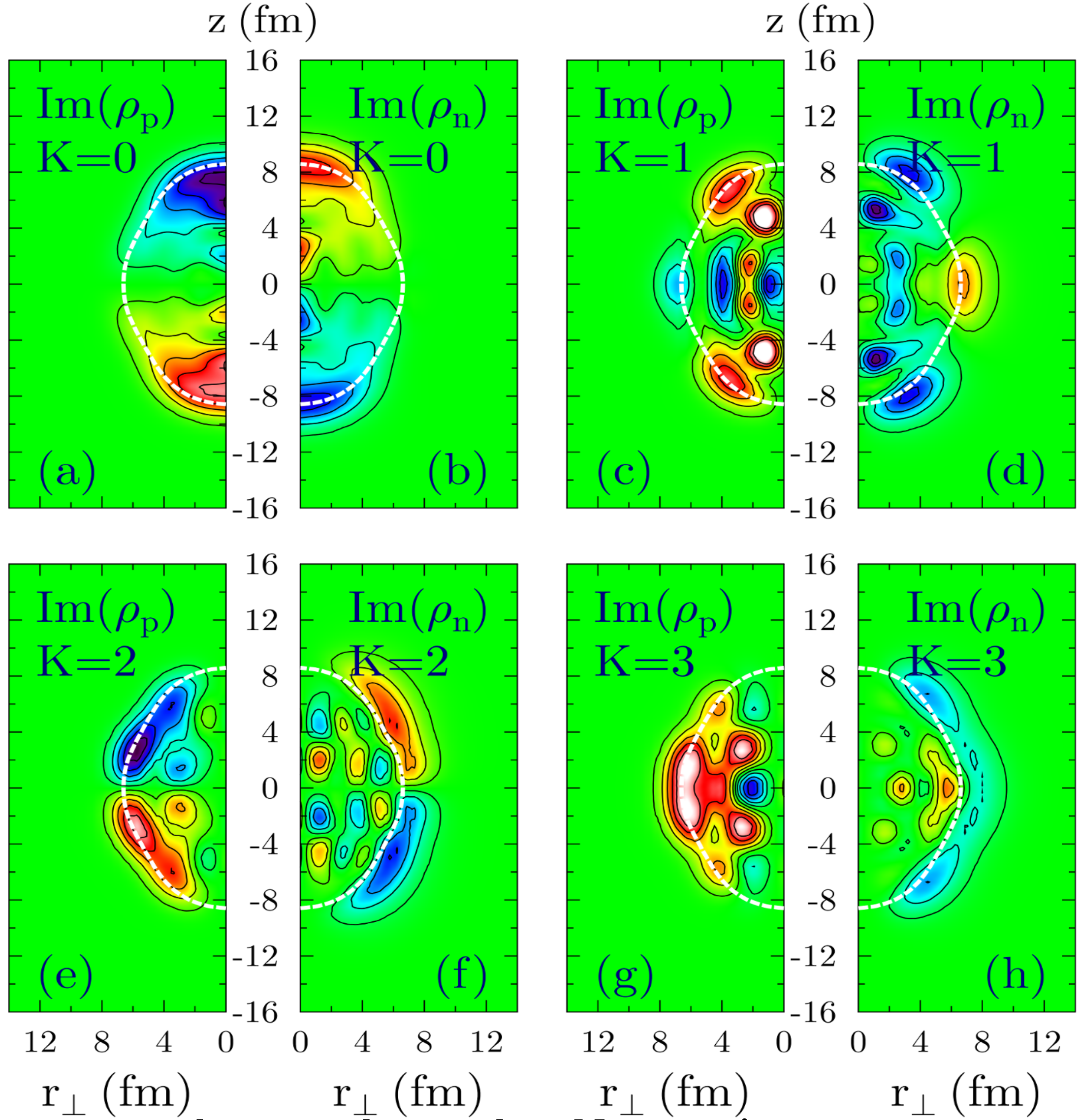


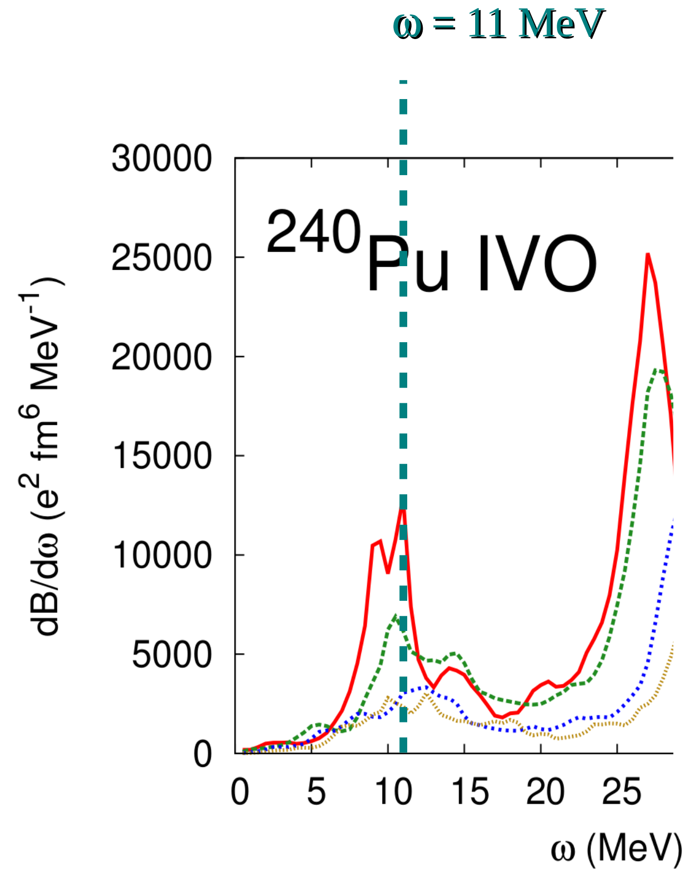
- Calculation of strength function trivially parallelizable

Multipole transitions with axial FAM-QRPA

- Induced transition density for isovector octupole operators shows octupole-like spatial distribution, and a notable collectivity

Induced iv octupole transition density in ^{240}Pu at ω = 11 MeV





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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
  - FAM implemented on axial coordinate space code (HFBAX)
  - New FAM module allows to compute arbitrary multipole mode with an axial code (HFBTHO)
- FAM can be trivially parallelized, allowing large scale surveys

- Sum rule technique has many applications, e.g. in EDF parameter optimization
- The newly developed FAM module allows systematic studies across significant portion of the nuclear chart (including actinides and superheavy nuclei). See talk by T. Oishi about the dipole excitations in rare-earth region