Calculation of the nuclear Schiff moment from DFT

EDMs: complementary experiments and theory connections
4 – 8 March 2024
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 parameter 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. When HFB equations have been solved, linear response can be used to generate excitations atop of the HFB state
- See talk by Karim Bennaceur

Nuclear Schiff moment

- As discussed in this workshop, various extensions of the standard model predict a much larger CP symmetry violation than present in the standard model. In atomic (or molecular) systems these effects interweave particle, nuclear, atomic and molecular physics.

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

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

- 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. The V_{PT} can be split into 3 + 2 parts, and the Schiff moment is parametrized as

$$S = a_0 g \bar{g}_0 + a_1 g \bar{g}_1 + a_2 g \bar{g}_2 + b_1 \bar{c}_1 + b_2 \bar{c}_2$$

- where a_i and b_i comes from nuclear structure calculation and $\bar{g}_i$ and $\bar{c}_i$ would be fixed from the observed EDM
- Because both operators have negative parity, the summation over *i* runs over opposite parity states compared to ground state.

Operators for Schiff moment

- The operators required for Schiff moment calculation are

$$\hat{S}_0 = \frac{e}{10}\sqrt{\frac{4\pi}{3}}\sum_i \left(r_i^3 - \frac{5}{3}\overline{r_{\rm ch}^2}\, r_i \right) Y_0^1(\Omega_i)$$

  where Y is spherical harmonic and

$$\begin{aligned}\hat{V}_{\rm PT}(\boldsymbol{r}_1-\boldsymbol{r}_2) = & -\frac{g m_\pi^2}{8\pi m_N}\Big\{(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\Big[\bar{g}_0\vec{\tau}_1\cdot\vec{\tau}_2 - \frac{\bar{g}_1}{2}(\tau_{1z}+\tau_{2z}) + \bar{g}_2(3\tau_{1z}\tau_{2z}-\vec{\tau}_1\cdot\vec{\tau}_2)\Big] \\ & -\frac{\bar{g}_1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)(\tau_{1z}-\tau_{2z})\Big\}\frac{\exp(-m_\pi|\boldsymbol{r}_1-\boldsymbol{r}_2|)}{m_\pi|\boldsymbol{r}_1-\boldsymbol{r}_2|^2}\left[1+\frac{1}{m_\pi|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right] \\ & +\frac{1}{2m_N^3}[\bar{c}_1+\bar{c}_2\vec{\tau}_1\cdot\vec{\tau}_2](\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\cdot\boldsymbol{\nabla}\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_2),\end{aligned}$$

- As can be seen, these operators have negative parity. That is, they connect states with opposite parity
- The $\bar{g}_i$ coefficients are related to the finite range part of V_{PT} and $\bar{c}_i$ coefficients to the contact part.

Nuclear Schiff moment and deformation

- As noted, the summation runs over opposite parity states compared to g.s.
- Depending on the nuclear structure, the first opposite parity state can be relatively low or rather high in energy. This has notable impact on the calculated Schiff moment due to the energy denominator $(E_0\text{-}E_i)^{-1}$.

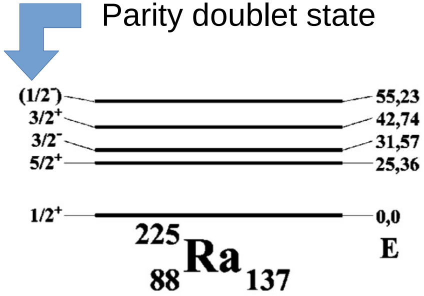
- In octupole deformed nuclei, a parity doublet state can be usually found at very low energy. For example, $1/2^-$ state at 55 keV in ^{225}Ra.
- In such kind of case, the Schiff moment can be approximated as

$$S \approx -2\frac{\langle\Psi_0|\hat{S}_0|\bar{\Psi}_0\rangle\langle\bar{\Psi}_0|\hat{V}_{PT}|\Psi_0\rangle}{\Delta E}$$

- where ΔE is the energy difference between ground state Ψ_0 and its parity doublet state Ψ_0.
- Smallness of energy denominator ΔE can enhance Schiff moment

- For nuclei without octupole deformation, like ^{199}Hg, the first opposite parity state is in much higher energy and summation must run over multiple states
- In this case, the linear response theory (i.e. QRPA) is a suitable method to compute the Schiff moment

Parity doublet state



J. Gasparro et al,
PRC 62 064305 (2000)

#	Nuclide	E_x [keV]	J^{π}_{order}
1	$^{199}_{80}Hg_{119}$	0.0	1/2-
2	$^{199}_{80}Hg_{119}$	158.37859 *10*	5/2-
3	$^{199}_{80}Hg_{119}$	208.20494 *10*	3/2-
4	$^{199}_{80}Hg_{119}$	403.51 *3*	3/2- *2*
5	$^{199}_{80}Hg_{119}$	413.84 *5*	5/2- *2*
6	$^{199}_{80}Hg_{119}$	455.462 *17*	1/2-,3/2-
7	$^{199}_{80}Hg_{119}$	492.297 *18*	3/2- *3*
8	$^{199}_{80}Hg_{119}$	532.48 *10*	13/2+
9	$^{199}_{80}Hg_{119}$	638 *3*	
10	$^{199}_{80}Hg_{119}$	667 *3*	5/2-,7/2-
11	$^{199}_{80}Hg_{119}$	667.4 *9*	1/2,3/2
12	$^{199}_{80}Hg_{119}$	695 ? *3*	

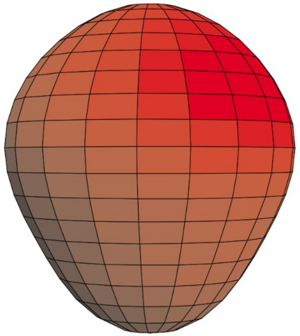
IAEA livechart

Octupole deformation and parity doublet state

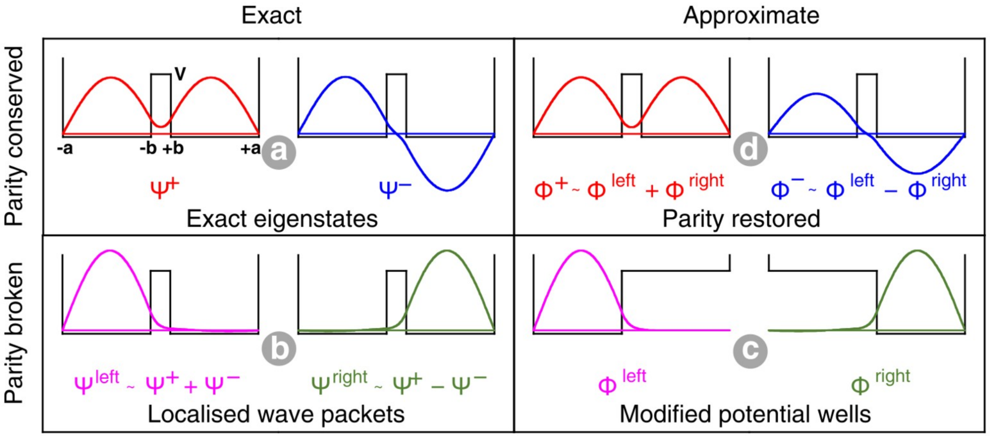
- In the symmetry-broken mean-field picture, octupole deformation shows up as a reflection asymmetric shape.
- Use of parity operator would flip the orientation of the nucleus
- Parity eigenstates can be constructed as

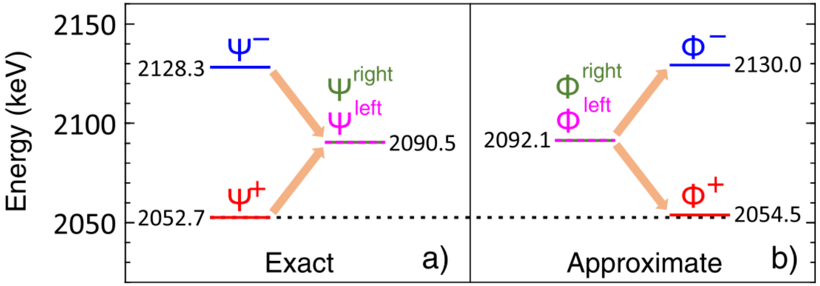
$$|\Phi^{\pm}\rangle = \frac{1}{\sqrt{2 \pm 2\epsilon}}(|\Phi^{\text{left}}\rangle \pm |\Phi^{\text{right}}\rangle)\,, \quad \epsilon = \langle\Phi^{\text{left}}|\Phi^{\text{right}}\rangle$$

- With sufficiently well separated left and right state, the energy difference between Φ^{+} and Φ^{-} states becomes small



Shape of 225Ra. J. Dobaczewski, J. Engel, PRL94, 232502 (2005)





Left: One-dimensional double symmetric potential well and corresponding wave-functions. Right: energies of symmetry broken and conserved states. From J. Sheikh et al, J. Phys. G: Nucl. Part. Phys. 48 (2021) 123001

Schiff moment and octupole deformation

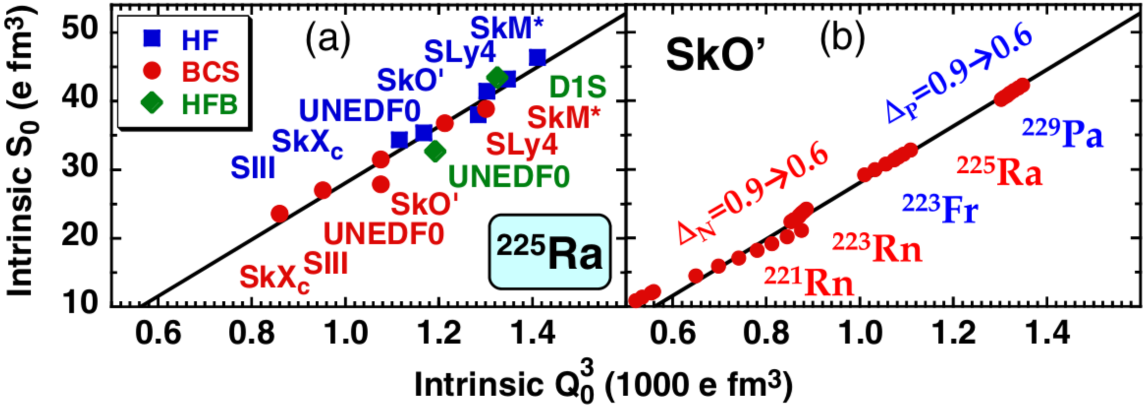
- In octupole deformed nuclei the intrinsic Schiff moment

$$\langle \Psi | \hat{S}_0 | \Psi \rangle$$

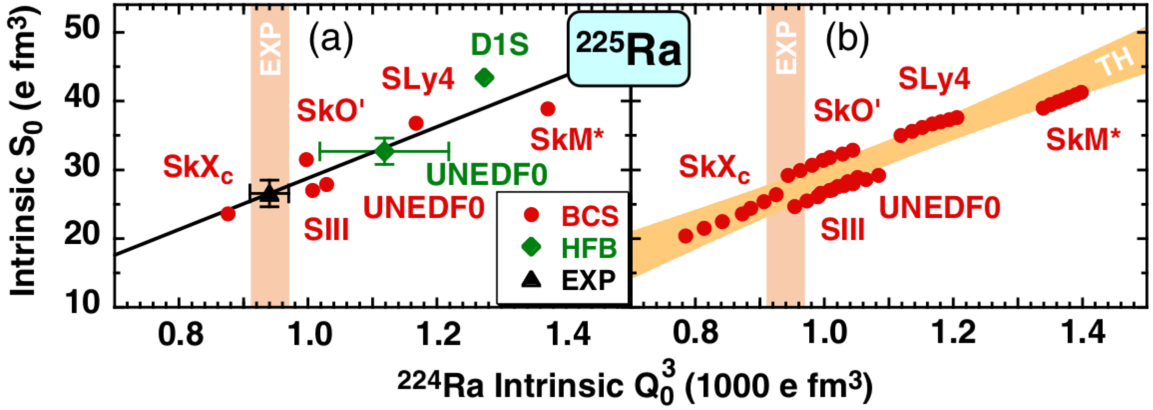
  correlates strongly with the octupole deformation (Q_3 moment)

- The bad thing is that there is deviation with the predicted intrinsic Q_3 value between various EDFs. Hence, deviations with predicted *S*.
- In addition, the strength of pairing correlations have noticeable effect

- The good thing is that intrinsic S_0 correlates strongly with intrinsic octupole moment in neighboring even-even nucleus
- This octupole moment can be estimated from gamma-transitions



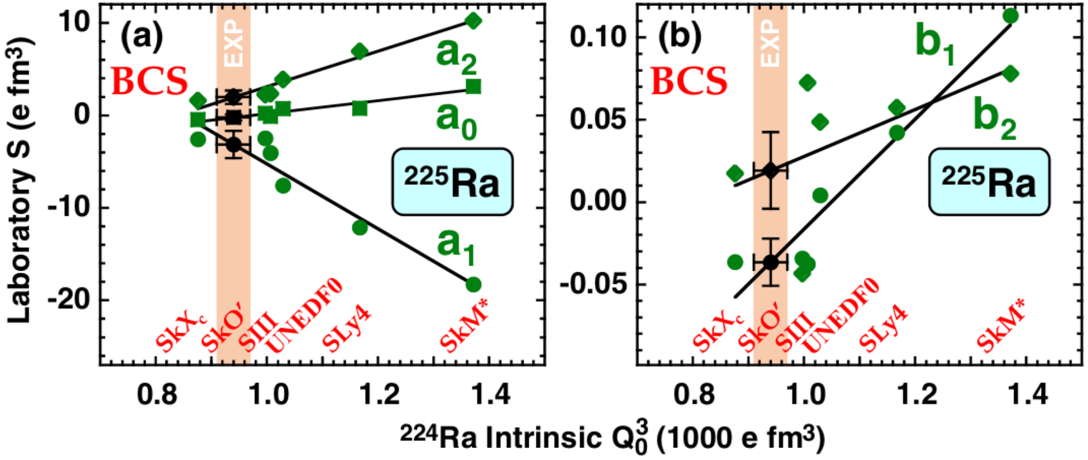
Up: Intrinsic Schiff moment vs intrinsic octupole moment. (a): for 225Ra.
(b): for various isotopes with SkO' EDF.
Below: (b) impact of variation of the pairing gap
J. Dobaczewski, et.al, Phys. Rev. Lett. 121, 232501 (2018)



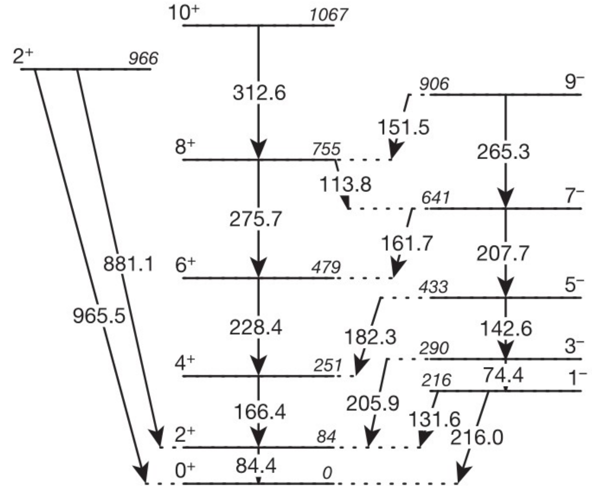
Schiff moment and octupole deformation

- The strong correlation with octupole moment carries out to the calculated Schiff moment in the laboratory frame
- Therefore, calculated Schiff moment value sensitive to octupole deformation properties of the EDF
- Experimental on closely correlated observables could help to reduce theoretical uncertainties

- For more information, see J. Dobaczewski, J. Engel, M.K., and P. Becker, Phys. Rev. Lett 121, 232501 (2018)



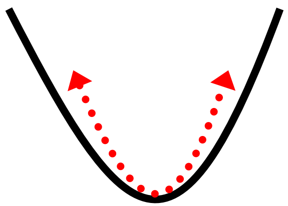
Schiff moment coefficients in 225Ra vs intrinsic octupole deformation in 224Ra for different Skyrme EDFs. J. Dobaczewski, et.al, PRL 121, 232501 (2018)



The level scheme of 224Ra. L.P. Gaffney, et al, Nature 497, 199 (2013).

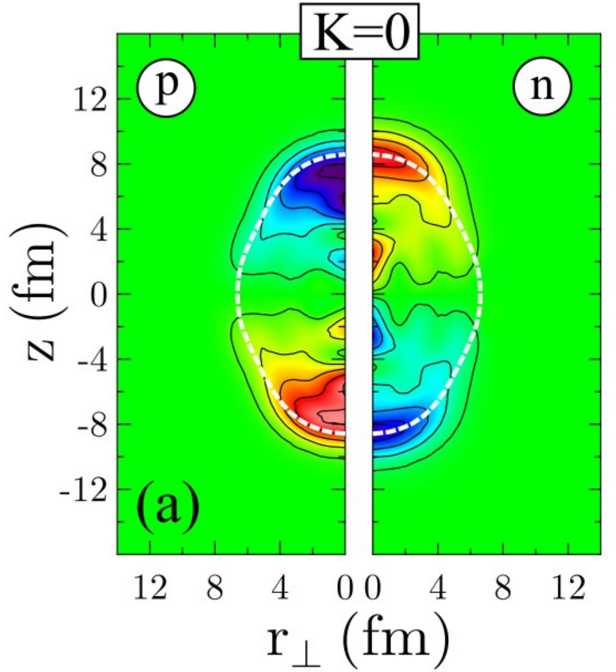
Linear response theory

- For nuclei without reflection asymmetric shape, the calculation includes summation over multiple states. For this kind of case, the superfluid linear response (QRPA) theory is suitable approach



- The QRPA describes small amplitude harmonic oscillations around the underlying mean-field state
- Various ways to derive the QRPA equations. One approach is to consider small amplitude limit of time-dependent Hartree-Fock or Hartree-Fock-Bogoliubov theory
- The time-dependent density matrix can be split to static and oscillating part

$$\rho(t) = \rho^0 + \rho^{(1)} e^{-i\omega t} + \rho^{(1)\dagger} e^{+i\omega t}$$



Oscillating part of density, isovector octupole, 240Pu. M.K., N. Hinohara, W. Nazarewicz, PRC 92, 051302(R) (2015)

- The QRPA excitation modes are now encoded in $\rho^{(1)}$ part.

Linear response theory

- Traditionally, QRPA has been formulated in its matrix form. By diagonalizing the QRPA matrix

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

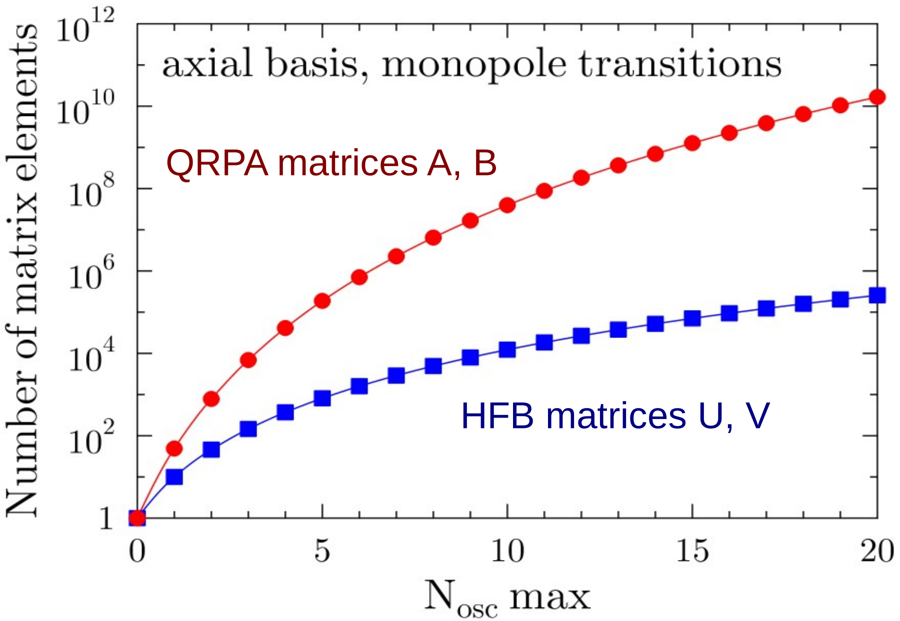
  QRPA eigenmodes are obtained

- When spherical symmetry becomes broken, the size of the QRPA becomes very large leading to steep increase in computational cost.

- To circumvent large numerical cost of MQRPA, two iterative QRPA methods have been developed: The finite amplitude method (FAM) and the iterative Arnoldi method

- The FAM can solve the QRPA problem with a modest CPU and memory cost, without any truncations
- Limitation: In basic formulation, only continuous transition strength function can be solved. Access to discrete states is more complicated

Number of matrix elements as a function of basis size



$\Rightarrow$ Iterative QRPA method required!

FAM-QRPA for odd-A nuclei

- The Schiff moment is usually calculated for odd-*A* nuclei

- In the HFB framework, odd-*A* nuclei can be calculated with quasiparticle blocking procedure. Instead of varying the HFB state, one needs to vary the state

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

  when solving the HFB equations.
- The quasiparticle index *a* is selected from low-lying q.p. states so that, e.g., its angular momentum *z*-projection corresponds the *j* of the nuclear ground state.

- Typically linear response (i.e. QRPA) has been formulated for even-even nuclei.
- The formulation of the odd-*A* QRPA introduces a new set of amplitudes. In addition to *X* and *Y*, *P* and *Q* amplitudes appear due to non-zero expectation values of $\langle b^+ b\rangle$ and $\langle b b^+\rangle$ in oscillating part of the density matrix

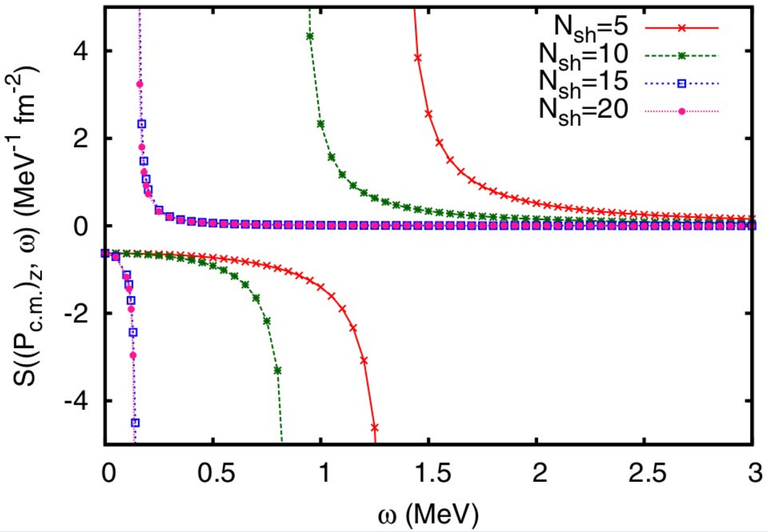
- Current FAM-QRPA implementation consist of HFBTHO code, which solves HFB equations and a FAM module, which is run after HFB calculation

- HFBTHO is limited time-reversal symmetric solutions. The odd-A nuclei are therefore calculated with equal filling approximation. Before FAM iterations, time-odd fields are solved non-self-consistently and HFB matrix is rediagonalized

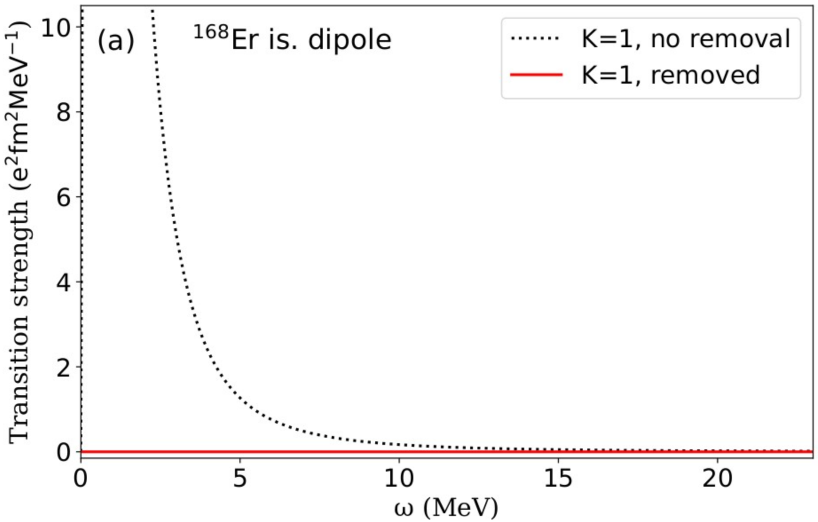
Spurious mode

- Due to broken translational symmetry, a spurious mode appears with $K^\pi = 0^-, 1^-$ 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).



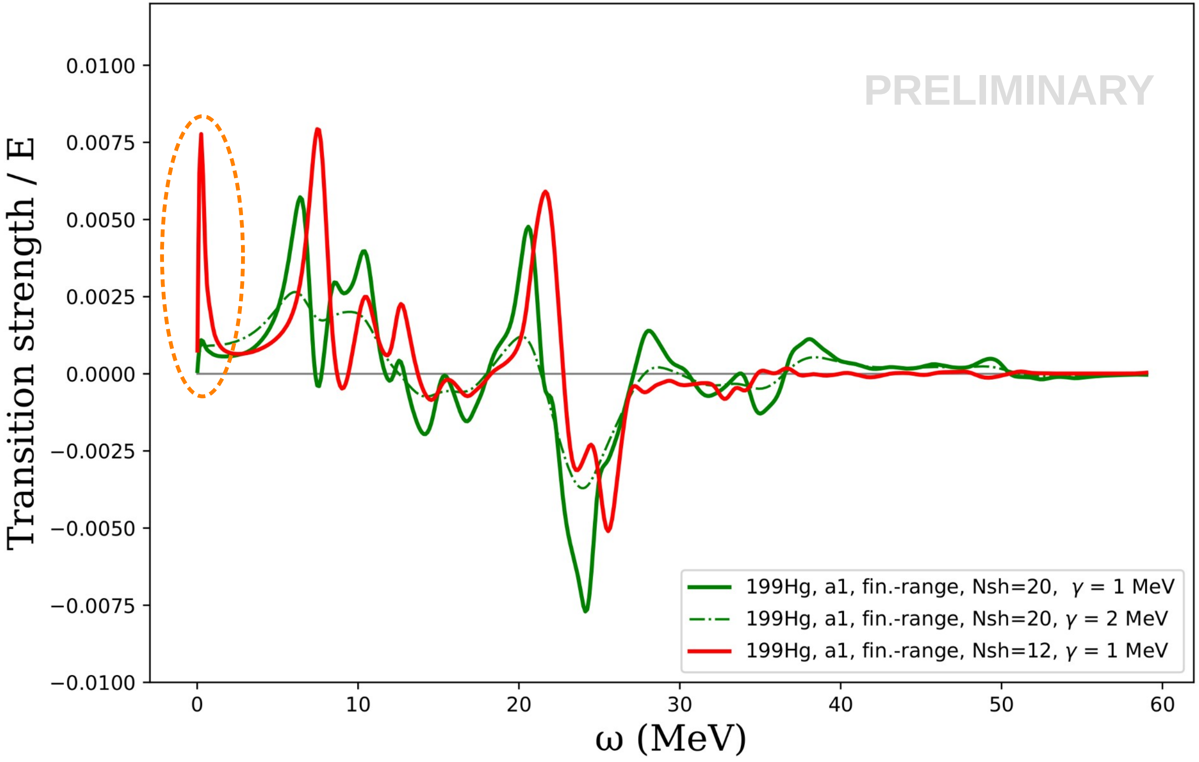
Transition strength of isoscalar dipole operator before and after removal of the spurious mode. M.K., J. Phys: Conf. Series 1643 012142 (2020)



Schiff moment, transition strength

- The calculated transition strength oscillates strongly. (Because of two different operators it can have also negative values)
- Removal of spurious mode only partially successful, although with N_{max} = 20 shells, it is almost completely removed.
- Smoothness depends also on the used width parameter γ.
- Computation of Schiff moment now requires numerical integration over energy ω, which might be prone to numerical error due to oscillating nature of the function.
- Alternative way: use the sum-rule method

Transition strength divided by energy denominator for *a*1 component in ^{199}Hg in units of *e* fm^3 / MeV. Results are with basis with N_{max} = 12 and 20.

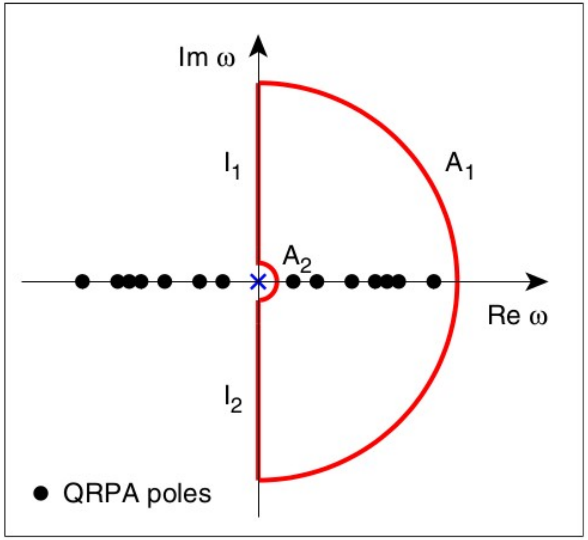


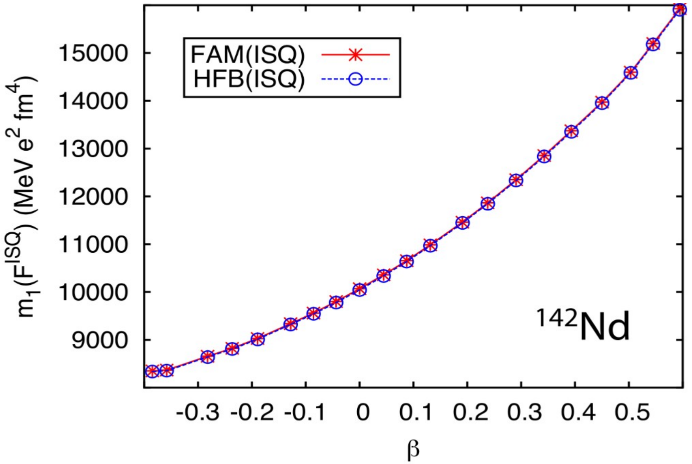
Sum rule method

- 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)

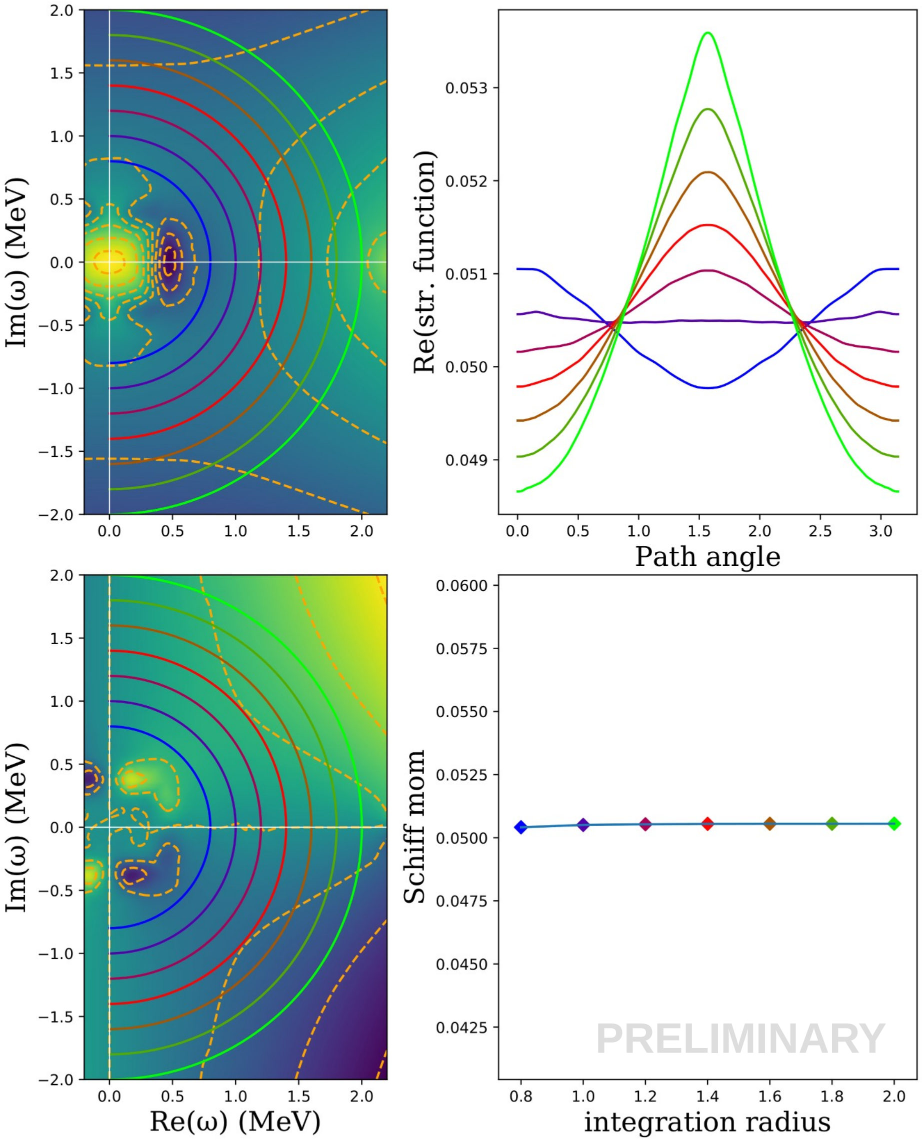
- The Schiff moment is obtained from inverse energy weight.
- It is actually enough to calculate the smaller arc A_2. Larger arc vanishes due to Jordan’s lemma and I_1 and I_2 cancel each other.
- The radius of A_2 should be selected so that the spurious mode is left outside of the contour





Strength function

- The contour integration method allows to circumvent the QRPA pole associated to the spurious center-of-mass motion
- Once outside of this pole, the computed Schiff moment is rather stable as a function of the A_2 radius.
- The figure on right shows real and imag. part of the strength function in the complex plane of energy ω. The arcs show different integration paths for A_2.
- Although the strength function differs for each path, the final result for Schiff moment is quite stable.



Time-odd part of the EDF

- Calculated Schiff moment depends on the EDF parameters, including those on time-odd part of the EDF

- Skyrme EDFs usually adjusted with time-even observables only. The parameters on time-odd part may not be well defined or constrained

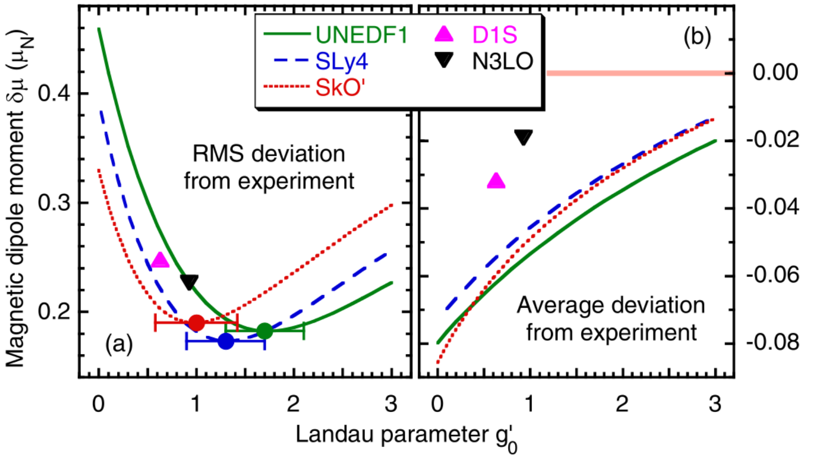
- Alternative way to parametrize time-odd part: Landau parameters
- Recent study on magnetic moments next to doubly-magic nuclei found that typical values are

$$g_0' \sim 1.4$$

- Earlier studies have deduced the other spin-channel parameter to be

$$g_0 \sim 0.4$$

RMS and average deviation of mag. moment as a function of g_0'. P.L. Sassarini, J. Dobaczewski, J. Bonnard, R.F. Garcia Ruiz, J. Phys. G 49 11LT01 (2022)



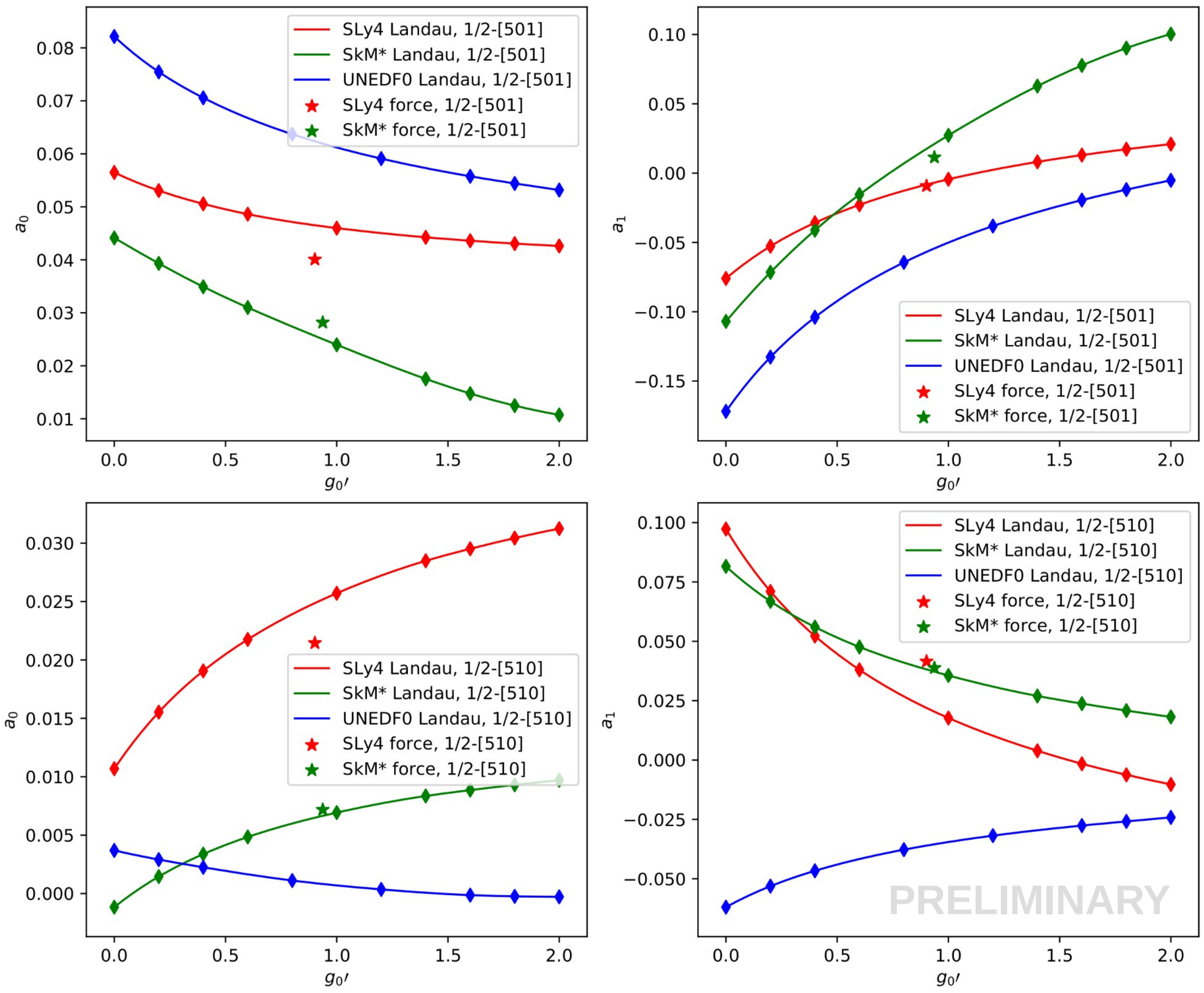
Results for ^{199}Hg

- Calculations as a function of g_0' with SLy4, SkM* and UNEDF0 EDFs. Also, results for SLy4, SkM* when time-odd part treated as in Skyrme force

- Two possible $K^\pi = 1/2^-$ blocking candidates in 199Hg: $1/2^-[501]$ and $1/2^-[510]$

  Results for these differ substantially

- Schiff moments behaves rather smoothly as a function of the Landau parameter. However, they also depend rather strong on it



Earlier results for ^{199}Hg

- Earlier calculations for 199Hg are summarized on table on right

- QRPA results from J.H. de Jesus and J. Engel, PRC 72, 045503 (2005) gave

  a_0 = 0.002 – 0.01 e fm^3
  a_1 = 0.057 – 0.09 e fm^3

  which is similar in magnitude to the results where $1/2^-$[510] state was blocked.
- This was, however, more simple calculation with spherically symmetric QRPA without q.p. blocking at HFB level

- Large scale SM calculations give a notably different result for the first and second $1/2^-$ state

Earlier results for a_i coefficients in ^{199}Hg in units of 10^{-2} e fm^3 from various different calculations. From K. Yanase and N. Shimizu, Phys. Rev. C 102, 065502 (2020).

	a_0	a_1	a_2
IPM ($m_\pi \to \infty$)	7.3	7.3	14.7
IPM	8.4	8.4	16.7
LSSM ($m_\pi \to \infty$)	8.8	9.2	19.0
LSSM	**8.0**	**7.8**	**14.7**
LSSM ($J^\pi = \frac{1}{2}{}^-_2$)	−0.05	0.4	1.3
IPM ($m_\pi \to \infty$) [36]	8.7	8.7	17.4
IPM ($m_\pi \to \infty$) [37,38]	5.8	5.8	11.6
IPM [37,38]	8.6	8.6	17.2
RPA [37,38]	0.04	5.5	0.9
IPM [39]	9.5	9.5	19.0
QRPA [39]	0.2 ↔ 1.0	5.7 ↔ 9.0	1.1 ↔ 2.5
HFB (SLy4) [40]	1.3	−0.6	2.4
HFB (SkM*) [40]	4.1	−2.7	6.9

Conclusions

- Various ways to compute nuclear Schiff moment with DFT based approachs
- With octupole deformed nuclei, strong enhancement of Schiff moment due to low-lying parity doublet state. Also, strong correlation with octupole moment and Schiff moment
- Linear response theory can be used for reflection symmetric nuclei. Requires its formulation for odd-*A* nuclei
- Spurious mode and strongly oscillating nature of the transition strength function poses a problem. This can be solved with the contour integration technique
- Obtained results depend on selection of the blocked q.p. state and parameters on the time-odd part of the EDF
- Things to consider in the future:
  - Remove equal filling approximation from HFB with linear response
  - Angular momentum and parity projection for octupole deformed nuclei
  - Use finite range based EDF
  - Proper uncertainty quantification (EDF parameters)

Schiff moment calculations with FAM-QRPA in collaboration with J. Engel

Backup slides

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

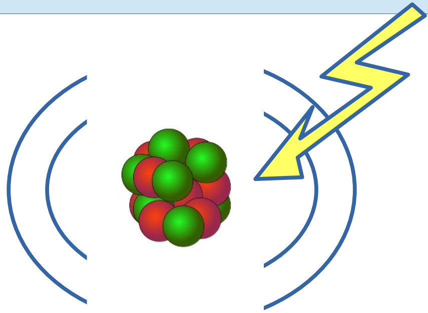
$$i\frac{d\delta\alpha_\mu(t)}{dt} = [H(t), \alpha_\mu(t)]$$

4) Define oscillating part as

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

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

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

Solve FAM eqs. iteratively for each ω.

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

FAM-QRPA for odd-A nuclei

- The Schiff moment requires formulation of the odd-*A* QRPA. 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 equal filling approx. (EFA) f_i = 1/2 for blocked q.p. and its conjugate state.

- EFA, however, does not allow time-odd fields, which would result to zero Schiff moment.
- Therefore, one should use full blocking

- In present HFBTHO implementation, HFB is first solved with EFA. Before FAM iterations, time-odd fields are solved and HFB matrix is rediagonalized

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

- With additional odd particle, there are also $\langle\alpha^+\alpha\rangle$ and $\langle\alpha\alpha^+\rangle$ 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

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

Thouless-Valatin moment of inertia

- When underlying HFB solution breaks some continuous symmetry, a symmetry restoring Nambu-Goldstone can appear on the QRPA solution

- 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 $\omega = 0$.
- We have showed that this give the same result as cranking calculation.
- This method could be used to obtain collective mass parameters

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