Finite amplitude method in axial basis

ICNT workshop “Physics of exotic nuclei:
Theoretical advances and challenges”

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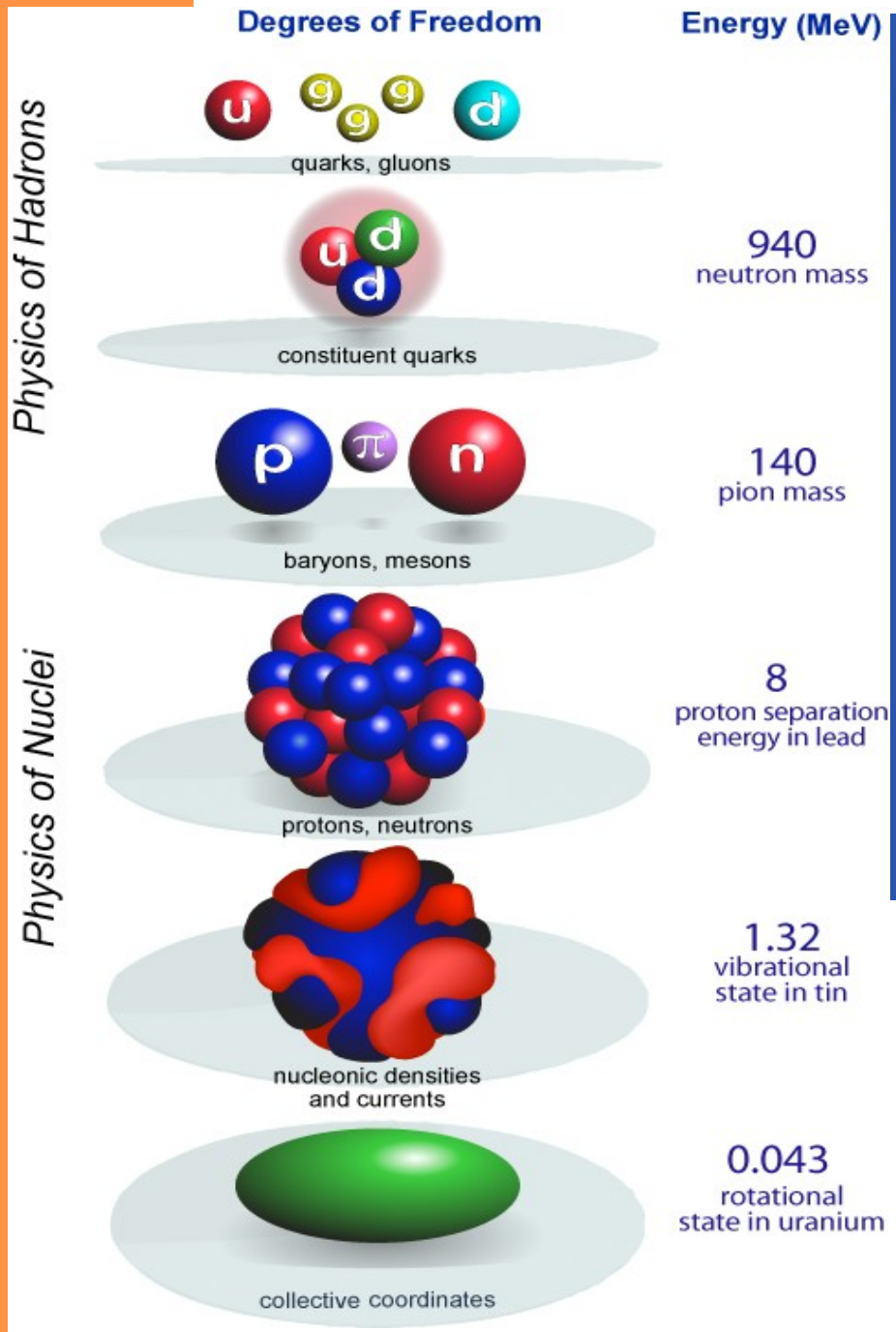
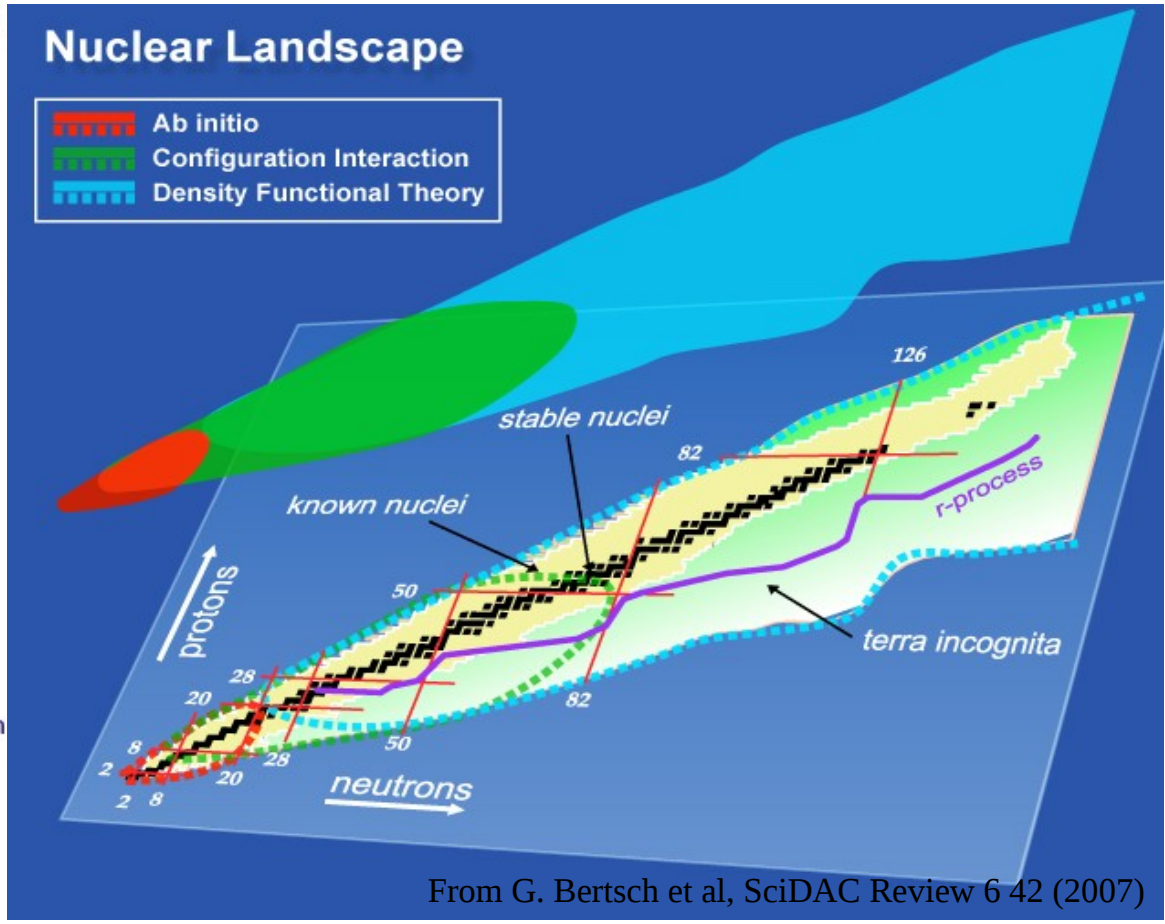
Proper degrees of freedom





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

- QCD is the underlying theory of nucleon-nucleon interaction, but it does not offer proper degrees of freedom to describe a nucleus with many particles

HFB and Skyrme energy density

Skyrme energy density:

$$H_t^{even}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J}J_t^2$$

$$H_t^{odd}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C^{\nabla j}\boldsymbol{s}_t\cdot\nabla\times\boldsymbol{j}_t + C^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t$$

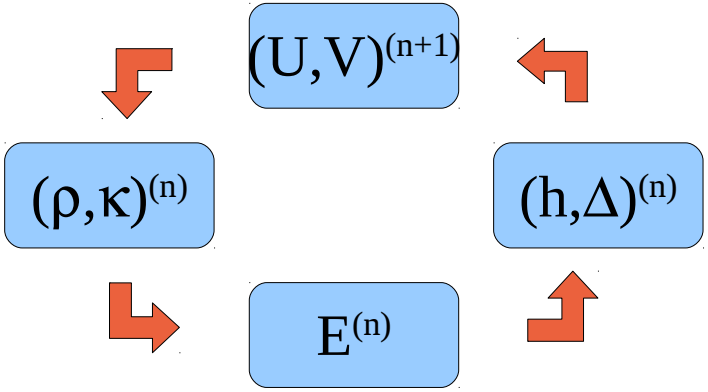
$$C_t^{\rho} = C_{t0}^{\rho} + C_{tD}^{\rho}\rho_0^{\gamma} \quad , \quad C_t^{s} = C_{t0}^{s} + C_{tD}^{s}\rho_0^{\gamma} \quad , \quad t=0,1$$

- Skyrme EDF is constructed from densities and their derivatives, multiplied by coupling constants
- Usually used in the framework of Hartree-Fock or Hartree-Fock-Bogoliubov theory
- HFB equations solved self-consistently (iterative process)

HFB equations:

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

$$h_{ij} = \frac{\partial E[\rho,\kappa]}{\partial \rho_{ij}} \quad , \quad \Delta_{ij} = \frac{\partial E[\rho,\kappa]}{\partial \kappa_{ij}}$$

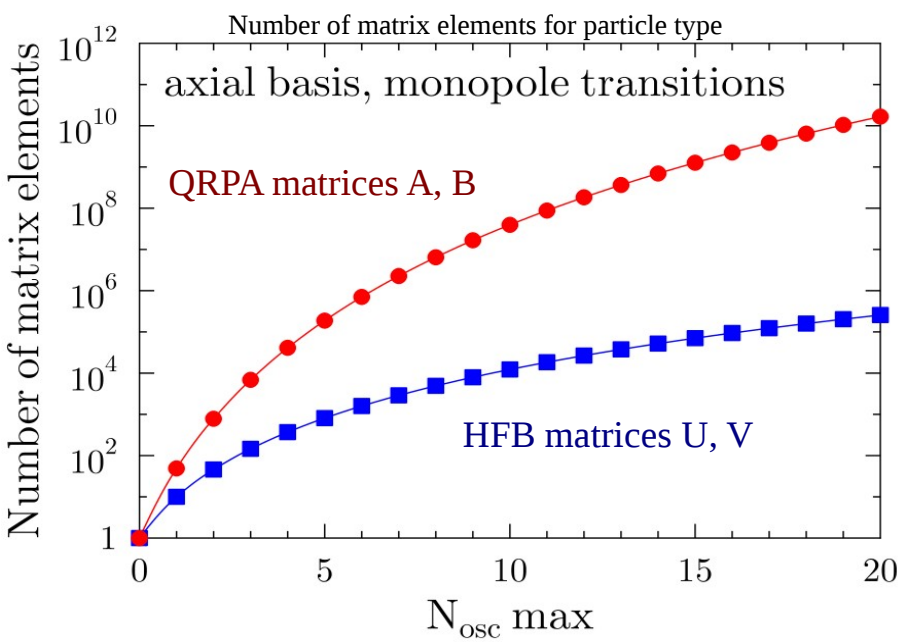


Linear response with matrix-QRPA

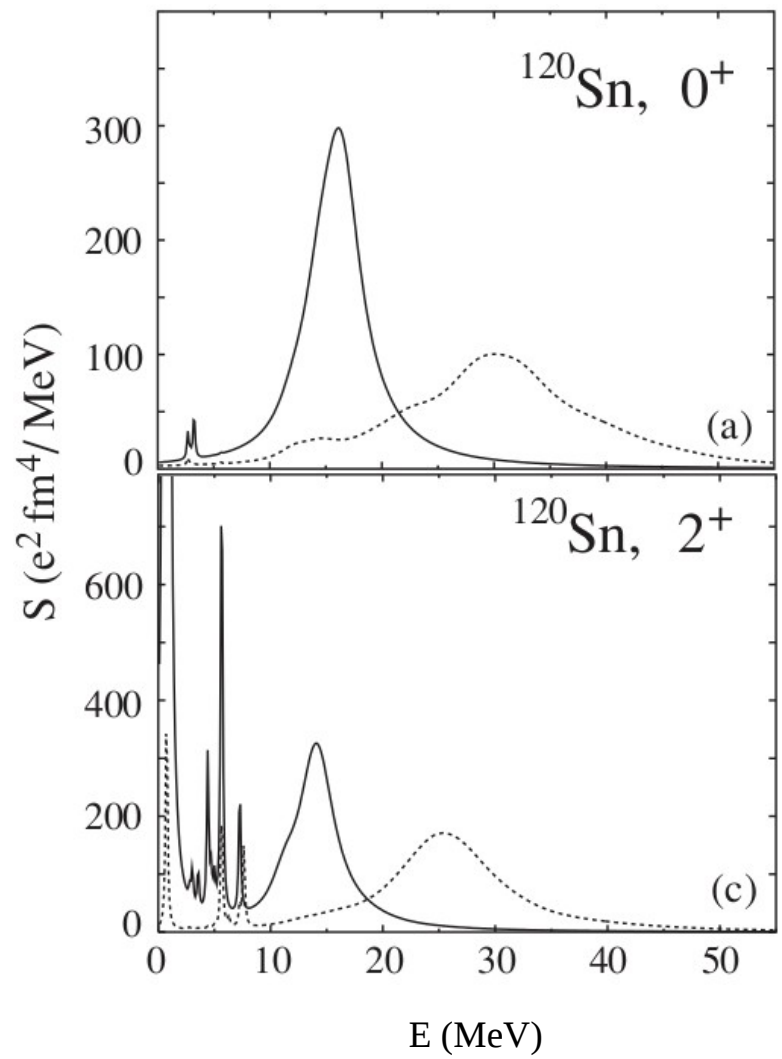
- QRPA traditionally formulated in the matrix form (MQRPA)

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

- Dimension of matrices A and B increases rapidly when basis size is increased
- Dimensions of MQRPA matrices usually reduced by introducing a cut-off parameter v_{crit} for the occupation of canonical states



J. Terasaki, et. al., PRC 71, 034310 (2005)

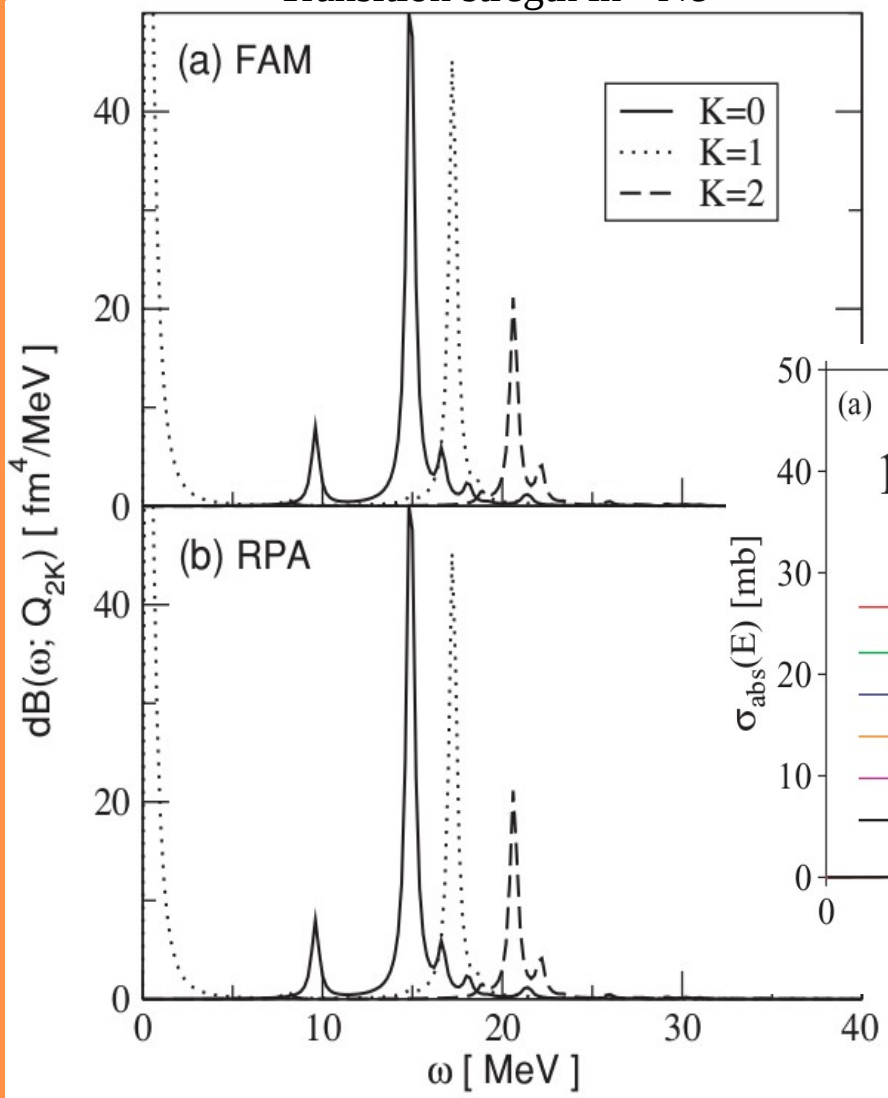


⇒ Iterative QRPA method required!

History of FAM-QRPA briefly

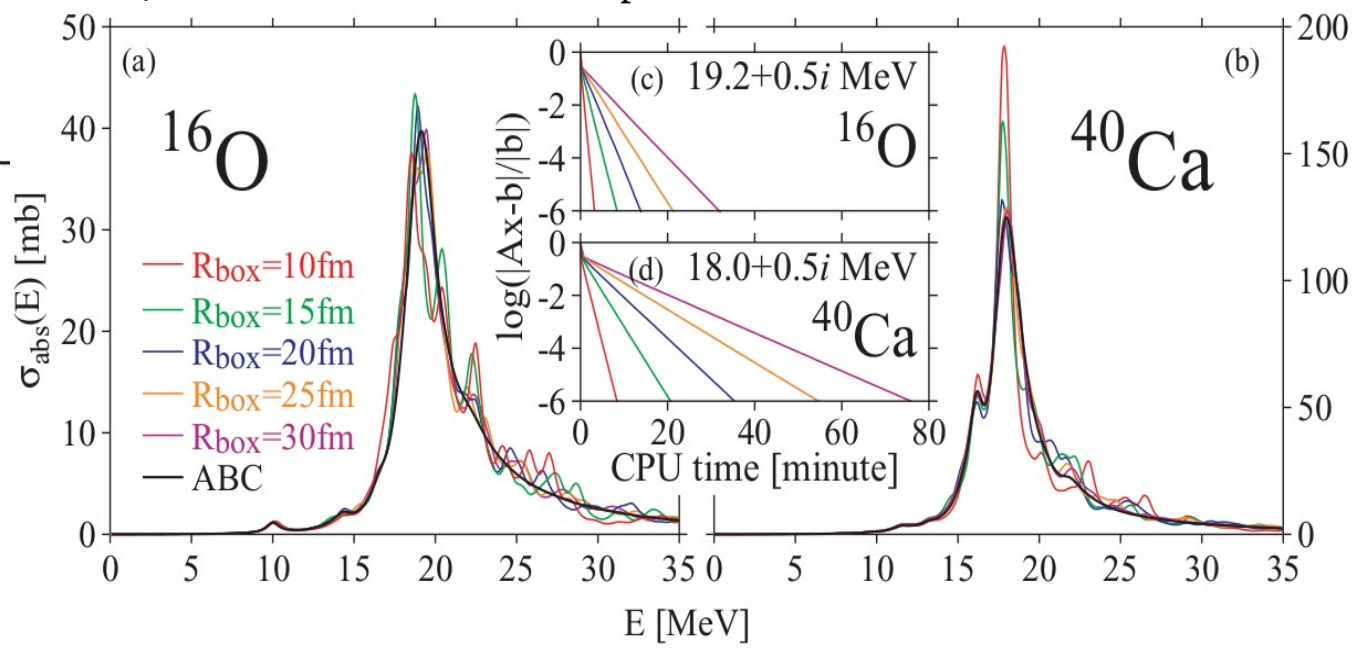
- FAM-QRPA method introduced in:
  T. Nakatsukasa, T. Inakura,
  K. Yabana, PRC 76, 024318 (2007)

Transition stregth in ^{20}Ne



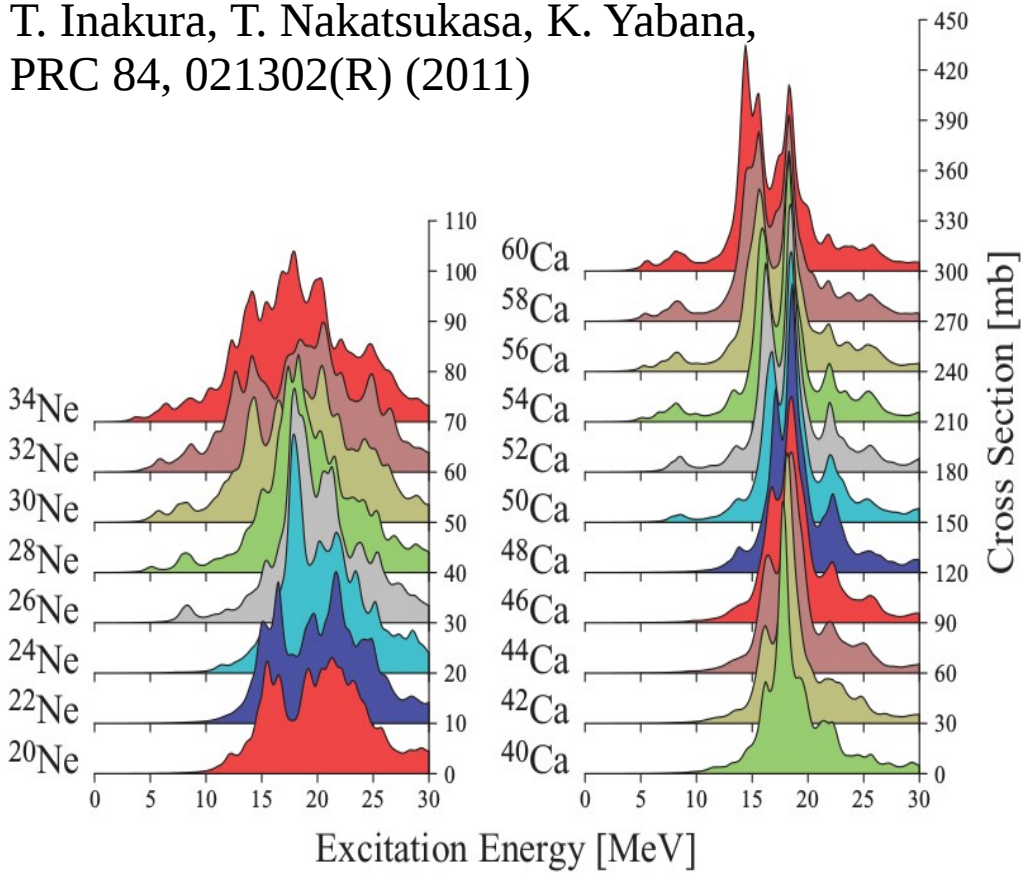
- Photoabsorption with Skyrme-EDF in 3D cartesian mesh studied:
  T. Inakura, T. Nakatsukasa, K. Yabana,
  PRC 80, 044301 (2009)

Photoabsorption cross section

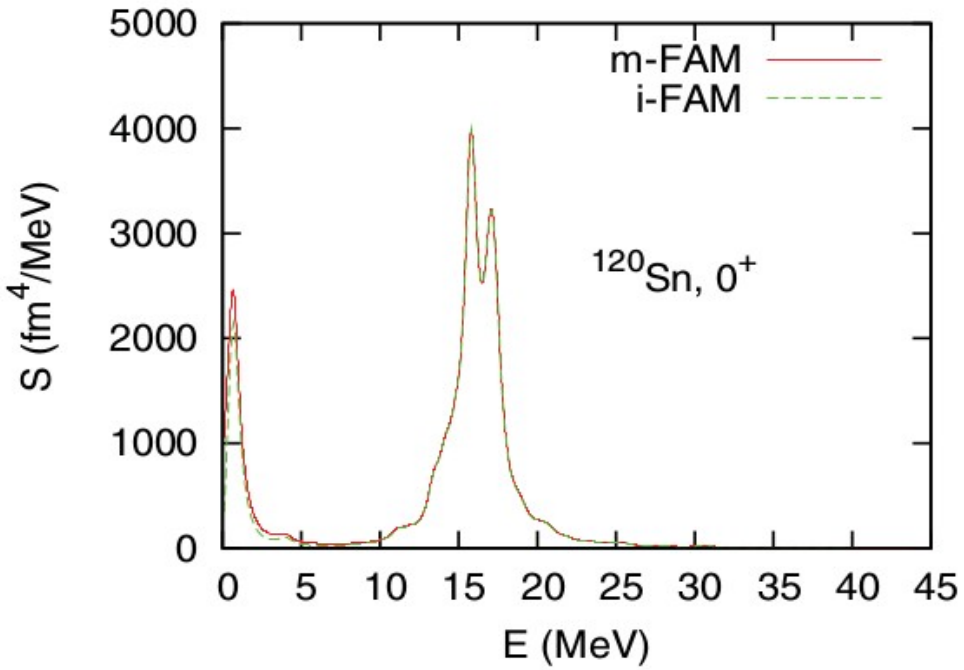


History of FAM-QRPA briefly (cont.)

- Pygmy dipole resonance studied with FAM in: T. Inakura, T. Nakatsukasa, K. Yabana, PRC 84, 021302(R) (2011)



- QRPA matrix elements with FAM: P. Avogadro, T. Nakatsukasa, PRC 87 014331 (2013)



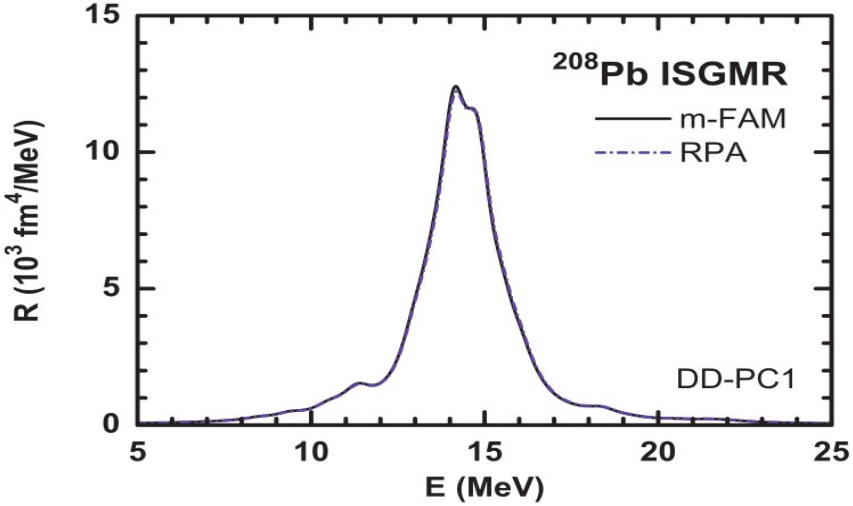
- Discrete states with FAM: N. Hinohara, M. Kortelainen, W. Nazarewicz, PRC C 87, 064309 (2013), **see talk by Nobuo Hinohara**

- Implementation to HFBTHO: M. Stoitsov, M. Kortelainen, T. Nakatsukasa, C. Losa, and W. Nazarewicz, PRC 84, 041305(R) (2011), see details later

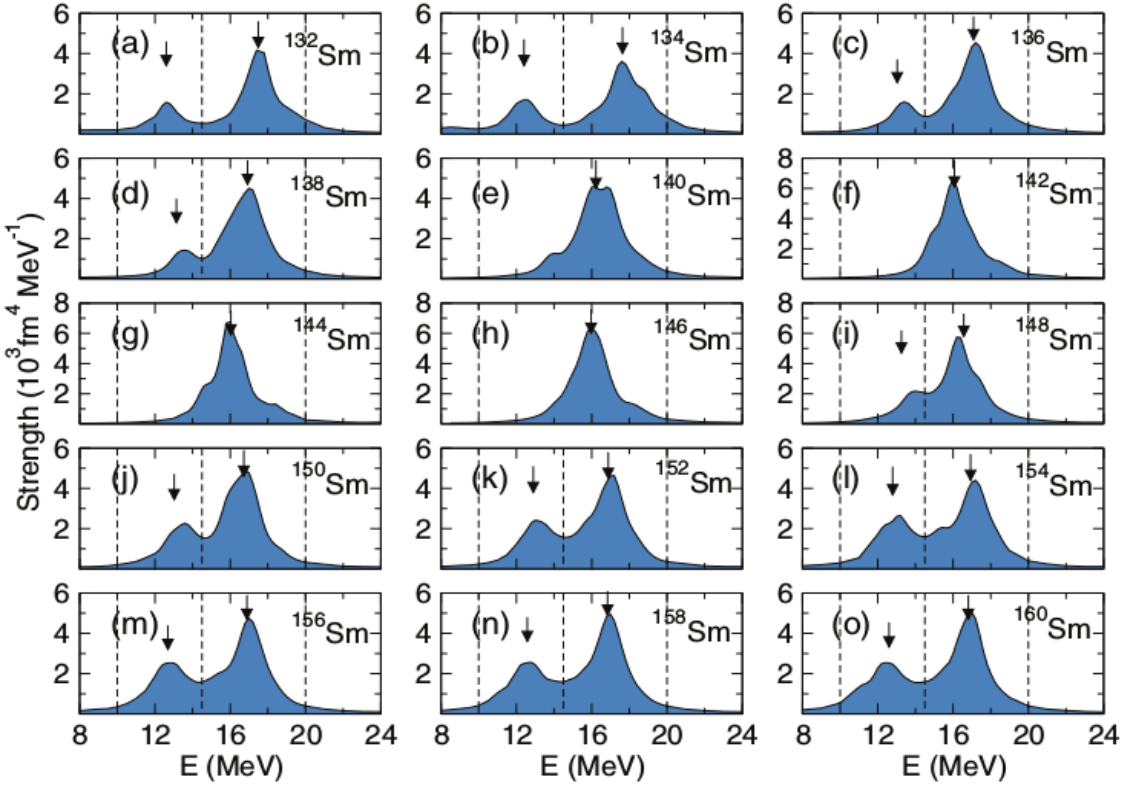
History of FAM-QRPA briefly (cont..)

FAM and relativistic mean field models

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

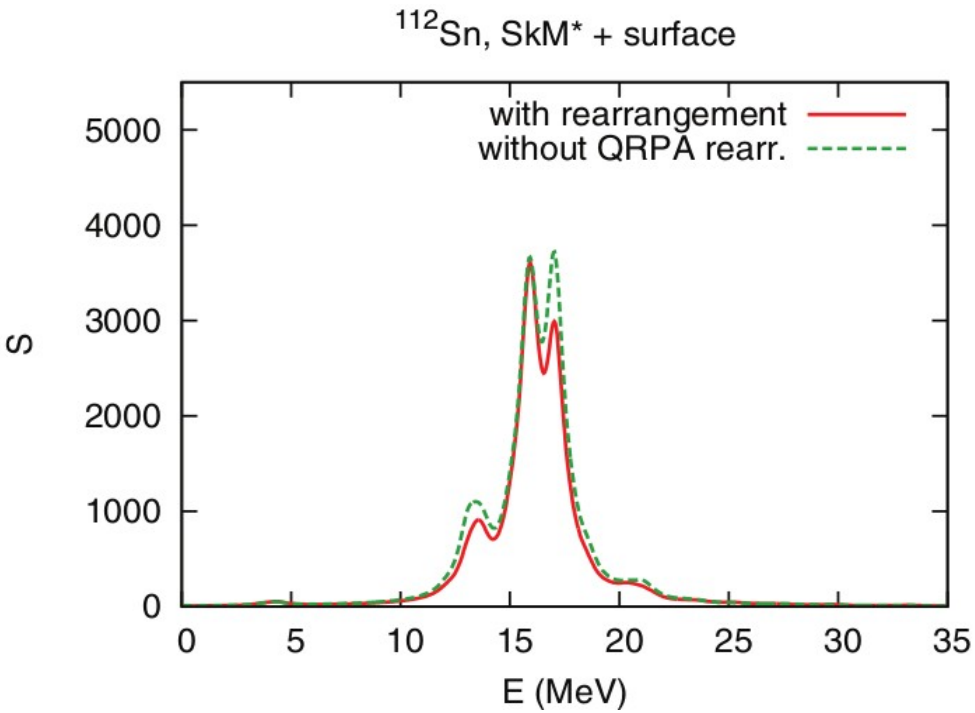


- FAM combined with axial RMF code: T. Niksic, N. Kralj, T. Tutis, D. Vretenar, P. Ring, PRC 88, 044327 (2013)

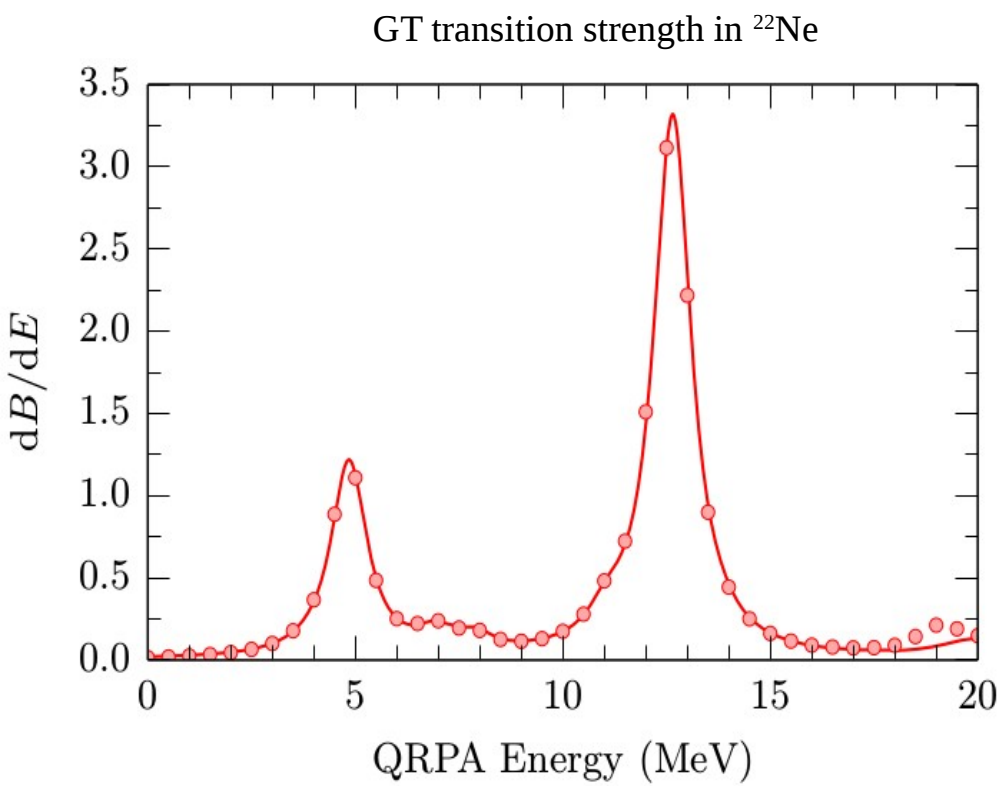


History of FAM-QRPA briefly (cont...)

- Effect of pairing channel to the position of the centroid: P. Avogadro, C.A. Bertulani, PRC 88, 044319 (2013)



- Beta-decays with FAM: M. T. Mustonen, T. Shafer, Z. Zenginerler, J. Engel, arXiv:1405.0254 (2014)



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

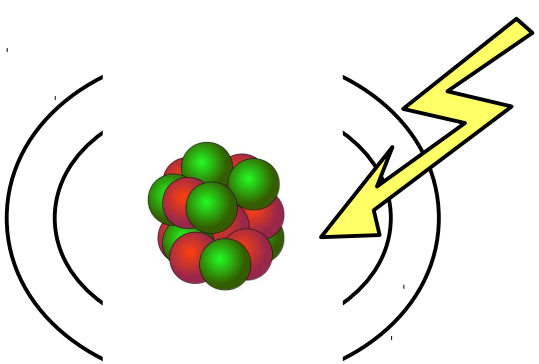
$$i\frac{d\,\delta\alpha_\mu(t)}{dt} = [H(t), \alpha_\mu(t)]$$

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



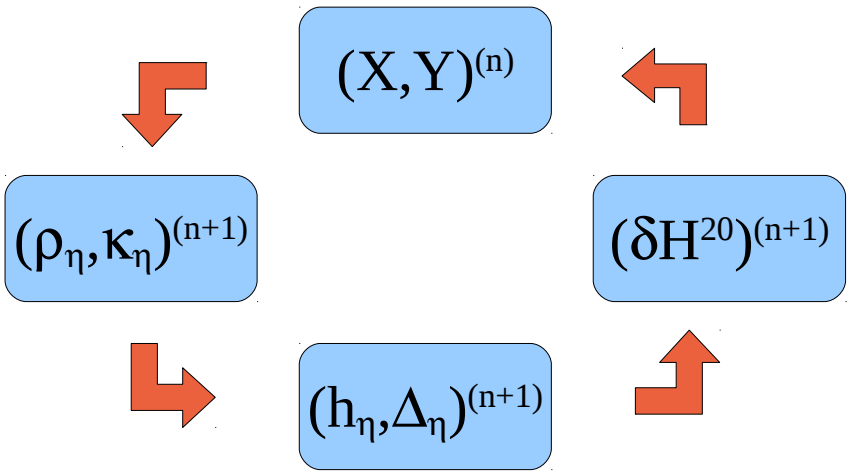
6) FAM equations then reads

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

Solving FAM-QRPA equations

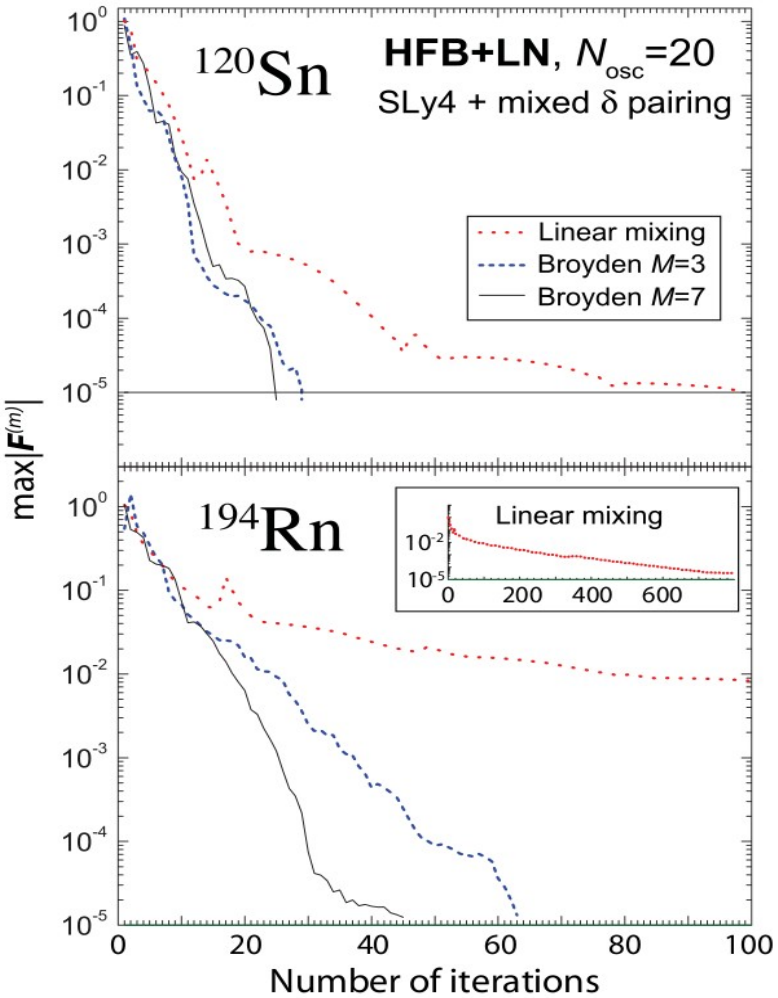
- To solve X and Y, write FAM equations as

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



- FAM equations are solved iteratively
- A small imaginary width introduced: $\omega \rightarrow \omega + i\gamma$
- Similarly as with HFB iterations, X and Y amplitudes eventually converge to solution
- Broyden method essential for the FAM (uses history of previous iterations to speed-up convergence)

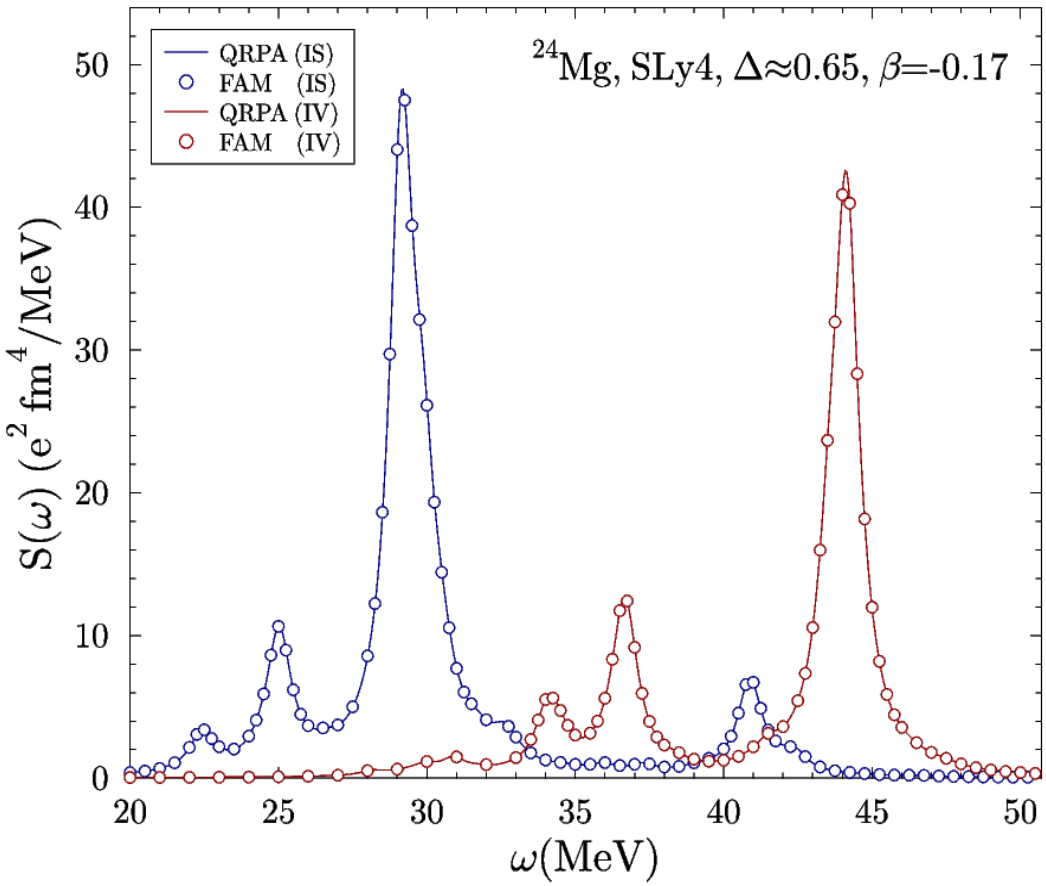
Broyden method: A. Baran, et. al., PRC78, 012318 (2008)

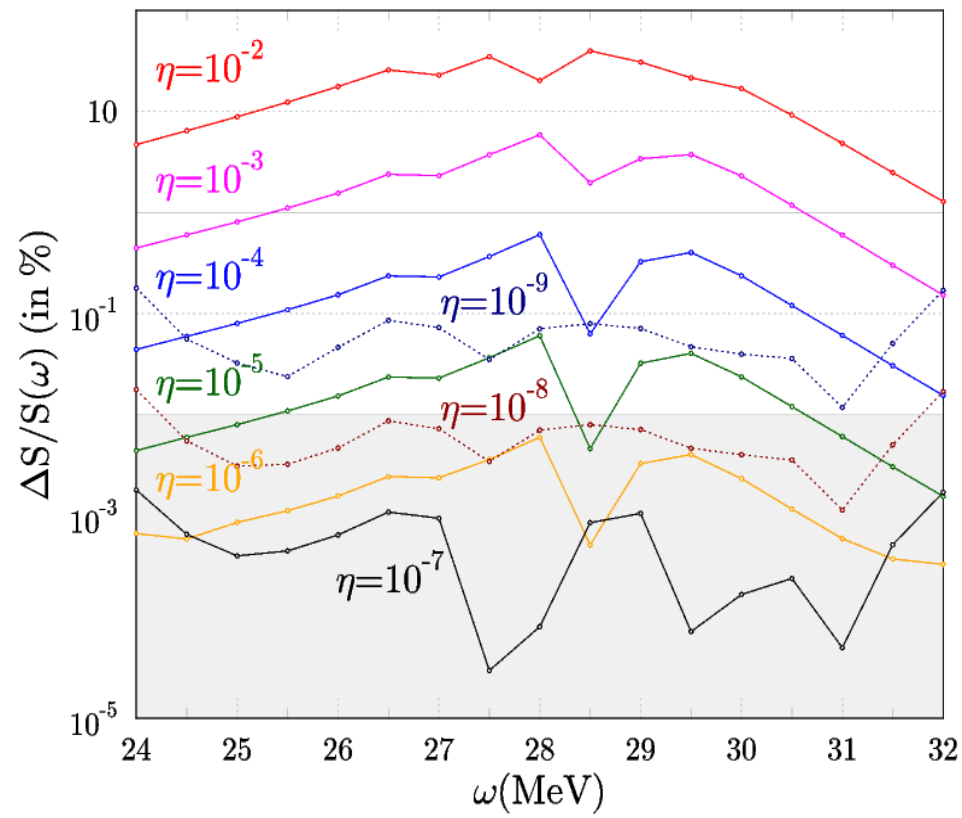


Example of ^{24}Mg with FAM and MQRPA

M. Stoitsov, M. Kortelainen, T. Nakatsukasa, C. Losa, W. Nazarewicz, PRC 84, 041305(R) (2011)

Monopole transition strength



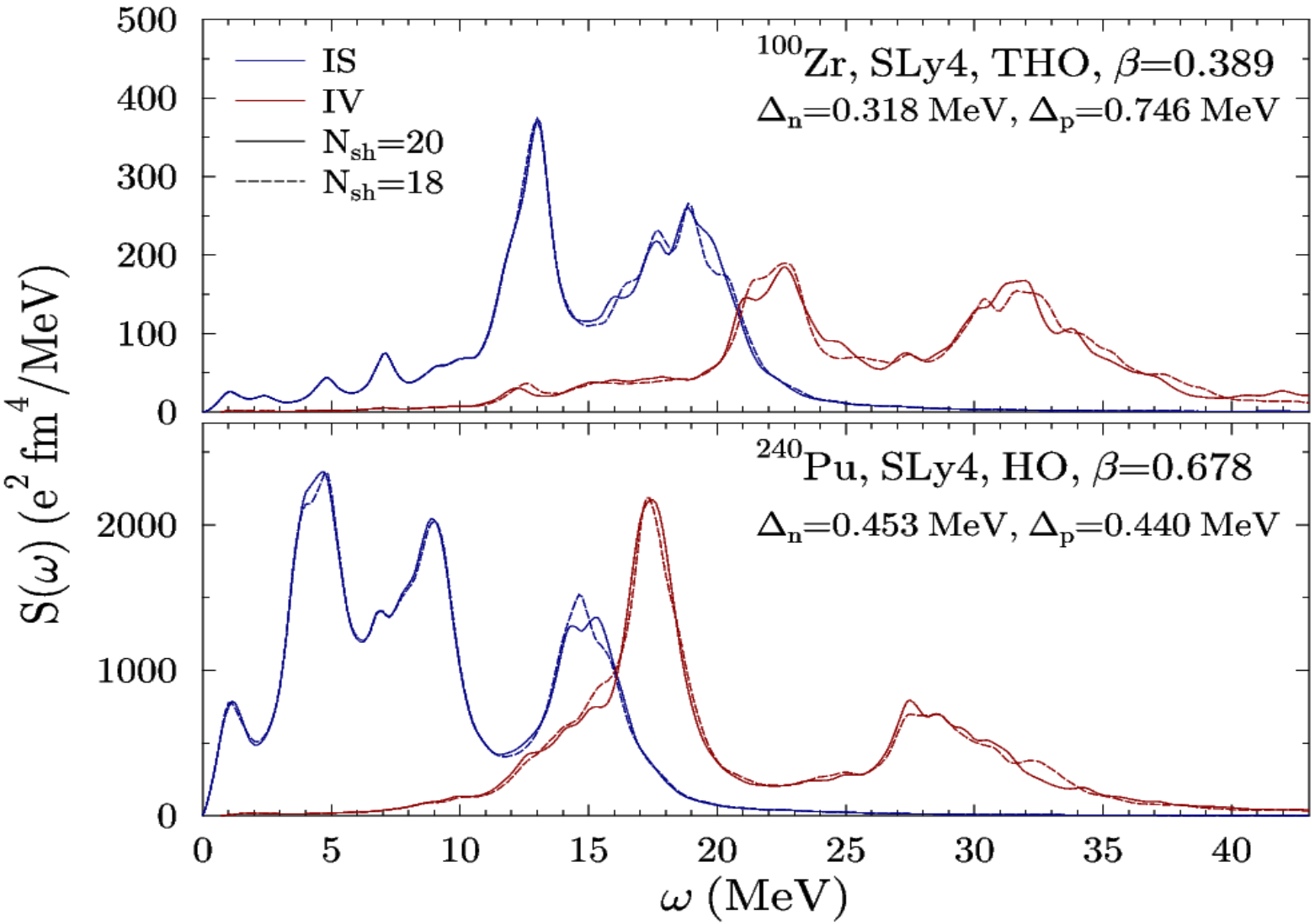


- FAM QRPA was implemented to axial HFBTHO code
- Results with FAM and matrix-QRPA agree.
- Results independent on expansion parameter η.

Monopole transition strength

M. Stoitsov, M. Kortelainen, T. Nakatsukasa,
C. Losa, W. Nazarewicz, PRC 84, 041305(R) (2011)

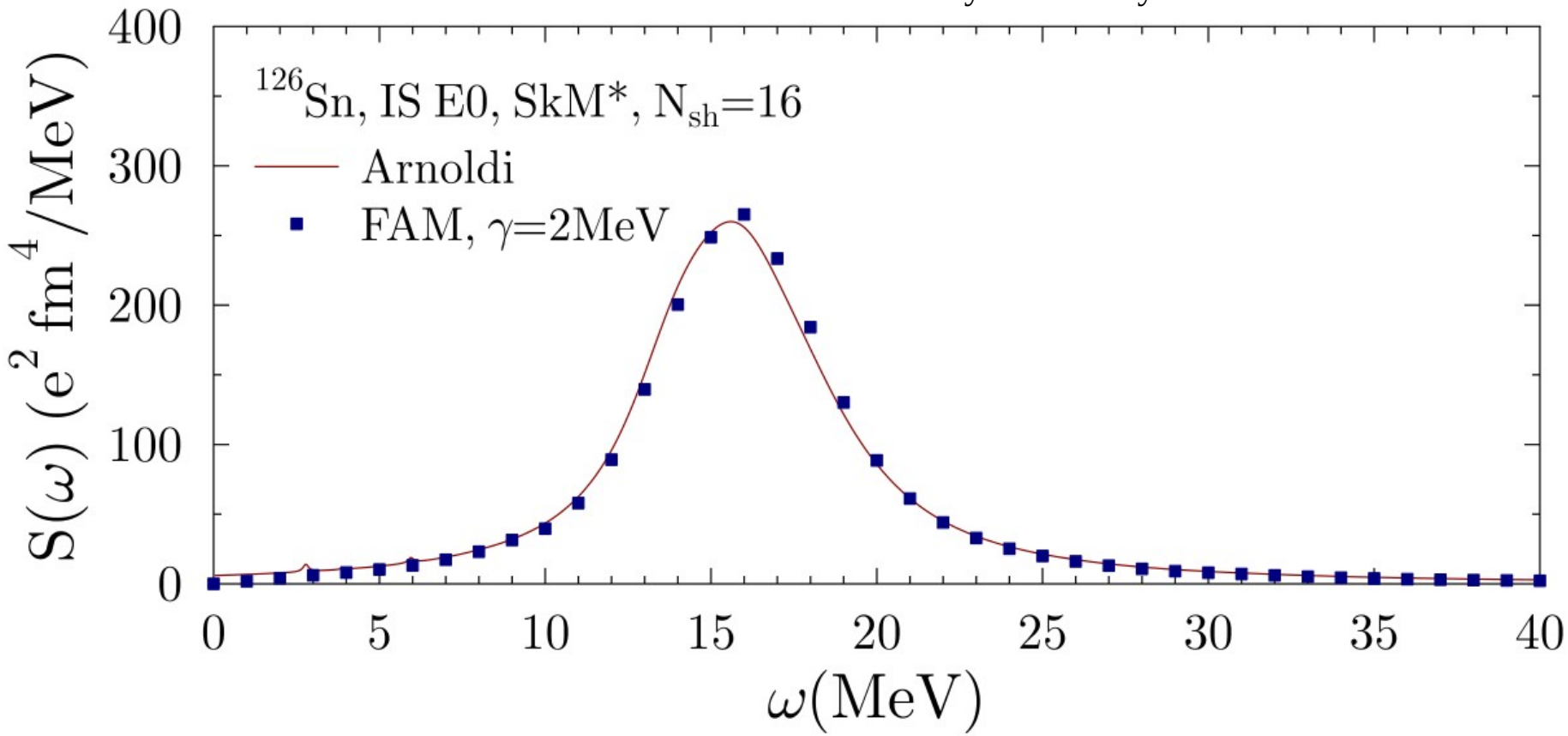
Monopole transition strength



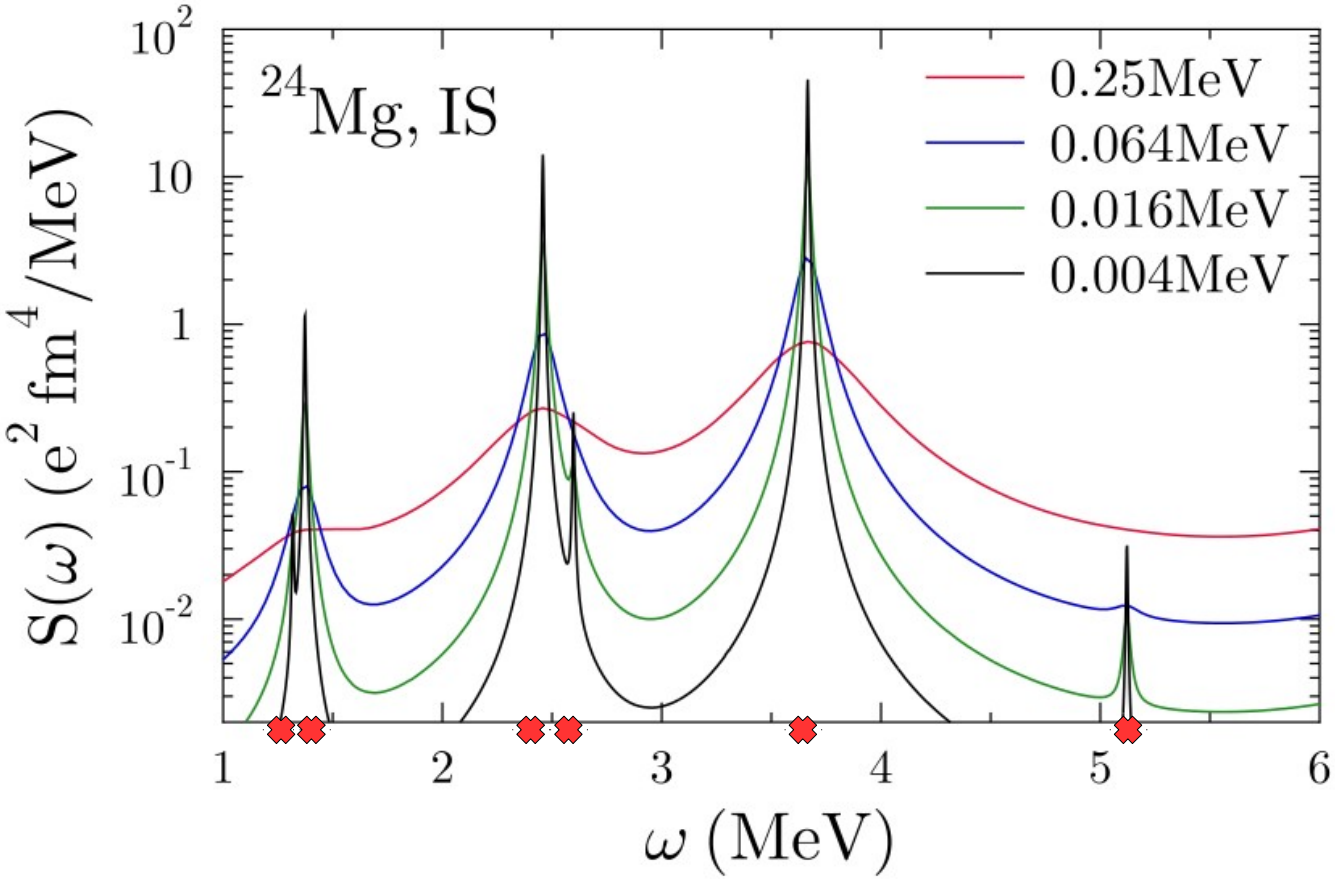
Comparison to iterative Arnoldi diagonalization

- FAM results can be compared to iterative Arnoldi diagonalization method (J. Toivanen, et. al., PRC 81, 034312 (2010))
- A test case of ^{126}Sn agrees well

Arnoldi calculation done by Petr Vesely with HOSPHE code



Discrete QRPA states with FAM



See talk by Nobuo Hinohara

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

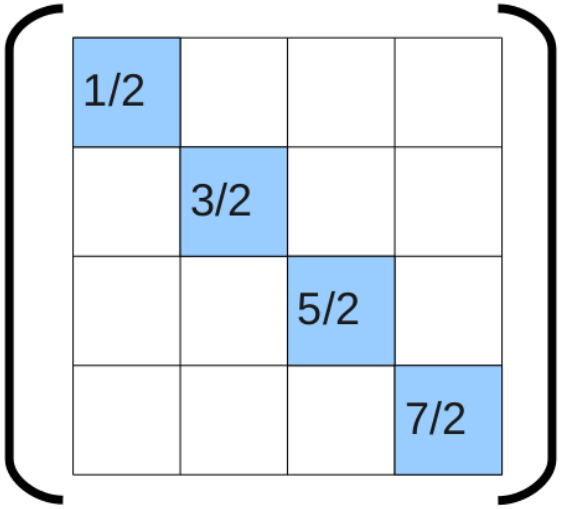
- Discrete QRPA states can be also accessed with FAM-QRPA
- Contour integration around the QRPA eigen-frequency, in complex plane, gives discrete QRPA amplitudes

K≠0 modes with axial FAM-QRPA

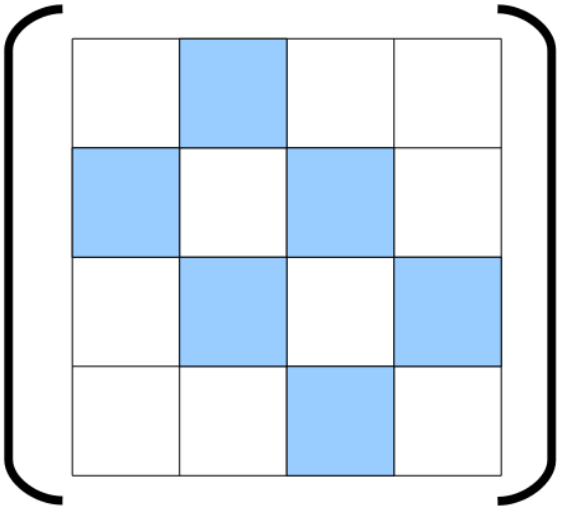
- Transition operator proportional to spherical harmonic $\mathbf{Y}_{LK}$
- K = 0 modes for E2 transitions can be calculated within the same block structure as the HFB
- In spherical nucleus, due to the Wigner-Eckart theorem, all K modes give the same transition strength function
- For deformed nuclei, all K modes needed
- For K ≠ 0 modes, the transition operator has a different block structure than HFB
- Need to explicitly linearize density dependent parts (expansion parameter η no longer needed)
- Implementation to HFBTHO

Matrix structure in axial basis for K ≠ 0 modes

$h_{HFB} =$



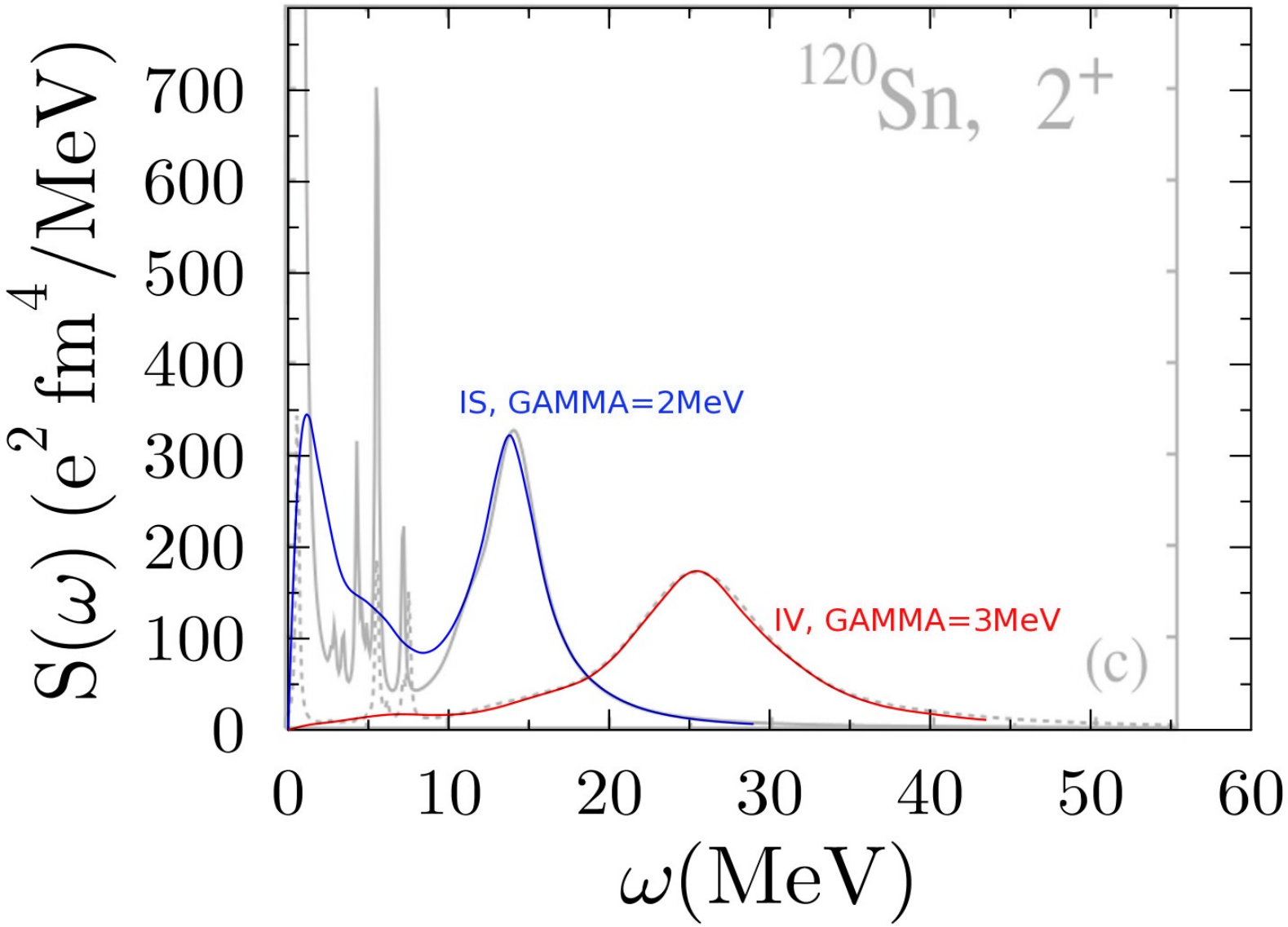
$F^{20} =$



In collaboration with N. Hinohara and W. Nazarewicz

E2 transition rates (spherical nucleus)

Comparison of FAM 2^+ calculation to results of J. Terasaki, et. al., PRC 71, 034310 (2005) (gray lines). Combined figure.



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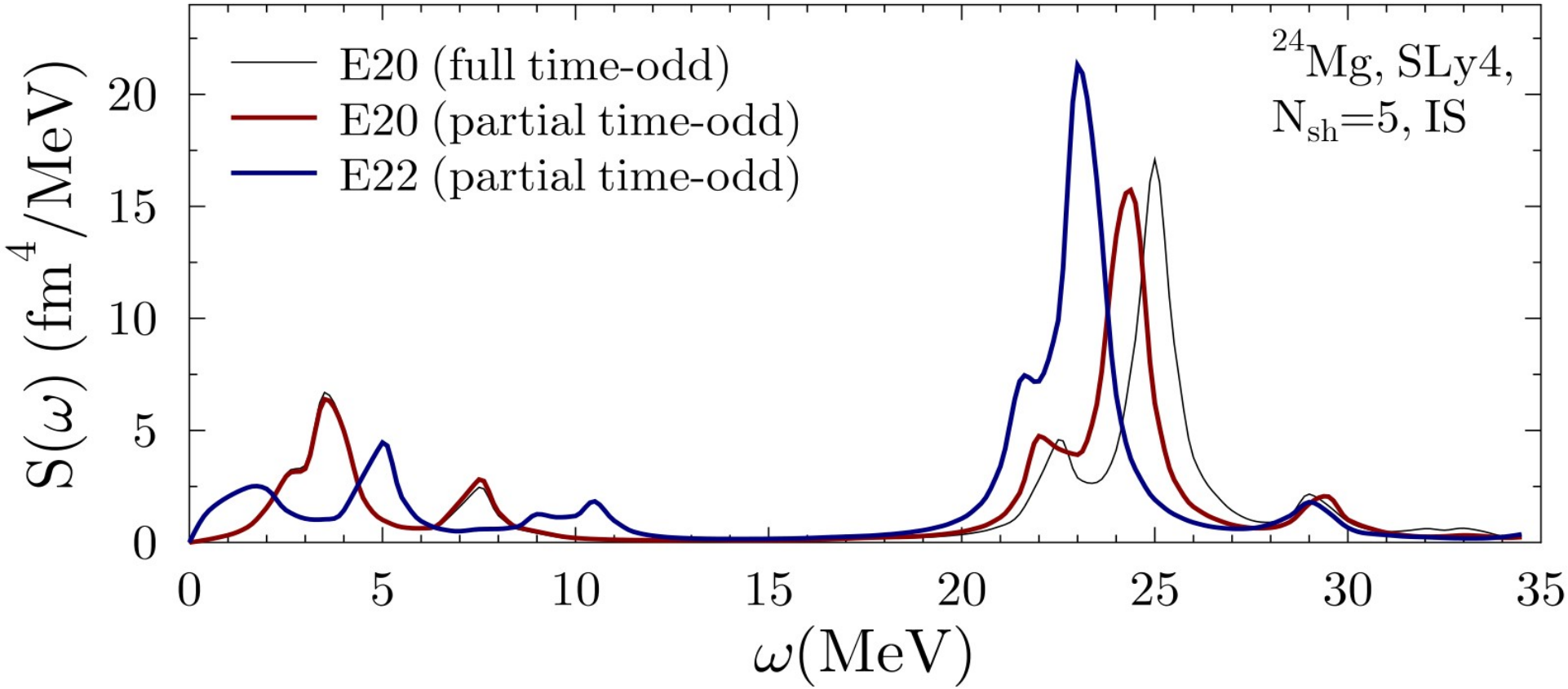
Test case of ^{24}Mg

PRELIMINARY

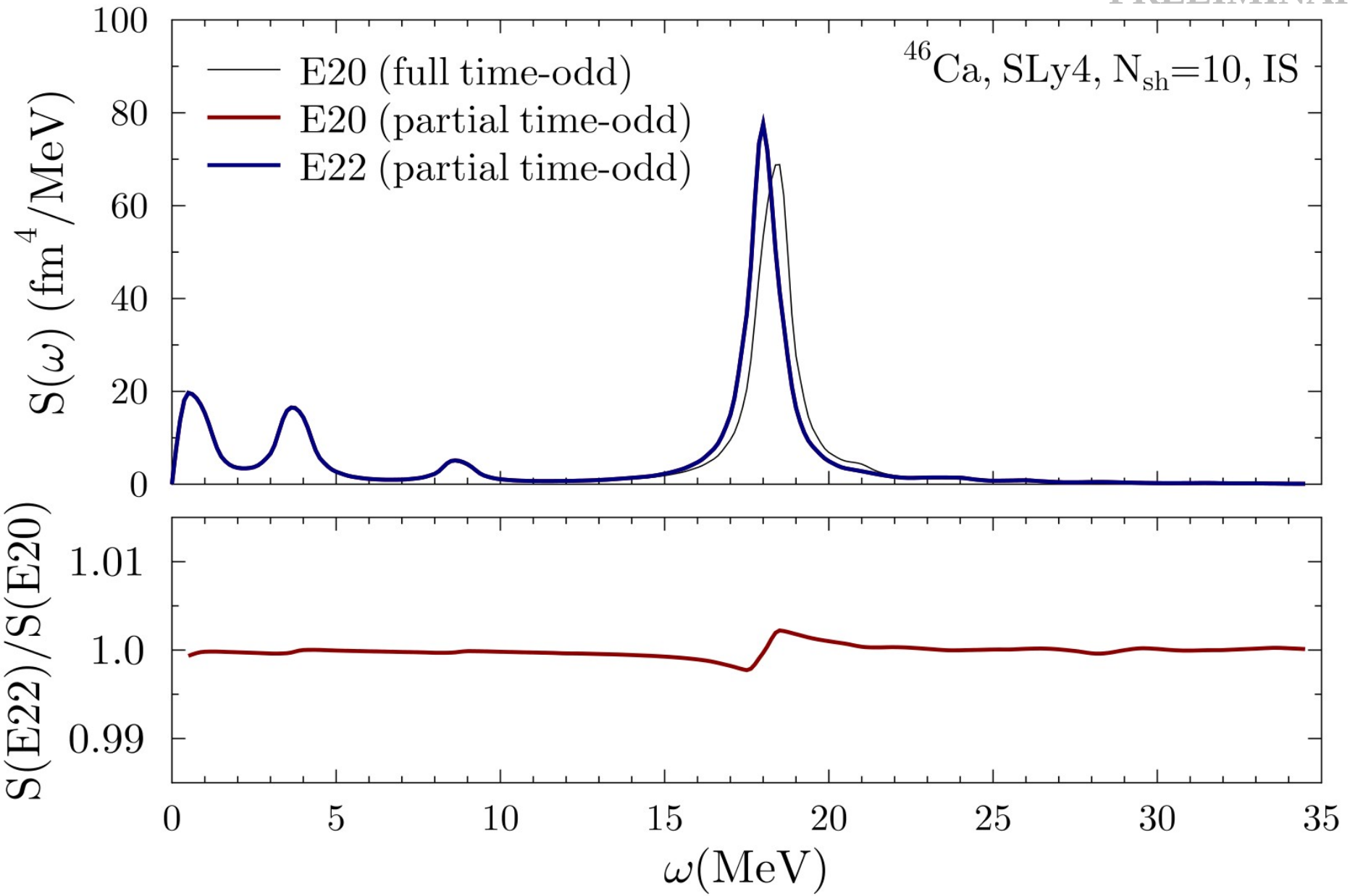


- Current FAM implementation in HFBTHO, with K≠0 modes, lacks some of the time-odd EDF components (**s.**∇×**j** -term)
- Test case of oblate deformed ^{24}Mg shows that this term has some impact

In collaboration with N. Hinohara and W. Nazarewicz

Testing spherical nuclei

PRELIMINARY



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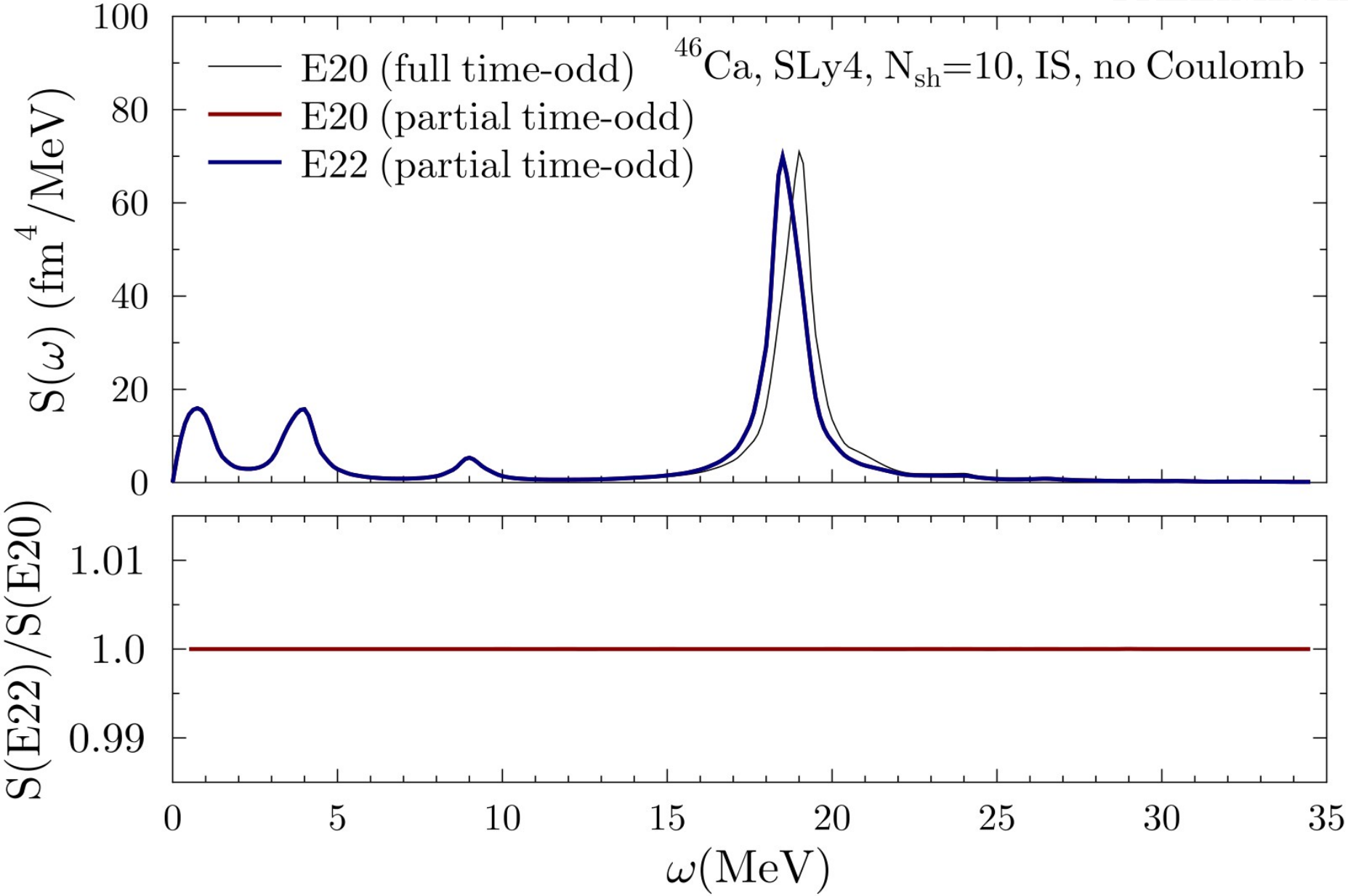
Testing spherical nuclei

PRELIMINARY



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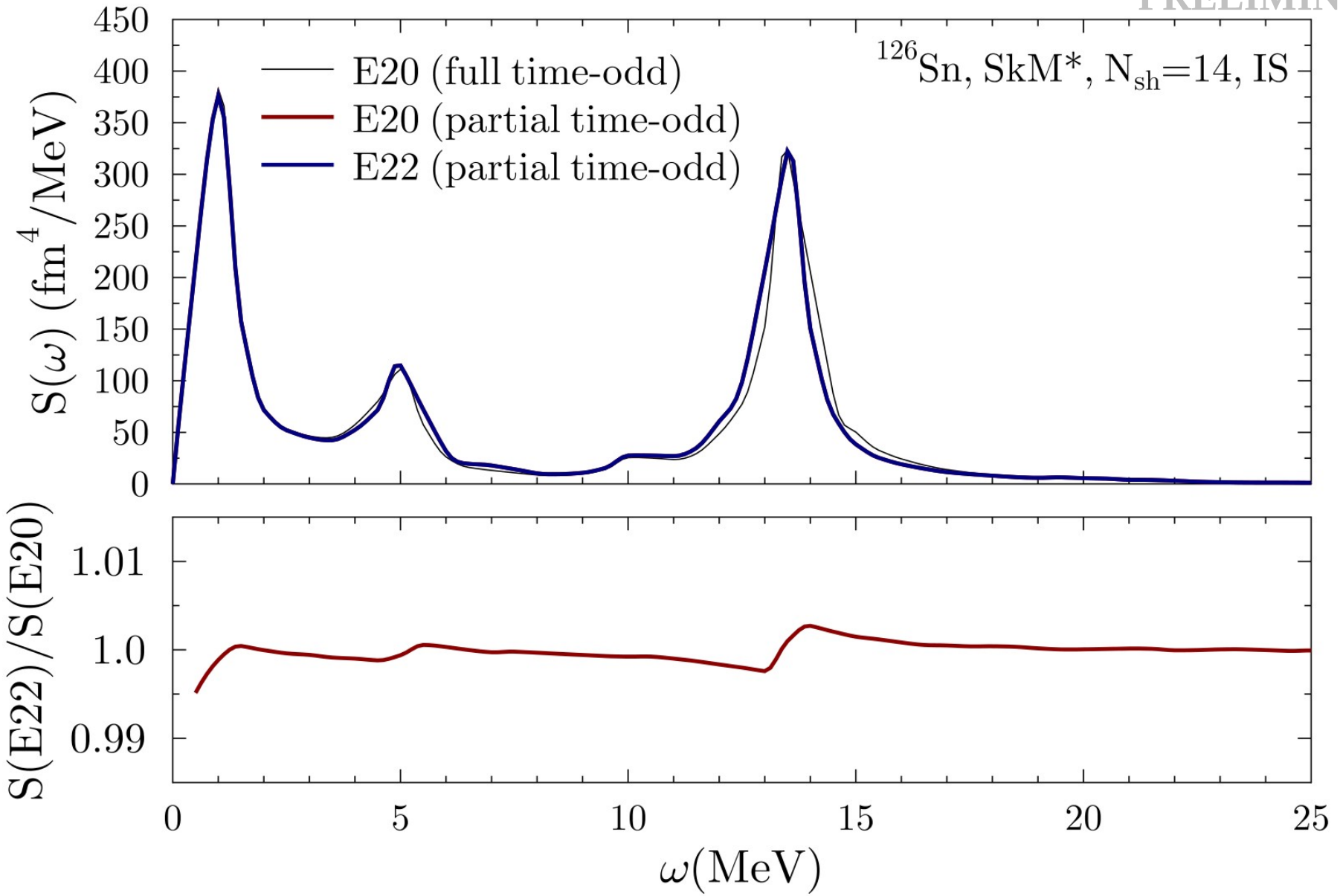
Testing spherical nuclei

PRELIMINARY



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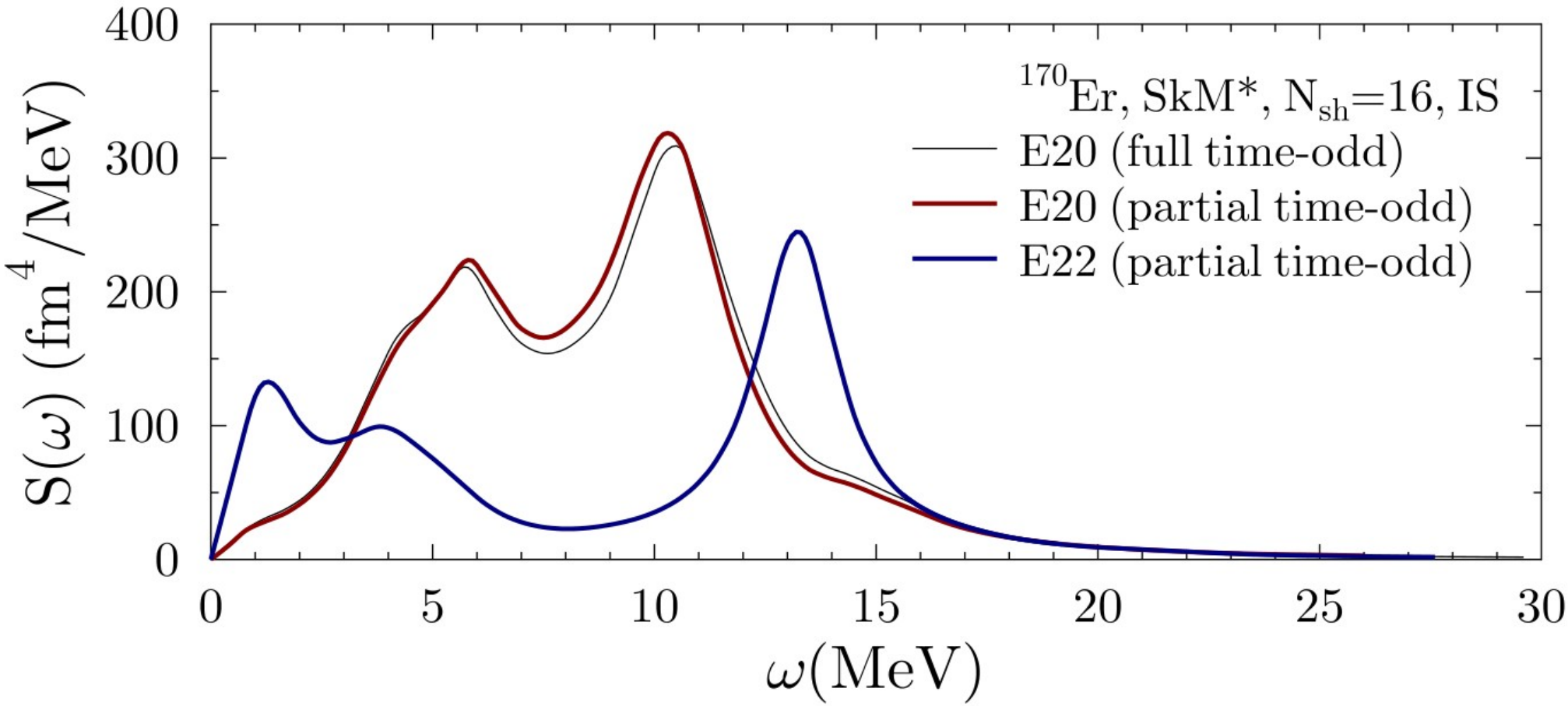
Isoscalar quadrupole stregth in ^{170}Er

PRELIMINARY



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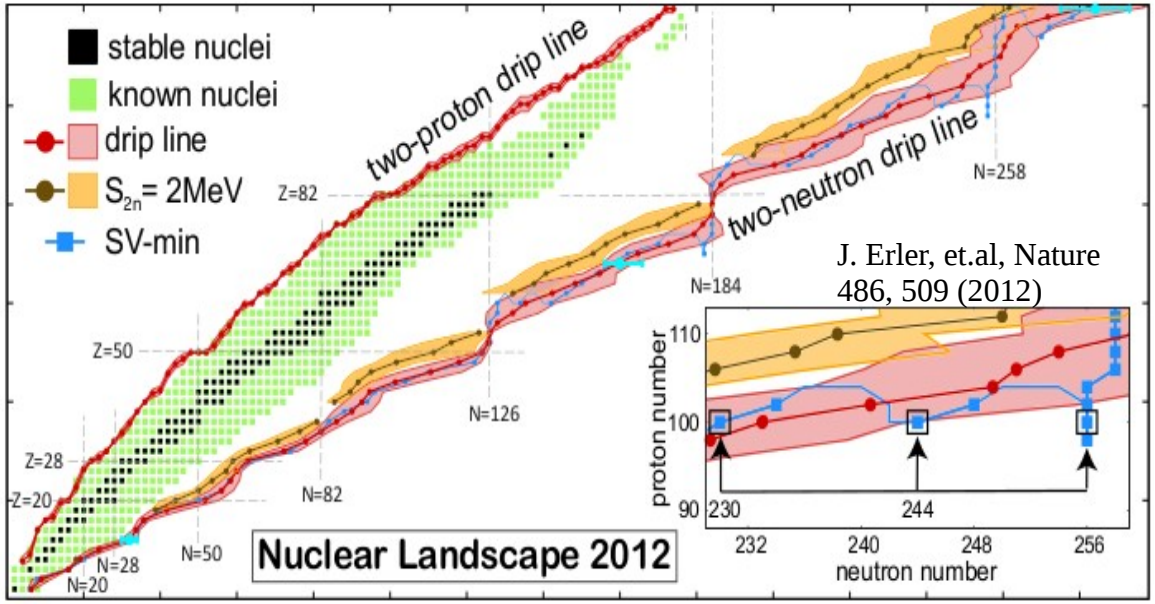
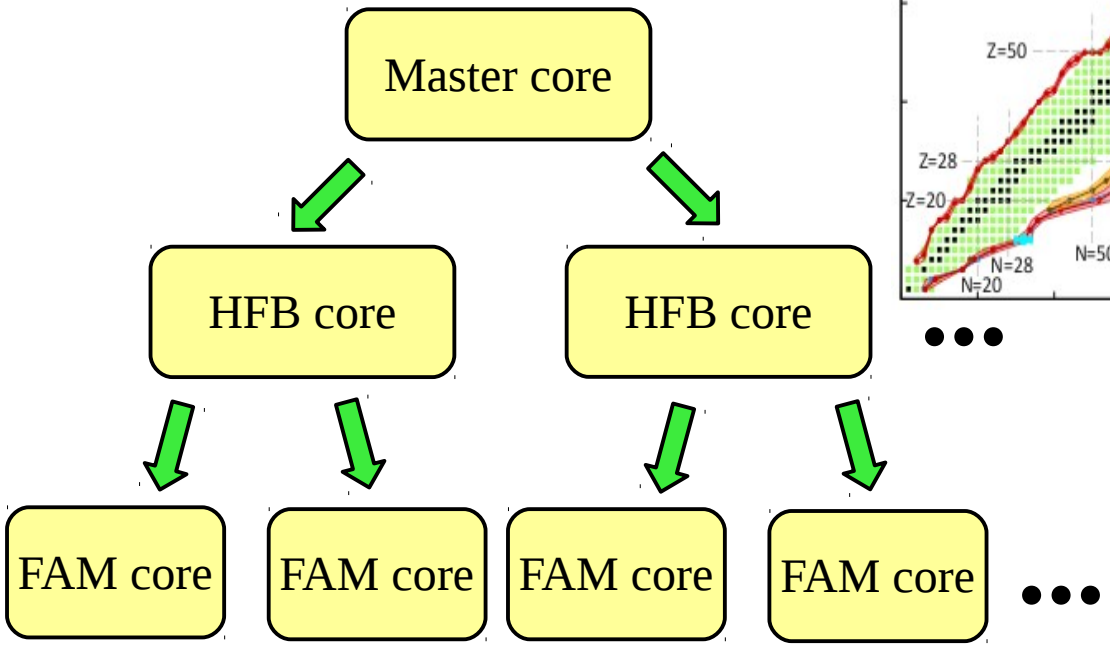
Parallelization of the FAM-QRPA



J. Erler, et.al, Nature 486, 509 (2012)



- New K ≠ 0 mode code requires substantially more CPU time
- MPI setup under construction, which would allow large scale surveys across the nuclear chart
- Can be parallelized (rather) trivially

Conclusions & Outlook

- Implementation of K $\neq$ 0 modes into the HFBTHO currently in progress (one time-odd term still missing)
- Computationally K $\neq$ 0 mode takes about two times more CPU time
- Another factor of ~2-8 to old FAM implementation, because densities are calculated from density matrices (instead of left-right method)

- Missing time-odd terms needs to be implemented
- Direct Coulomb may need some improvements: At the moment it is the largest source of discrepancy between K=0 and K=2 modes in spherical nuclei
- Parallelization of the FAM module
- Magnetic transitions
- Novel EDFs and FAM?