Iterative linear response methods for atomic nuclei

Lepton flavour change in nuclei workshop
14 – 17 April 2025
ECT* Trento

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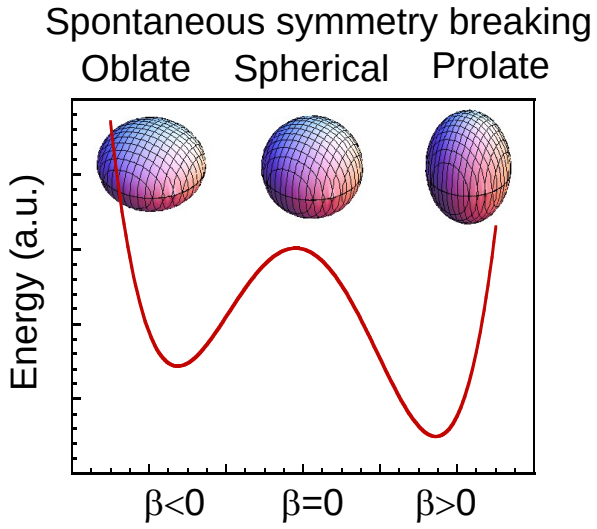
DFT based models (very short recap)

- DFT is presently the only fully microscopical approach which can be applied throughout the entire nuclear chart
- Key element is the energy density functional (EDF). Encodes complex nuclear interactions into energy density
- Parameters of the EDF needs to be adjusted to empirical input. Some parameters better constrained than others. For example, time-odd part of the EDF not so well constrained
- To solve the many-body wave function, one needs to solve Hartree-Fock-Bogoliubov (HFB) equations. This gives quasiparticle states and the self-consistent mean-field.
- HFB equations can be solved by using a set of basis states or in coordinate space

- Spontaneous symmetry breaking important element.
  Allows to incorporate various correlations into the wave-function.
  Example: nuclear deformation
- In principle, symmetries broken at mean-field level should be restored. This is computationally costly and often neglected.



- Many methods to access excited states.
- This presentation focuses only on the linear response theory.
- See also talk by Jacek Dobaczewski

HFB equations

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

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

  where *h* and Δ are the nuclear mean field and pairing field. λ denotes chemical potential.
- By solving this equation, we obtain the quasiparticle energies E_k and the matrices *U* and *V* which determine the generalized Bogoliubov quasiparticle transformation and the HFB vacuum state

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \,, \quad \beta_k |\mathrm{HFB}\rangle = 0$$

- Nuclei with odd particle number are described as having one quasiparticle atop of the HFB vacuum:

$$\beta_k^\dagger |\mathrm{HFB}\rangle$$

- In this case, the effect of blocking needs to be taken into account when solving HFB eq.

Some terminology

- Linear response approach is sometimes referred as a random-phase-approximation (RPA)
- The RPA was developed at early 1950's by Bohm and Pines. In they work, they considered collective plasma oscillations in electron gas.

- The name "RPA" originated from one of their four requirements for collectivity assumption. Quoting from D. Bohm and D. Pines, Phys. Rev. 82, 625 (1951):

> (3) We distinguish between two kinds of response of the electrons to a wave. One of these is in phase with the wave, so that the phase difference between the particle response and the wave producing it is independent of the position of the particle. This is the response which contributes to the organized behavior of the system. The other response has a phase difference with the wave producing it which depends on the position of the particle. Because of the general random location of the particles, this second response tends to average out to zero when we consider a large number of electrons, and we shall neglect the contributions arising from this. This procedure we call the "random phase approximation."

- Although the "RPA" is probably not very descriptive for the method, the name got stuck.
- The superfuild version of RPA is called as the quasiparticle-RPA (QRPA)

QRPA in search for physics beyond the SM

- Many experiments which search for physics beyond the standard model use atomic nucleus as a laboratory
- For this reason precise, nuclear structure input is required

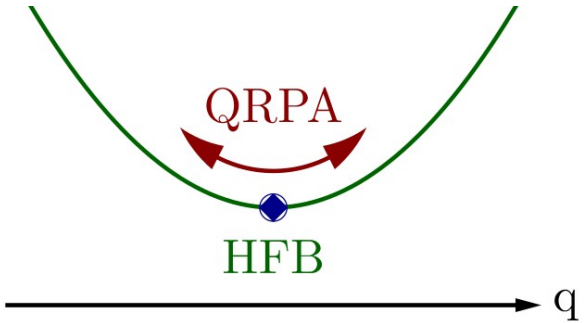
- QRPA has been used to model nuclear structure for such cases. An (incomplete) list:
  - Neutrinoless double-beta-decay: Connected to neutrino mass and its type (Dirac or Majorana mass)
  - Nuclear Schiff moment: Connected to search for electric dipole moment
  - Nuclear anapole moment: Originating from parity nonconserving interactions
  - WIMP-nucleus scattering (within MQPM framework): Direct search of dark matter
  - Muon-electron conversion

Linear response

- To access dynamical properties of the superfluid nuclei, in the framework of nuclear DFT, linear response (that is, the QRPA) is one of the most often employed method
- There are numerous ways to derive the (Q)RPA equations:
  - By using the equations of the motion method.
  - By starting from the time-dependent Hartree-Fock (for RPA) or HFB theory (for QRPA), and taking a small amplitude limit.
  - By linearizing two-particle two-hole excitations (RPA)
  - From perturbation theory with Green's functions, by considering certain kind of diagrams.

- All these lead to the same set of equations
- Essentially linear response (or QRPA) describes small amplitude oscillations around the HFB state

QRPA oscillations around the HFB state (schematically)

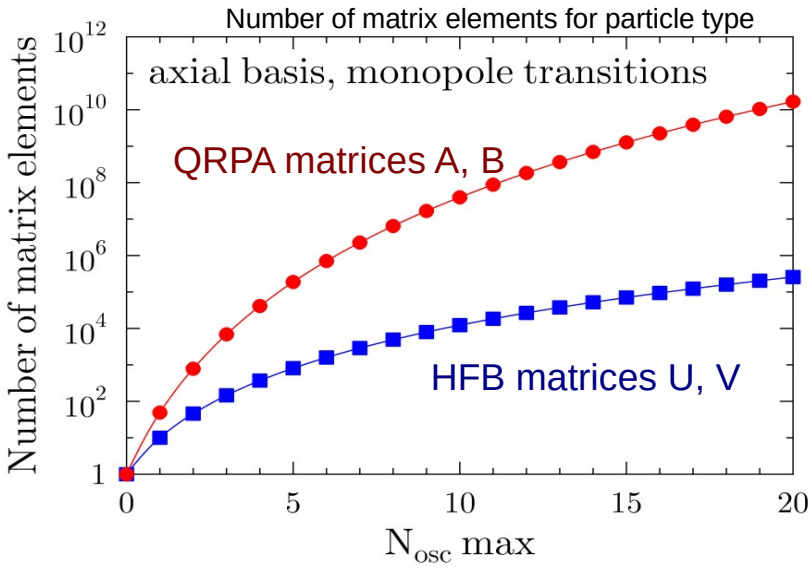


Why to use iterative linear response methods?

- In the past, the QRPA has been often formulated in its matrix form
- 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, described with X and Y amplitudes



- Unfortunately, computational cost of matrix QRPA becomes huge when spherical symmetry is broken
- This has been usually mitigated by introducing truncations on the used quasiparticle basis (which can lead to other problems)

- To avoid large CPU time cost, iterative linear response methods have been developed.
- Two examples: Finite amplitude method (FAM) and iterative Arnoldi diagonalization.

The finite amplitude method

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

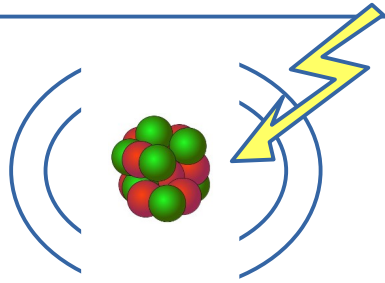
$$i\frac{d\delta\alpha_\mu(t)}{dt} = [H(t), \alpha_\mu(t)]$$

4) Define oscillating part as

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

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

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

7) Introduce a small imaginary width as

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

Solve FAM eqs. iteratively for each ω.

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

At the present, several FAM impelmentations exists, from spherical codes to axial and 3D Cartesian ones, utilizing many different EDF frameworks

FAM and nuclei with an odd particle number

- The FAM method can be also formulated for odd nuclei. This can be done either with exact blocking or with so-called equal filling approximation (EFA)
- The generalized density matrix at the HFB level for odd nuclei is

$$\mathrm{R}_0 = \begin{pmatrix} f & 0 \\ 0 & 1-f \end{pmatrix}$$

where f_i is otherwise zero except 1 for blocked quasiparticle state.

- In EFA f_i = 1/2 for blocked q.p. state and its time-reversed conjugate state.
- EFA, however, does not allow time-odd fields at the HFB level. This prevents computation of some particular operators

- In the normal even-even case, the induced density matrix contains only $\langle\beta^+\beta^+\rangle$ and $\langle\beta\beta\rangle$ type of terms.

- With additional odd particle, there are also $\langle\beta^+\beta\rangle$ and $\langle\beta\beta^+\rangle$ type of amplitudes, denoted here as *P* and *Q*.

$$\delta R = \begin{pmatrix} P(\omega) & X(\omega) \\ -Y(\omega) & -Q(\omega) \end{pmatrix}$$

- These new amplitudes are solved at the same time with *X* and *Y*, during the FAM iterations. The FAM eqs. are now

$$(E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) = -(1-f_\mu-f_\nu)(\delta H^{20}(\omega) - F^{20})_{\mu\nu}$$
$$(E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) = -(1-f_\mu-f_\nu)(\delta H^{02}(\omega) - F^{02})_{\mu\nu}$$
$$(E_\mu - E_\nu - \omega)P_{\mu\nu}(\omega) = -(f_\nu-f_\mu)(\delta H^{11}(\omega) - F^{11})_{\mu\nu}$$
$$(E_\mu - E_\nu + \omega)Q_{\mu\nu}(\omega) = -(f_\nu-f_\mu)(\delta H^{\bar{1}\bar{1}}(\omega) - F^{\bar{1}\bar{1}})_{\mu\nu}$$

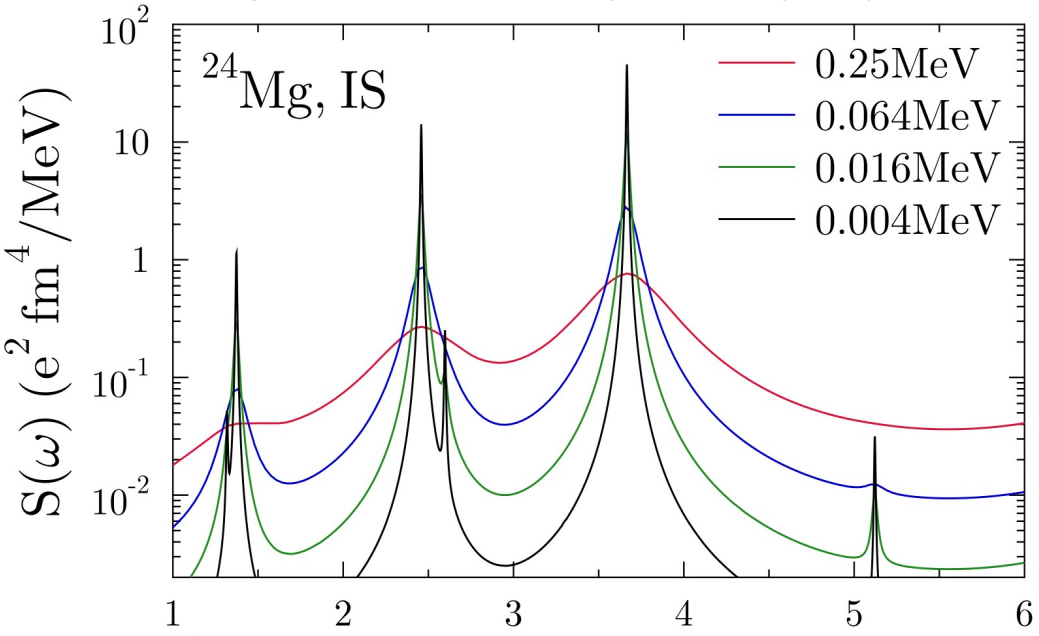
Afaik, no actual implementations yet for exact, self-consistent, blocking case

FAM and discrete low-lying states

- The FAM equations are usually solved with a given imaginary component γ in ω
- Depending on the value of γ, the QRPA poles show up more or less sharp peaks
- By scanning through real part of ω, transition strength function can be computed

- Does not give transitions rates to individual states
- Discrete low-lying states can be accessed via contour integration technique
- Similar technique also for computation of various energy weighted sum rules

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



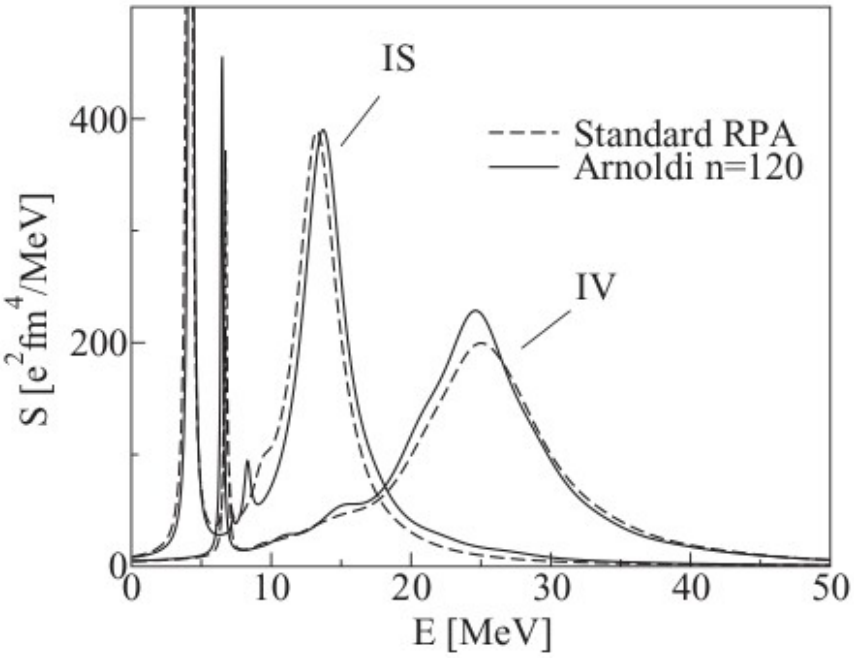
Discrete states: N. Hinohara, M. K., W. Nazarewicz, Phys. Rev. C 87, 064309 (2013)
Sum rules: N. Hinohara, M.K., W. Nazarewicz, E. Olsen, PRC 91, 044323 (2015)

Iterative Arnoldi diagonalization

- Another iterative methods is the iterative Arnoldi diagonalization, interoduced in J. Toivanen et al, Phys. Rev. C 81, 034312 (2010)
- Method is based on finding an approximation on eigenvalues and -vectors in Krylov subspace (similarly to non-Hermitian Lanczos method)

- Resulting transition strength approaches to matrix QRPA and FAM ones with increasing number of iterations
- Original formulation for computation of transition strength function. Later, expanded to computation individual states in B. G. Carlsson et al, Phys. Rev. C 86, 014307 (2012)

2+ states in 132Sn. J. Toivanen et al, PRC81, 034312 (2010)



What about beta decays?

- The FAM equations were given as

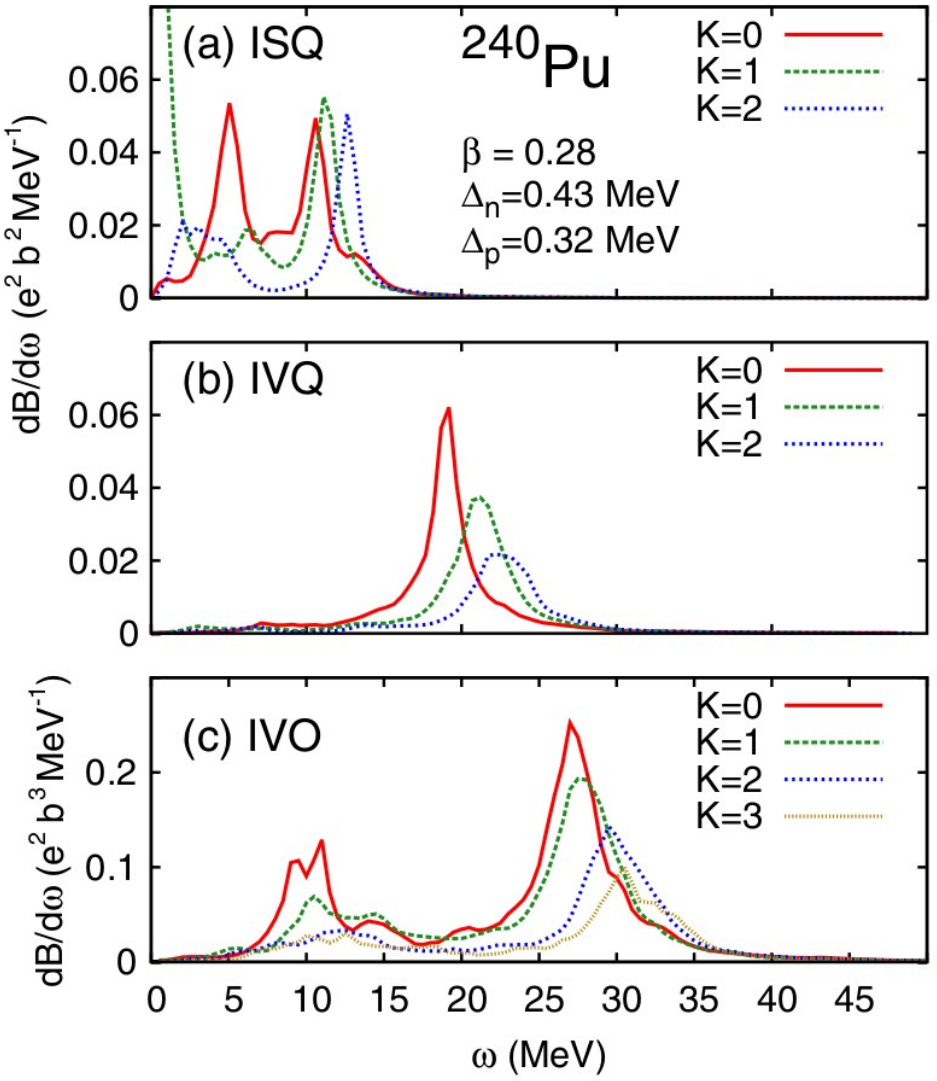
$$(E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) = F^{20}_{\mu\nu}$$
$$(E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) = F^{02}_{\mu\nu}$$

- So far, we have considered like-particle QRPA. That is, we take index μ and ν to be of the same particle type (proton or neutron)
- In this case the FAM describes transitions where initial and final state are in the same nucleus
- Due to nucleon-nucleon interaction in H^{20} and H^{02}, proton and neutron amplitudes are coupled, when solving FAM eqs.

- Beta transitions can be addressed with pnFAM (i.e. pnQRPA)
- In this case, the external field *F* tries to change protons to neutrons or other way around
- One of the indexes in {μ,ν} is a proton index and the other is a neutron index
- In addition to β-decays, pnQRPA can be applied processes such as muon capture or double-beta-decays

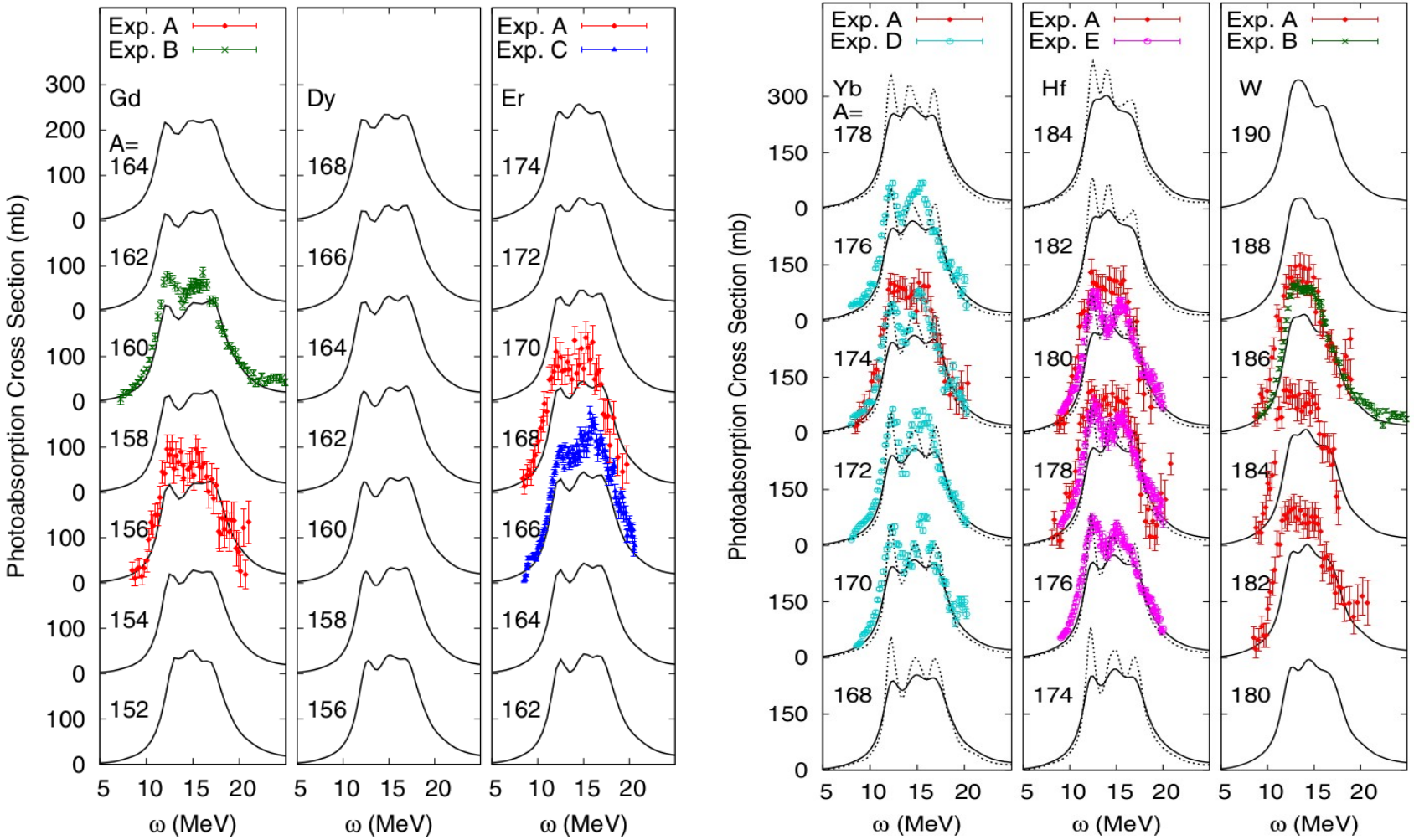
FAM and multipole transition strength functions

- The FAM is very suitable tool to compute transition strength functions. That is, transition strength from the ground state to excited state at energy ω
- The method allows to run calculations for very heavy deformed nuclei without any truncations in the quasiparticle basis with reasonable CPU and memory cost
- Trivially parallelizable: Each value of ω can be run independently in its own MPI process



Transition strength functions (isoscalar quadrupole, isovector quadrupole and isovector octupole) in ^{240}Pu from FAM-QRPA with SLy4. From M.K., et al, Phys. Rev. C 92, 051302(R) (2015)

Photoabsorption in heavy nuclei

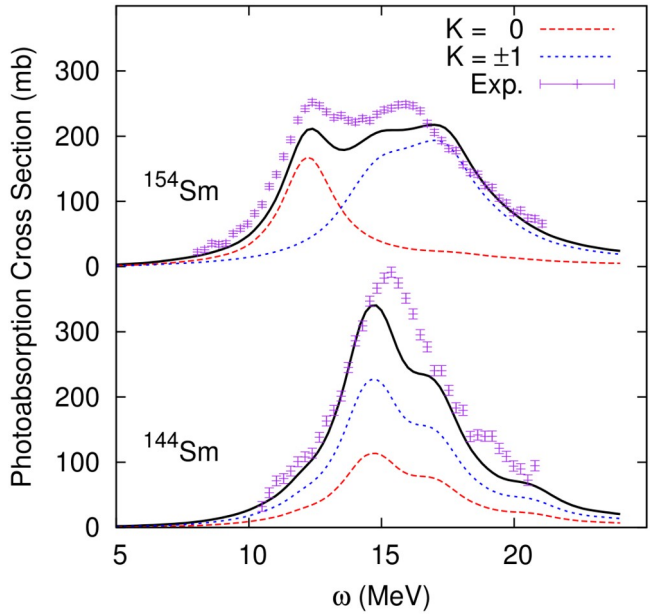


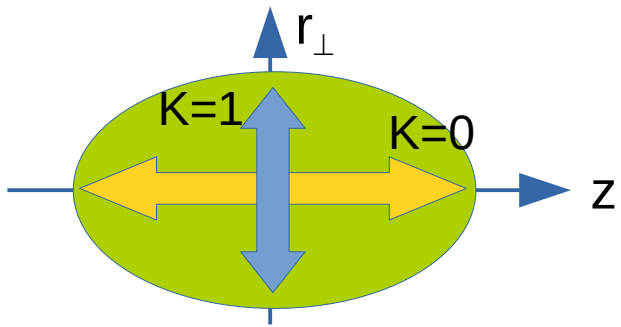
From T. Oishi, M.K., N. Hinohara, PRC 93, 034329 (2016)

Deformation and splitting of giant resonances

- 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.

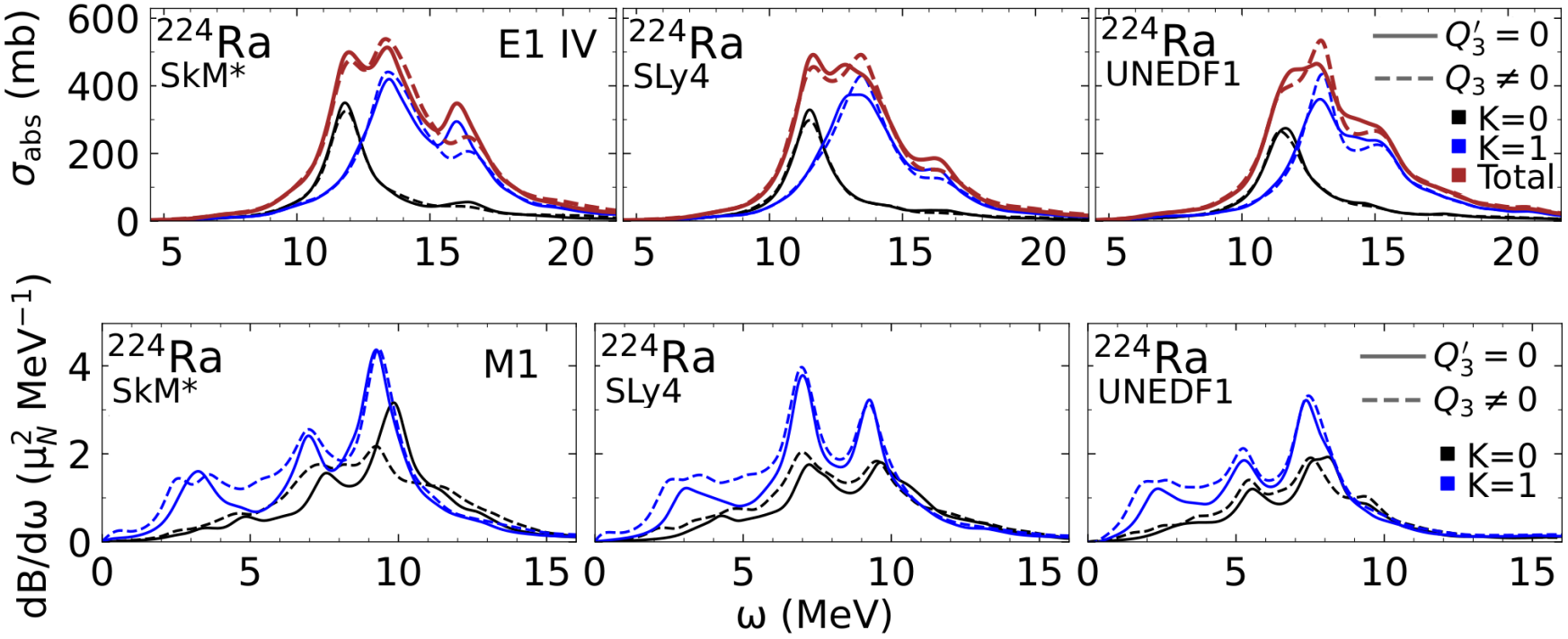
Photoabsorption in Sm isotopes from FAM-QRPA with SkM*. From T. Oishi, et.al, Phys. Rev. C 93, 034329 (2016)





Transition strength function and octupole deformation

- We are currently investigating the impact of octupole deformation (i.e. a pear-shape deformation) on the transition strength functions.
- For photoabsorption cross section, the impact seems to be small. However, for M1 transitions, a notable difference can be seen at the low-lying transition strength
- Work done by Manu Kanerva



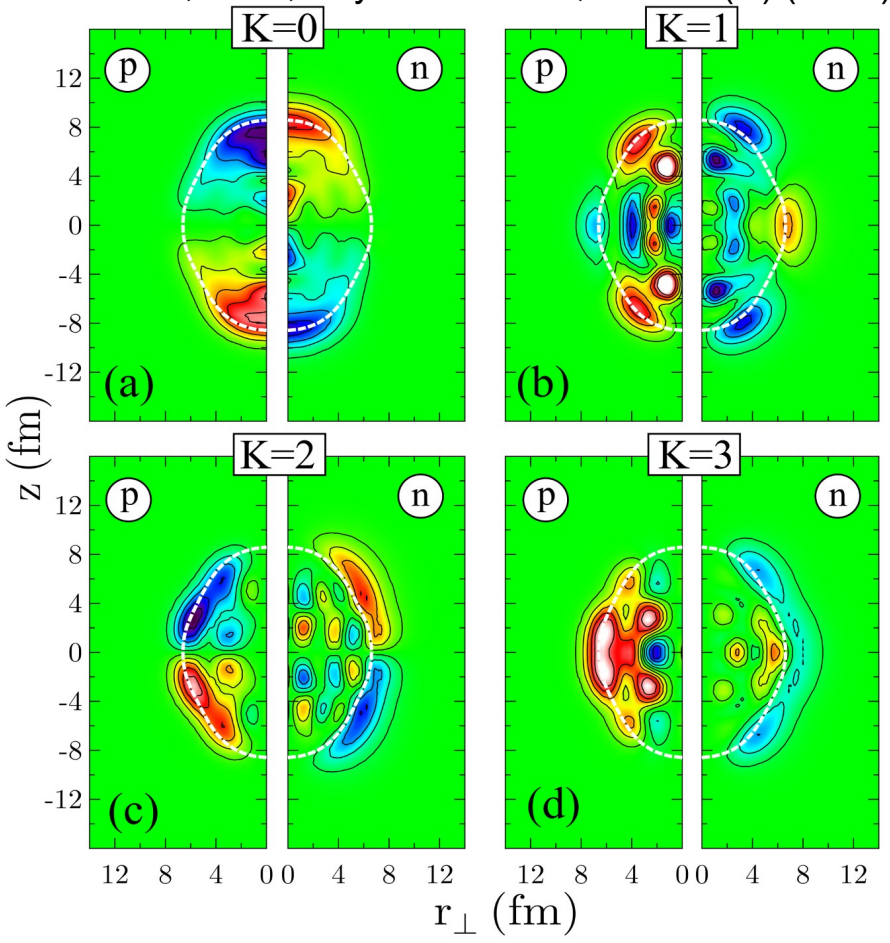
Induced transition densities

- The QRPA corresponds to a small amplitude oscillations around the static HFB density ρ_0.
- The oscillating part of the density is determined by the QRPA amplitudes as

$$\rho_{\mathrm{f}} = UXV^T + V^*Y^TU^\dagger$$

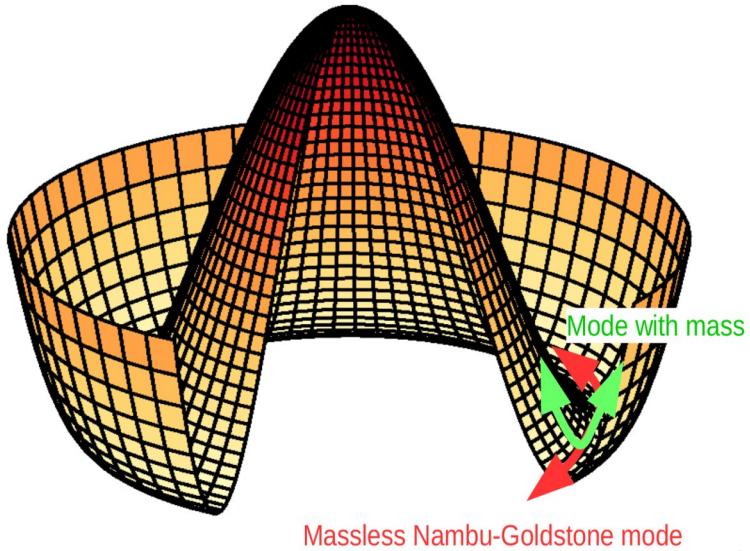
- For example, with isovector octupole operator, the induced transitions densities show a clear octupole-like shapes (see the fig)
- Low-lying iv. octupole modes in 240Pu show collectivity: The induced density covers large portion of the nuclear volume

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

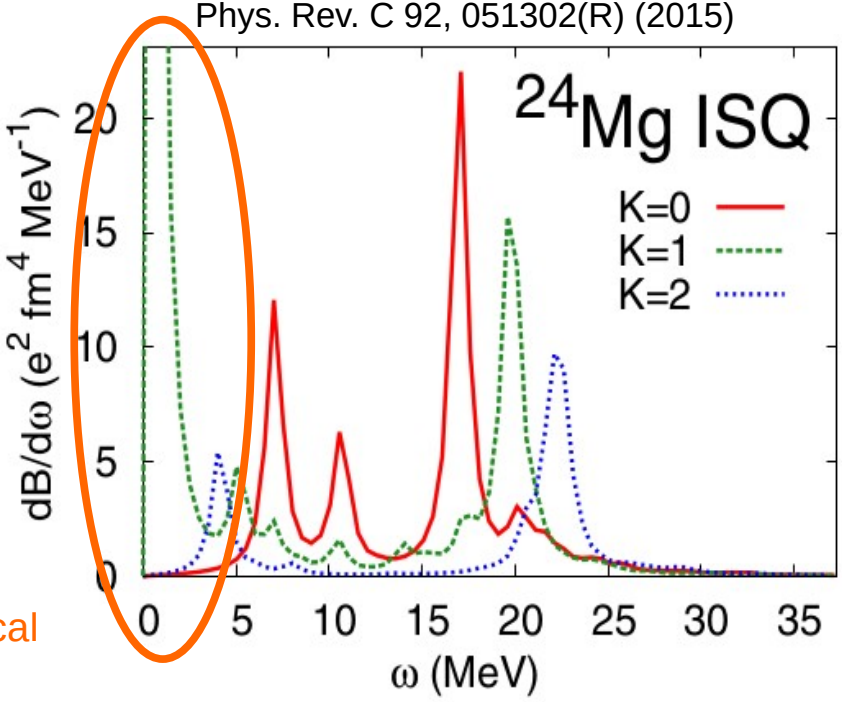


Spurious mode

- If the underlying HFB solution breaks some symmetry, this may cause a spurious QRPA mode to appear
- The spurious mode appears at zero energy
- This corresponds to the well-known Nambu-Goldstone (NG) mode
- The type of the spurious mode depends on which of the symmetry was broken



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

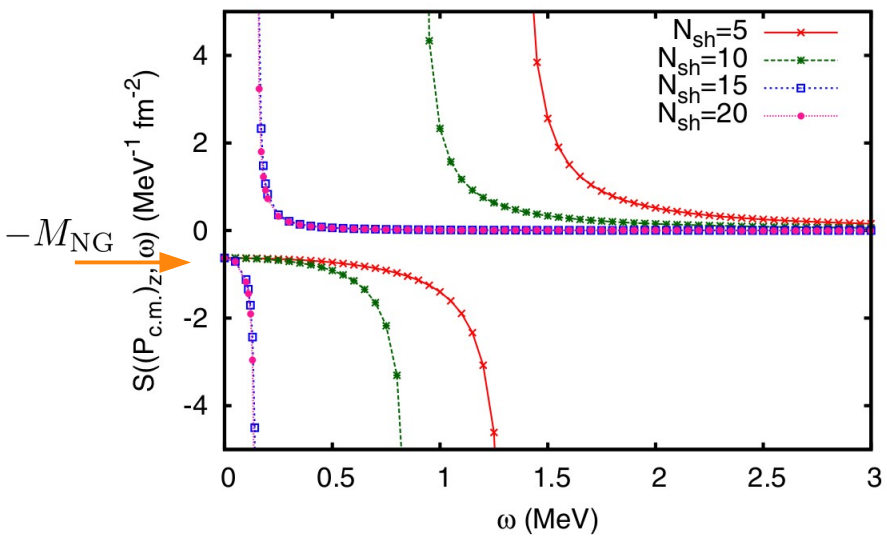


Spurious mode due to breaking of the spherical symmetry

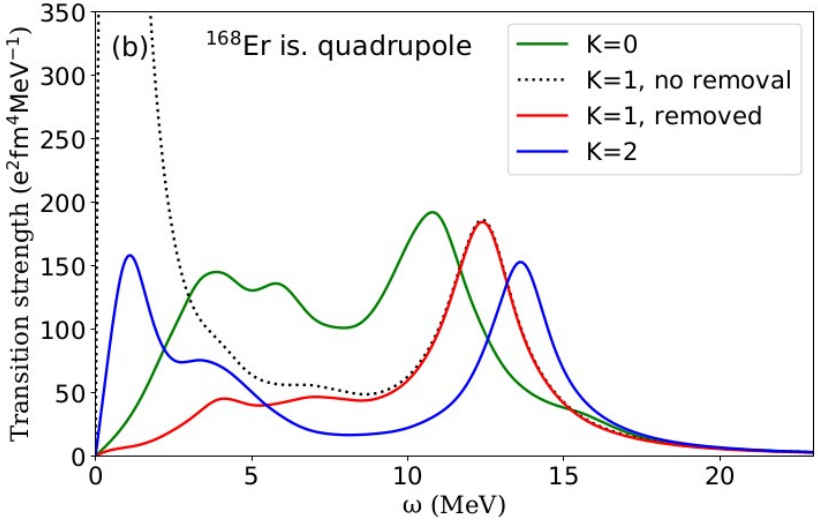
Spurious mode and its removal

- Due to broken translational symmetry, a spurious mode appears with $K^\pi = 0^-, 1^-$ operators. For broken rotation symmetry spurious mode appears with $K^\pi = 1^+$ operators.
- This Nambu-Goldstone mode should be in principle be decoupled from physical modes and be located at zero excitation energy.
- Due to finite size of the basis, spurious mode is located at finite excitation energy $\omega > 0$.
- Spurious mode can be removed from transition strength, leaving only physical modes. However, due to finite basis size, this may not be perfect for more complicated operators

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



Transition strength of isoscalar quadrupole operator before and after removal of the spurious mode. M.K., J. Phys: Conf. Series 1643 012142 (2020)



Thouless-Valatin moment of inertia

- Spurious NG mode can be used to obtain the Thouless-Valatin moment of inertia. It is obtained at $\omega = 0$ from strength function S as

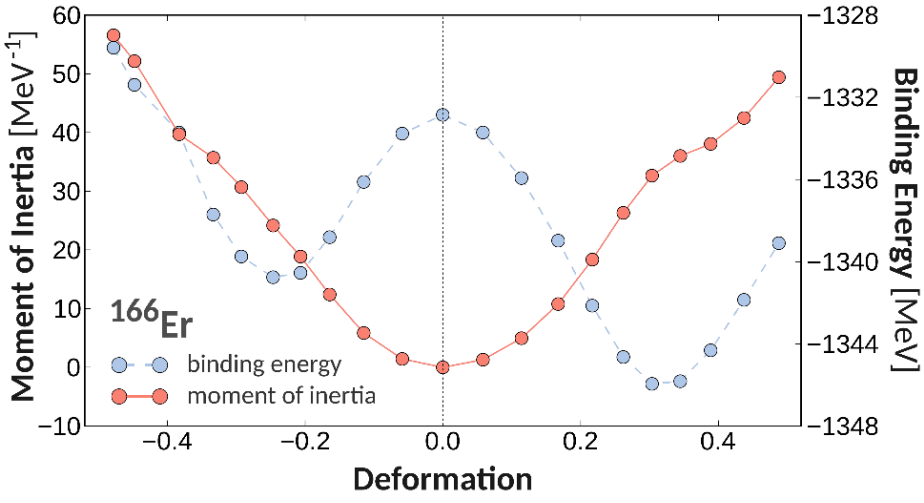
$$-M_{\mathrm{NG}} = S(\hat{P}, \omega = 0)$$

- For example, nuclear deformation breaks rotational symmetry. This leads to appearance of suprious mode on $K^{\pi} = 1^{+}$ channel.
- By applying J_y operator on the FAM calculation, the moment of inertia can be obtained at $\omega = 0$.
- This gives the same result for moment of inertia as cranking calculation.

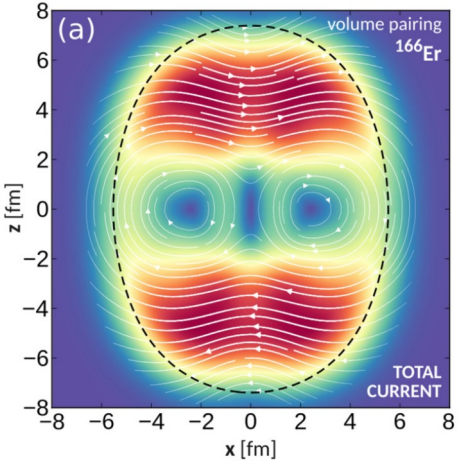
- This method can be used to obtain collective mass parameters for various collective Hamiltonian modes

- Nuclear superfluidity has a notable impact on the moment of inertia

Rotational TV inertia as a function of deformation
K.Petrik, M.K., Phys. Rev. C 97, 034321 (2018)



Superfluid flow in ^{166}Er, coming from the response to J_y operator.
PRC97, 034321 (2018)



Beyond QRPA: quasiparticle-vibration coupling

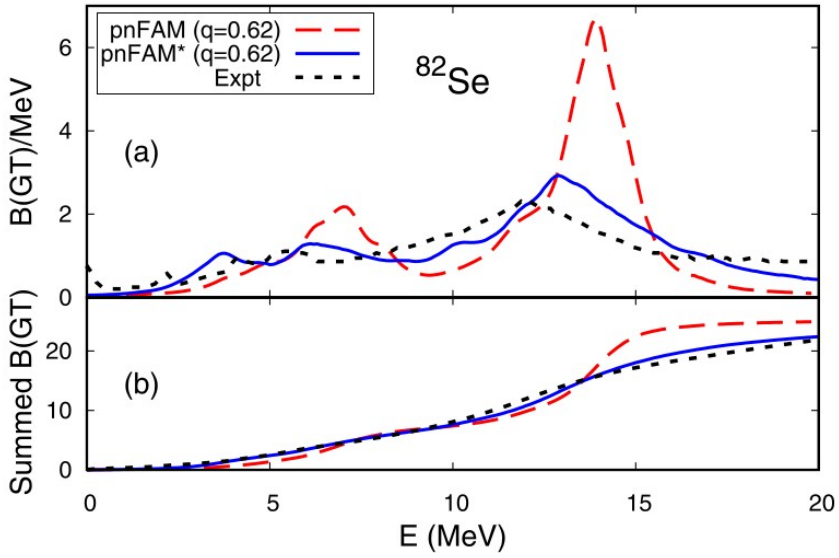
- As was earlier discussed, QRPA corresponds to small amplitude oscillations (i.e. assumption of adiabaticy)
- However, this assumption may not work well at the higher frequency

- We have recently studied the impact phonon coupling in pnFAM for Gamow-Teller (GT) transitions
- In this formulation, the like-particle FAM amplitudes are used to construct a “spreading matrix” *W*, generating an additional term on FAM eqs:

$$[\tilde{W}(\omega)X(\omega)]_{\pi\nu} = \sum_{\pi'\nu'} \tilde{W}_{\pi,\nu,\pi'\nu'} X_{\pi'\nu'}$$

- The inclusion of the phonon coupling improves the GT transition strength function when compared to experimental results

Gamow-Teller strength distribution with pnFAM and with quasiparticle-vibration couling included (pnFAM*)



See details in:
Q. Liu, J. Engel, N. Hinohara, M.K., Phys. Rev C 109, 044308 (2024)

Side note: Nuclear Schiff moment with FAM

- The observation of a non-zero electric dipole moment (EDM) in an atom ground state would implicate a violation of charge-parity (CP) symmetry, originating from a beyond standard model physics
- Various extensions of the standard model predict a much larger CP symmetry violation than present in the standard model. Presently, some of the tightest constraints for CP violation comes from EDM experiments

- Due to the screening effects, the nuclear quantity which induces the atomic EDM is the nuclear Schiff moment. It can be calculated as

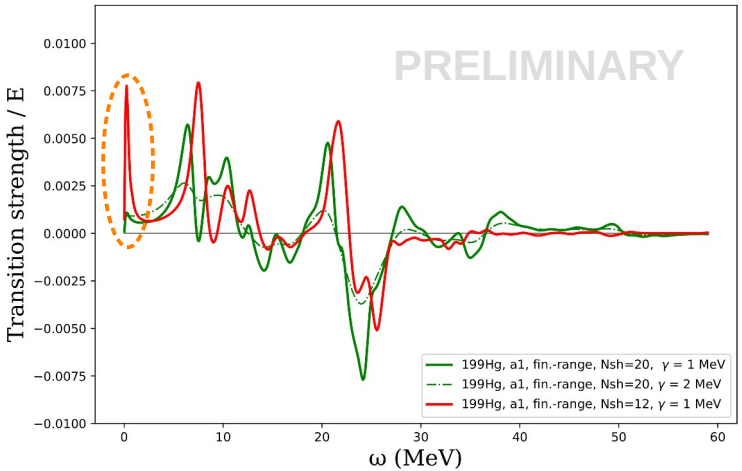
$$S \equiv \langle \Psi_0 | \hat{S}_0 | \Psi_0 \rangle \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_0 | \Psi_i \rangle \langle \Psi_i | \hat{V}_{PT} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.}$$

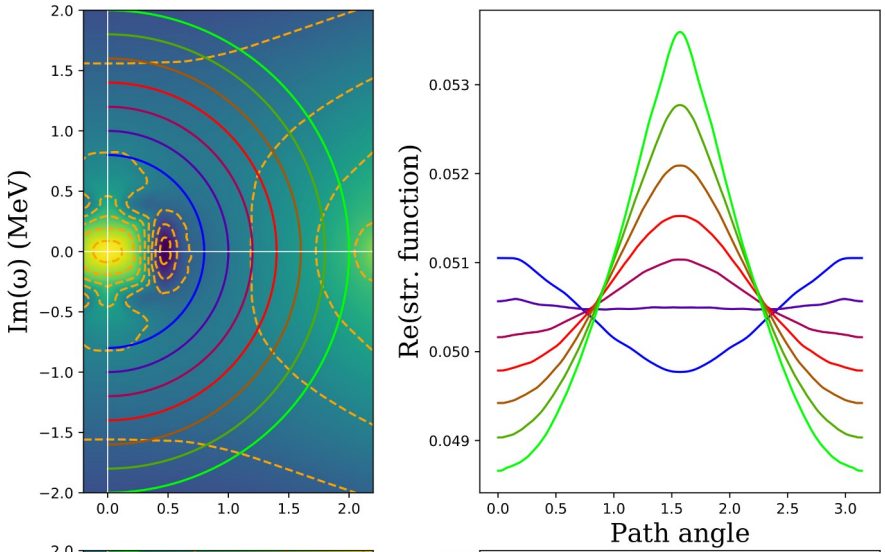
where S_0 is the Schiff operator, V_{PT} is the parity an time-reversal violating interaction, and Ψ_0 is the nuclear ground state

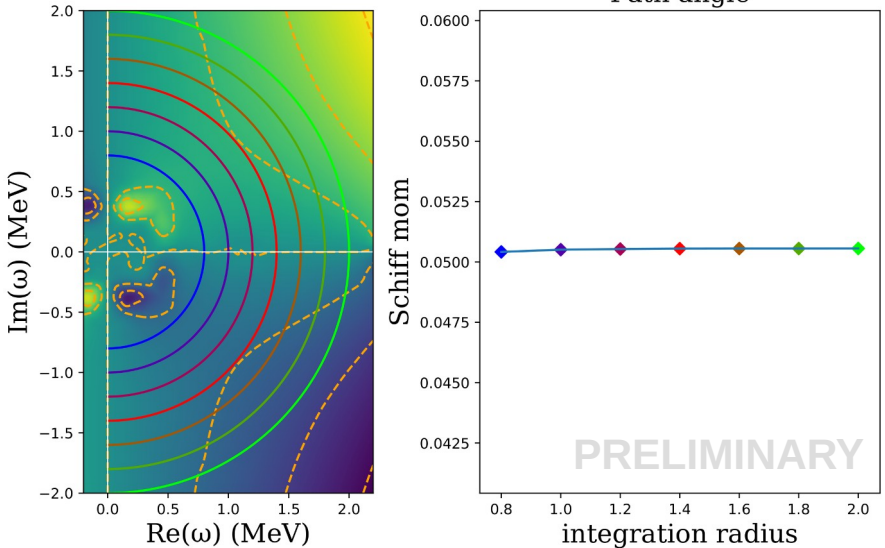
- For certain kind of nuclei the FAM can be used to compute the Schiff moment

Side note: Nuclear Schiff moment with FAM

- Ongoing project, in collaboration with J. Engel, to compute nuclear Schiff moment from linear response theory
- Due to interference of two different operators, the transition strength function oscillates strongly
- A better suited approach is to use the contour integration technique developed for sum rules
- This allows also to circumvent the pole associated to spurious mode







Operators for $\mu^- \rightarrow e^-$ conversion

- The operator connected to nuclear structure aspects in muon-electron conversion is

$$\hat{\boldsymbol{T}}_{\lambda\kappa\gamma,\mu}(qr) = j_\kappa(qr)\left[i^\kappa \boldsymbol{Y}_\kappa(\hat{\boldsymbol{r}})\sigma_\gamma\right]_{\lambda\mu}$$

- This is used to compute vector and axial-vector transition strengths for incoherent part of the process as

$$S_V = \frac{1}{2J_i+1}\sum_f \left(\frac{q_f}{m_\mu}\right)^2 \sum_\lambda |\langle f\|\hat{\boldsymbol{T}}_{\lambda\lambda\gamma=0}\|i\rangle|^2$$

$$S_A = \frac{1}{2J_i+1}\sum_f \left(\frac{q_f}{m_\mu}\right)^2 \sum_{\lambda\kappa} |\langle f\|\hat{\boldsymbol{T}}_{\lambda\kappa\gamma=1}\|i\rangle|^2$$

- Spherical Bessel function $j_k(qr)$ can be approximated as a polynomial when argument qr is not too large.
- Linear response theory is very much suitable for computation of this kind of transition strength functions
- For the ground-state to ground-state part of the process, DFT-based approaches should also work very well

Eqs. from J. Kostensalo et al, PRC 98, 065504 (2018)

Summary

- The linear response theory is a very versatile tool for nuclear structure calculations for various processes
- Iterative linear response methods allow calculations with reasonable CPU and memory cost for heavy deformed nuclei
- In addition to transition strength function, these methods can be used to compute mass parameters microscopically for various collective Hamiltonian models
- Nuclei with an odd particle number not much yet addressed with linear response methods. They would offer many interesting opportunities
- Ongoing project to compute nuclear Schiff moment
- FAM could be utilized for nuclear structure calculations for the $\mu^- \rightarrow e^-$ conversion process

Backup slides

Spurious mode and its removal

- Physical FAM amplitudes can be obtained from calculated ones by removing spurious component as

$$X^{\rm phys}_{\mu\nu} = X^{\rm cal}_{\mu\nu} - \lambda_P \hat{P}_{\mu\nu} - \lambda_Q \hat{Q}_{\mu\nu}$$
$$Y^{\rm phys}_{\mu\nu} = Y^{\rm cal}_{\mu\nu} + \lambda_P \hat{P}^*_{\mu\nu} + \lambda_Q \hat{Q}^*_{\mu\nu}$$

- Here $P \equiv P^{20}$ and $Q \equiv Q^{20}$ are some operators, connected to broken symmetry, with canonical commutation relation

$$[\hat{Q}, \hat{P}] = i$$

- The operator Q may not have an analytical form in all cases. In such kind of situation, it can be obtained from response to *P* operator at zero frequency as

$$\hat{Q} = -i \frac{X(0) + Y^*(0)}{S(\hat{P}, 0)}$$

where $S(P,0)$ is the computed strength function of *P* at ω = 0.

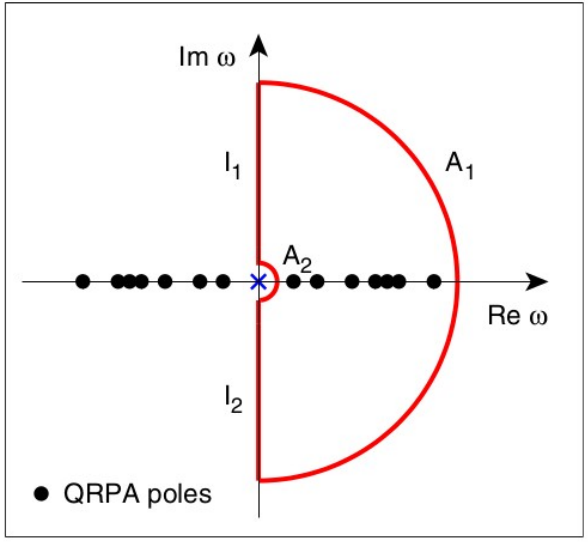
- See more information at N. Hinohara, PRC 92, 034321 (2015)

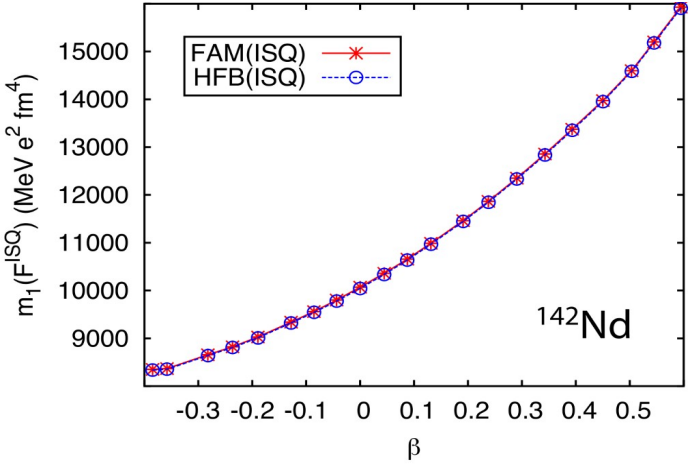
Sum rule method

- Energy weighted 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
- See N. Hinohara, M. Kortelainen, W. Nazarewicz, and E. Olsen, PRC 91, 044323 (2015)

- Depending on the selected energy weight, not all of the parts of the contour are required to be calculated.
- For example, with inverse energy weight, it is actually enough to calculate the smaller arc A_2. Larger arc vanishes due to Jordan's lemma and I_1 and I_2 cancel each other.
- The radius of A_2 should be selected so that the spurious mode is left outside of the contour





Giant resonances

- Giant resonances are small amplitude, high frequency modes, having typically large collectivity. Usually, around the giant resonance energy, there are numerous states close to each other
- Most important ones are the giant dipole, quadrupole and monopole resonances. These can be observed, for example, with photo-nuclear reactions or electron scattering experiments
- Semiclassically, giant resonances can thought to be shape or spin oscillations of neutron and proton matter
- There is no isoscalar dipole resonance, since this would just correspond to movement of the center of mass

Giant dipole resonance, exp. result

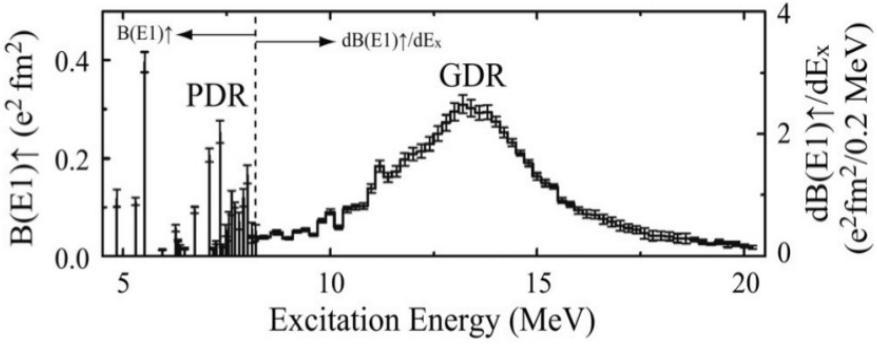


Fig. 5. Total $B(E1)$ strength distribution of ^{208}Pb deduced from the present work. The bump centered at ~ 13 MeV corresponds to the giant dipole resonance, and the strength concentration at around 7–9 MeV to the pygmy dipole resonance.

A. Tamii, et. al., Eur. Phys. J. A 50, 28 (2014)

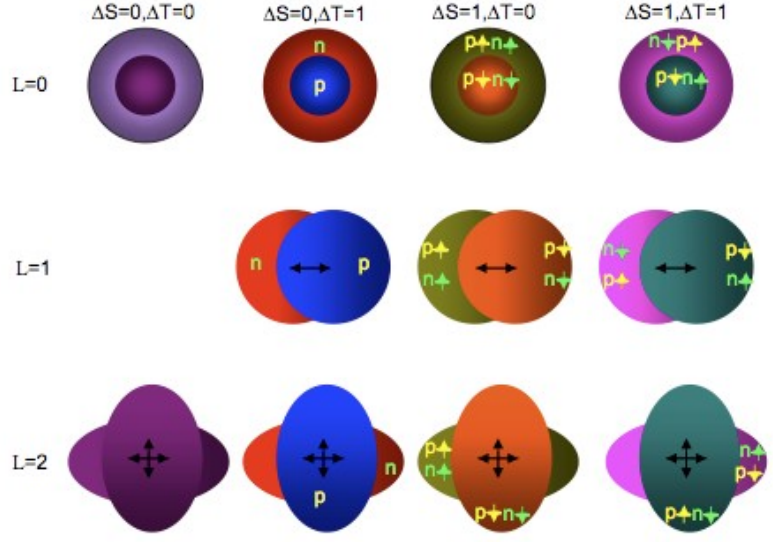


Fig. from Texas A&M Univ., Cyclotron Institute