Finite amplitude method for low-lying collective modes and QRPA sum rules

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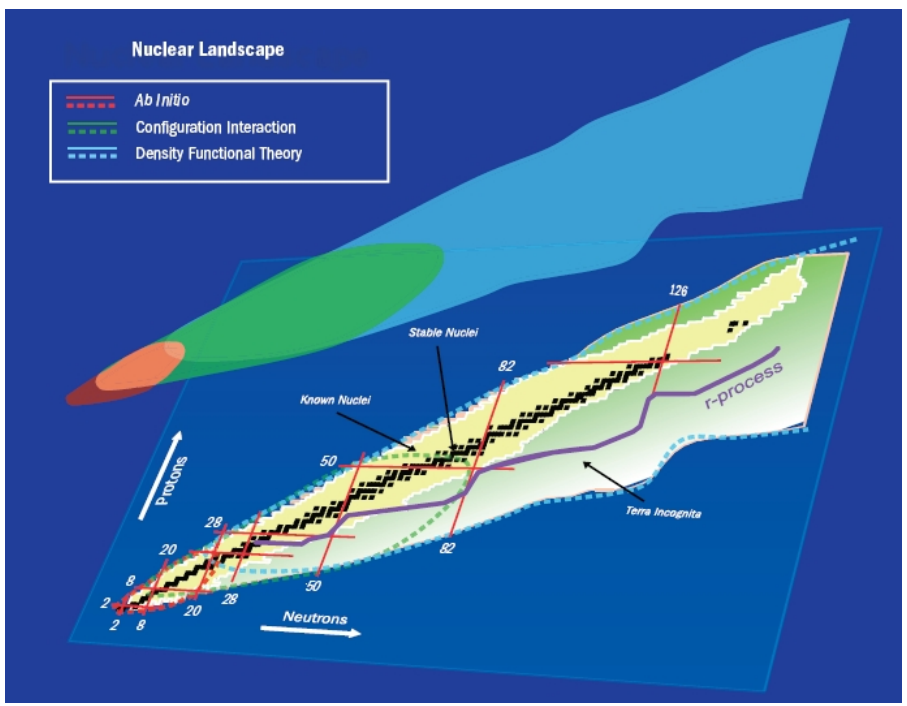
Density functional theory

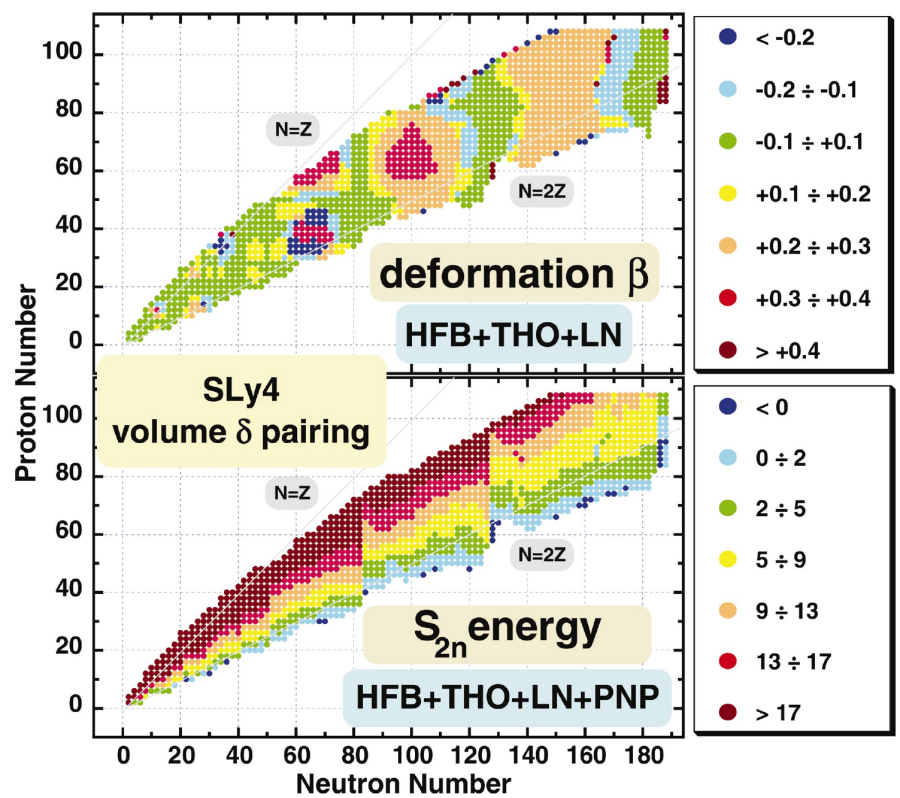
- self-consistent approach for medium/heavy mass nuclei
- universal energy density functionals (UNEDF)

UNEDF2: Kortelainen et al., arXiv:1312.1746

- functionals fitted to ground state and matter properties

ground state properties





Stoitsov et al., Phys. Rev. **C68**,054312 (2003)

Excited States

- Collective/single-particle excitation
  - low-lying state:
    - shell structure, pairing, deformations
  - giant resonances:
    - incompressibility, symmetry energy
  - not used in the functional parameter fitting
    - time-odd coupling constants

- Quasiparticle random-phase approximation (QRPA)
  - small amplitude limit of time-dependent DFT
  - harmonic approximation/linear response
  - matrix formulation: generalized eigenvalue problem
    - diagonalization of two-body residual interaction part
    - requires high-performance computing

QRPA (matrix formulation, MQRPA)

$$\hat{H} = \sum_{ij} t_{ij}\hat{c}_i^\dagger \hat{c}_j + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k \qquad \hat{H}' = \hat{H} - \sum_\tau \lambda^{(\tau)}\hat{N}^{(\tau)}$$

HFB $\quad \hat{a}_\mu |\phi_{\rm HFB}\rangle = 0 \qquad \hat{a}_\mu = \sum_k (V^*_{k\mu}\hat{c}_k^\dagger + U^*_{k\mu}\hat{c}_k)$

$$\hat{H}' = \langle \hat{H}' \rangle + \sum_\mu E_\mu \hat{a}_\mu^\dagger \hat{a}_\mu + \sum_{\mu\nu\mu'\nu'} (\hat{a}_\mu^\dagger \hat{a}_\nu^\dagger \quad \hat{a}_\nu \hat{a}_\mu) \begin{pmatrix} A_{\mu\nu,\mu'\nu'} & B_{\mu\nu,\mu'\nu'} \\ B^*_{\mu\nu,\mu'\nu'} & A^*_{\mu\nu,\mu'\nu'} \end{pmatrix} \begin{pmatrix} \hat{a}_{\mu'}^\dagger \hat{a}_{\nu'}^\dagger \\ \hat{a}_{\nu'}\hat{a}_{\mu'} \end{pmatrix} + \cdots$$

$$= \langle \hat{H}' \rangle + \sum_\mu E_\mu \hat{a}_\mu^\dagger \hat{a}_\mu + \sum_\lambda \omega_\lambda \hat{O}_\lambda^\dagger \hat{O}_\lambda + \cdots$$

QRPA equation (matrix formulation)

$$[\hat{H}', \hat{O}_\lambda^\dagger] = \omega_\lambda \hat{O}_\lambda^\dagger \quad \Longleftrightarrow \quad \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\lambda \\ Y^\lambda \end{pmatrix} = \omega_\lambda \begin{pmatrix} X^\lambda \\ -Y^\lambda \end{pmatrix}$$

$$\hat{O}_\lambda^\dagger = \sum_{\mu\nu} X^\lambda_{\mu\nu}\hat{a}_\mu^\dagger \hat{a}_\nu^\dagger - Y^\lambda_{\mu\nu}\hat{a}_\nu \hat{a}_\mu$$

dimension: $10^{6\text{-}10}$

normalization $\quad \sum_{\mu<\nu} X^\lambda_{\mu\nu} X^{\lambda'*}_{\mu\nu} - Y^\lambda_{\mu\nu} Y^{\lambda'*}_{\mu\nu} = \delta_{\lambda\lambda'}$

heavy calculation using large memory storage for DFT

- Terasaki and Engel, PRC82,034326 (2010)
- Yoshida and Nakatsukasa, PRC83, 021304(R) (2011)
- Losa et al., PRC81,064307 (2010)

Which quantities do we need from QRPA?

(matrix) QRPA solutions

- eigenvalues: excitation energies
- eigenvectors: QRPA two-quasiparticle amplitudes (X,Y)
- strength functions (from X and Y)

- **collective low-lying states**:

  excitation energies, amplitudes of (several) discrete states

- **giant resonances**:

  structure of the strength functions (smeared)

- **sum rules**:

  energies, strength functions of all excited states

Which quantities do we need from QRPA?

(matrix) QRPA solutions

- eigenvalues: excitation energies
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- strength functions (from X and Y)

- **collective low-lying states**: → complex-energy FAM

  excitation energies, amplitudes of (several) discrete states

- **giant resonances**: → original FAM

  structure of the strength functions (smeared)

- **sum rules**: → complex energy FAM

  energies, strength functions of all excited states

Goal: to develop efficient technique for QRPA problems using FAM

Finite amplitude method (FAM)

Nakatsukasa et al., PRC76,024318(2007)

- Talk by Markus (this morning)
- linear response of an external field

- Efficient solution of (Q)RPA:
  without computing two-body residual interactions (AB matrix)
  AB matrix ~ N_{qp}^4, induced field ~ N_{qp}^2
- Easy to implement:
  minor extension to existing HFB code
- No model space truncation at the QRPA level:
  Full two-quasiparticle model space can be used

implementations:

3D-HF-RPA: Nakatsukasa et al (2007) 1D-HFB-QRPA: Avogadro PRC84 (2011)
2D-HFBTHO-QRPA: Stoitsov et al PRC84(2011), pn-QRPA Mustonen et al (2014)
1D-RHF-RPA: Liang et al PRC87(2013), 2D-RHB-QRPA: Niksic PRC88(2014)

technique to compute AB matrix: Avogadro et al PRC87(2013)

FAM

frequency ω fixed during iteration

Nakatsukasa et al., PRC76,024318(2007)

weak time-dependent external field (η: small parameter)

$$\hat{F}(t) = \eta \left\{ \hat{F}(\omega) e^{-i\omega t} + \hat{F}^\dagger(\omega) e^{i\omega t} \right\}$$

$$\hat{A}^\dagger_{\mu\nu} = \hat{a}^\dagger_\mu \hat{a}^\dagger_\nu, \hat{B}_{\mu\nu} = \hat{a}^\dagger_\mu \hat{a}_\nu.$$

$$\hat{F}(\omega) = \frac{1}{2} \sum_{\mu\nu} \left\{ F^{20}_{\mu\nu}(\omega) \hat{A}^\dagger_{\mu\nu} + F^{02}_{\mu\nu}(\omega) \hat{A}_{\mu\nu} \right\} + \sum_{\mu\nu} F^{11}_{\mu\nu}(\omega) \hat{B}_{\mu\nu}$$

TDHFB equation

$$i \frac{\partial \hat{a}_\mu(t)}{\partial t} = [\hat{H}(t) + \hat{F}(t), \hat{a}_\mu(t)]$$

first order in η

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

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

FAM equation

FAM: equivalent to QRPA

oscillation of the quasiparticles

$$\hat{a}_\mu(t) = \{ \hat{a}_\mu + \delta \hat{a}_\mu(t) \} e^{iE_\mu t},$$

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

induced field

$$\hat{H}(t) = \hat{H}_0 + \delta \hat{H}(t) \qquad \hat{H}_0 = \sum_\mu E_\mu \hat{B}_{\mu\mu}$$

$$\delta \hat{H}(t) = \eta \left\{ \delta \hat{H}(\omega) e^{-i\omega t} + \delta \hat{H}^\dagger(\omega) e^{i\omega t} \right\}$$

Advantage of FAM

- avoid using two-body A and B (QRPA) matrices in induced field δH(t)
- iterative solution (no diagonalization)

induced field (one-body, contains information of AB matrices)

$$\delta H^{20}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} \{A_{\mu\nu,\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}\} X_{\mu'\nu'}(\omega) + B_{\mu\nu,\mu'\nu'} Y_{\mu'\nu'}(\omega)$$

$$\delta H^{02}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} B^*_{\mu\nu,\mu'\nu'} X_{\mu'\nu'}(\omega) + \left\{A^*_{\mu\nu,\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}\right\} Y_{\mu'\nu'}(\omega)$$

oscillation of quasiparticles changes the densities

$$\rho(t) = \rho_{\rm HFB} + \eta(\delta\rho(\omega)e^{-i\omega t} + {\rm h.c.})$$

$$\kappa(t) = \kappa_{\rm HFB} + \eta(\delta\kappa^{(+)}(\omega)e^{-i\omega t} + \delta\kappa^{(-)}(\omega)e^{i\omega t})$$

$$\delta\rho(\omega) = UXV^T + V^*Y^TU^\dagger$$

$$\delta\kappa^{(+)}(\omega) = UXU^T + V^*Y^TV^\dagger,$$

$$\delta\kappa^{(-)}(\omega) = V^*X^\dagger V^\dagger + UY^*U^T,$$

induced field is numerically evaluated using finite amplitude ($\eta \sim 10^{-7}$)

$$\delta h(\omega) = \frac{h\left[\rho_\eta, \kappa^{(+)}_\eta, \kappa^{(-)*}_\eta\right] - h\left[\rho, \kappa, \kappa^*\right]}{\eta},$$

$$\delta\Delta^{(+)}(\omega) = \frac{\Delta\left[\rho_\eta, \kappa^{(+)}_\eta, \kappa^{(-)*}_\eta\right] - \Delta\left[\rho, \kappa, \kappa^*\right]}{\eta},$$

$$\delta\Delta^{(-)}(\omega) = \frac{\Delta\left[\rho_\eta, \kappa^{(-)}_\eta, \kappa^{(+)*}_\eta\right] - \Delta\left[\rho, \kappa, \kappa^*\right]}{\eta},$$

$$\delta H^{20}_{\mu\nu}(\omega) = \Big(U^\dagger\delta h V^* - V^\dagger\delta\Delta^{(-)*}V^* + U^\dagger\delta\Delta^{(+)}U^* - V^\dagger\delta h^T U^*\Big)_{\mu\nu}$$

$$\delta H^{02}_{\mu\nu}(\omega) = \Big(-V^T\delta h U + U^T\delta\Delta^{(-)*}U - V^T\delta\Delta^{(+)}V + U^T\delta h^T V\Big)_{\mu\nu}.$$

code for h[ρ] can be based on existing HFB

FAM

need to use complex ω <-> smeared strength function

for real ω, strength function is always zero

$$\frac{dB(\omega,F)}{d\omega} = \sum_{i>0} |\langle i|\hat{F}|0\rangle|^2 \delta(\omega-\Omega_i)$$

$$\frac{dB(\hat{F},\omega)}{d\omega}(\omega_\gamma) = -\frac{1}{\pi}\mathrm{Im}S(\hat{F},\omega+i\gamma) = \frac{\gamma}{\pi}\sum_i \left\{ \frac{|\langle i|\hat{F}|0\rangle|^2}{(\Omega_i-\omega)^2+\gamma^2} - \frac{|\langle 0|\hat{F}|i\rangle|^2}{(\Omega_i+\omega)^2+\gamma^2} \right\}$$

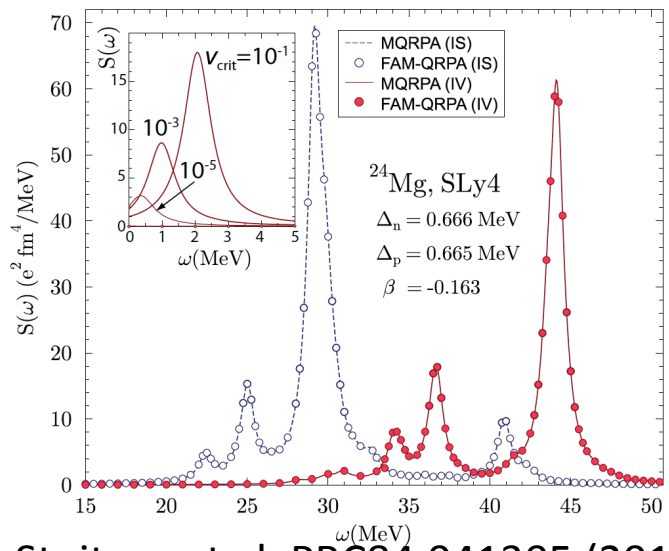
The strength function from FAM

$$S(F,\omega) = \sum_{\mu<\nu} F^{20*}_{\mu\nu} X_{\mu\nu}(\omega) + F^{02*}_{\mu\nu} Y_{\mu\nu}(\omega)$$

$$S(\hat{F},\omega_\gamma) = -\sum_\nu \left\{ \frac{|\langle\nu|\hat{F}|0\rangle|^2}{\Omega_\nu-\omega_\gamma} + \frac{|\langle 0|\hat{F}|\nu\rangle|^2}{\Omega_\nu+\omega_\gamma} \right\}$$

$$X_{\mu\nu}(\omega_\gamma) = -\sum_i \left\{ \frac{X^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega_\gamma} + \frac{Y^{i*}_{\mu\nu}\langle 0|\hat{F}|i\rangle}{\Omega_i+\omega_\gamma} \right\}$$

$$Y_{\mu\nu}(\omega_\gamma) = -\sum_i \left\{ \frac{Y^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega_\gamma} + \frac{X^{i*}_{\mu\nu}\langle 0|\hat{F}|i\rangle}{\Omega_i+\omega_\gamma} \right\}$$



Stoitsov et al, PRC84,041305 (2011)

The imaginary part γ gives the Lorentzian-smeared QRPA width

FAM with fixed width γ: same strength distribution as smeared QRPA

FAM for discrete low-lying states

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

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$$\begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]^{-1} \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

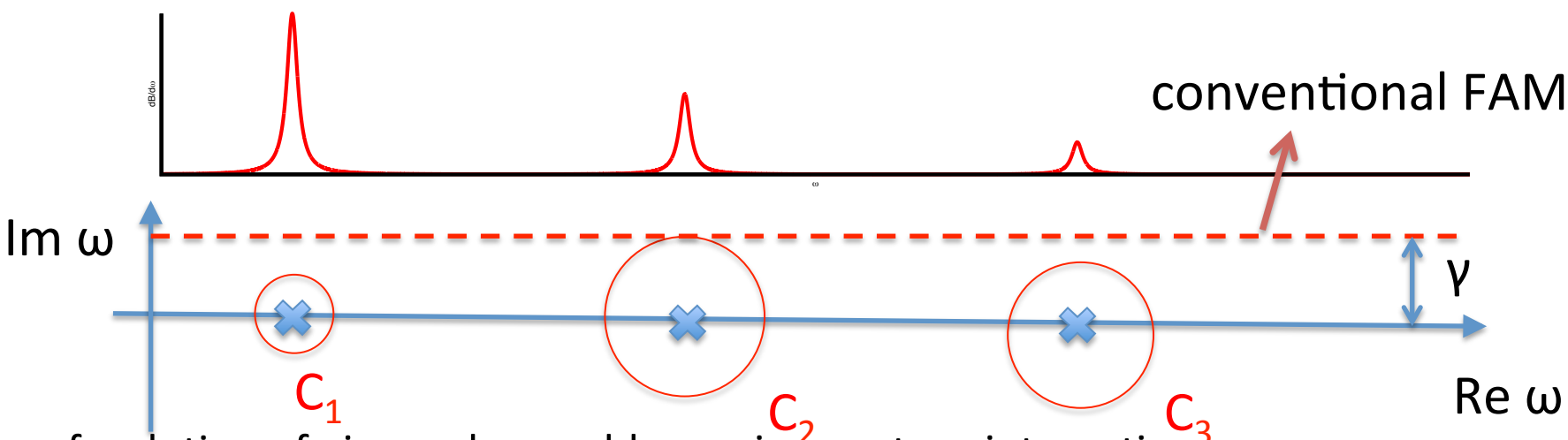
→ first-order poles at ω = Ωi (QRPA energies)

Contour integration

$$\frac{1}{2\pi i} \oint_{C_i} \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} d\omega = \langle i|\hat{F}|0\rangle \begin{pmatrix} X^i \\ Y^i \end{pmatrix}$$

X(ω), Y(ω): FAM amplitudes

X, Y: QRPA eigenvectors



cf. solution of eigenvalue problem using contour integration

Sakurai and Sugiura J. Comp. App. Math 159, 119 (2003).

FAM for discrete low-lying states

two ways to compute the strength function

A. from complex integrations of X and Y FAM amplitudes

$$|\langle i|\hat{F}|0\rangle|^2 = \sum_{\mu<\nu}\left\{\left|\frac{1}{2\pi i}\oint_{C_i} X_{\mu\nu}(\omega)d\omega\right|^2 - \left|\frac{1}{2\pi i}\oint_{C_i} Y_{\mu\nu}(\omega)d\omega\right|^2\right\}$$

then we can have all the QRPA X_i and Y_i amplitudes

$$X^i_{\mu\nu} = e^{-i\theta}|\langle i|\hat{F}|0\rangle|^{-1}\frac{1}{2\pi i}\oint_{C_i} X_{\mu\nu}(\omega_\gamma)d\omega_\gamma,$$

$$Y^i_{\mu\nu} = e^{-i\theta}|\langle i|\hat{F}|0\rangle|^{-1}\frac{1}{2\pi i}\oint_{C_i} Y_{\mu\nu}(\omega_\gamma)d\omega_\gamma.$$

C, D

$$\langle i|\hat{F}|0\rangle = \langle\Phi_0|[\hat{O}_i,\hat{F}]|\Phi_0\rangle = \sum_{\mu<\nu}(X^{i*}_{\mu\nu}F^{20}_{\mu\nu} + Y^{i*}_{\mu\nu}F^{02}_{\mu\nu})$$

X_i, Y_i are independent of the choice of operator F

QRPA energy

$$\Omega_i^2 = \frac{1}{|\langle i|\hat{F}|0\rangle|^2}\sum_{\mu<\nu}\left\{\left|\frac{1}{2\pi i}\oint_{C_i}(E_\mu+E_\nu)X_{\mu\nu}(\omega)+\delta H^{20}_{\mu\nu}(\omega)d\omega\right|^2 - \left|\frac{1}{2\pi i}\oint_{C_i}(E_\mu+E_\nu)Y_{\mu\nu}(\omega)+\delta H^{02}_{\mu\nu}(\omega)d\omega\right|^2\right\}$$

complex-energy FAM: strength function, QRPA amplitudes, energy

Numerical comparison with MQRPA

FAM code for K=0 developed in Stoitsov et al., PRC84, 041305 (2011)

^{24}Mg, oblate configuration (HFBTHO, SLy4) 5 oscillator shells

isoscalar/isovector monopole excitation

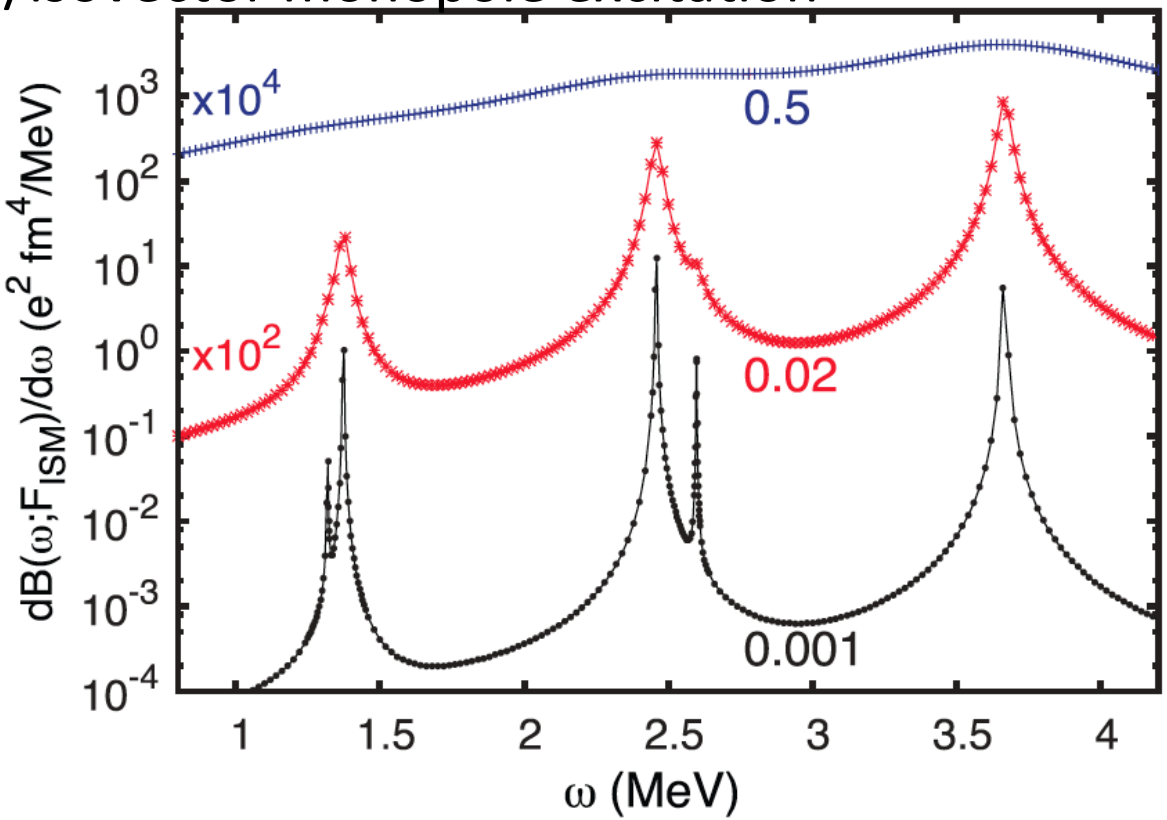


FIG. 1. (Color online) The low-lying isoscalar monopole strength at the oblate HFB minimum of ^{24}Mg calculated with the conventional FAM-QRPA using three values of smearing width γ (in MeV).

Numerical comparison with MQRPA

contour: circle, radius=0.02 MeV, discretized with 11 points

Ω_i (MeV)		isoscalar monopole strength (e^2fm^4)			
MQRPA	FAM	MQRPA	FAM-A	FAM-C	FAM-D
1.3185	1.3183	5.729(−4)	5.771(−4)	5.776(−4)	5.781(−4)
1.3731	1.3731	1.539(−2)	1.511(−2)	1.510(−2)	1.511(−2)
2.4582	2.4581	0.1796	0.1780	0.1784	0.1783
2.5998	2.5975	2.957(−3)	3.056(−3)	3.060(−3)	3.057(−3)
3.6687	3.6657	0.5776	0.5755	0.5788	0.5788
5.1185	5.1212	3.539(−4)	3.744(−4)	4.360(−4)	4.345(−4)
7.4108	7.4084	0.4900	0.4820	0.4848	0.4848

FAM-A: directly from the contour integration

FAM-C: from QRPA X_i and Y_i amplitudes
calculated from isoscalar monopole FAM

FAM-D: from QRPA X_i and Y_i amplitudes
calculated from isovector monopole FAM

QRPA X and Y do not depend on external fields

Numerical comparison with MQRPA

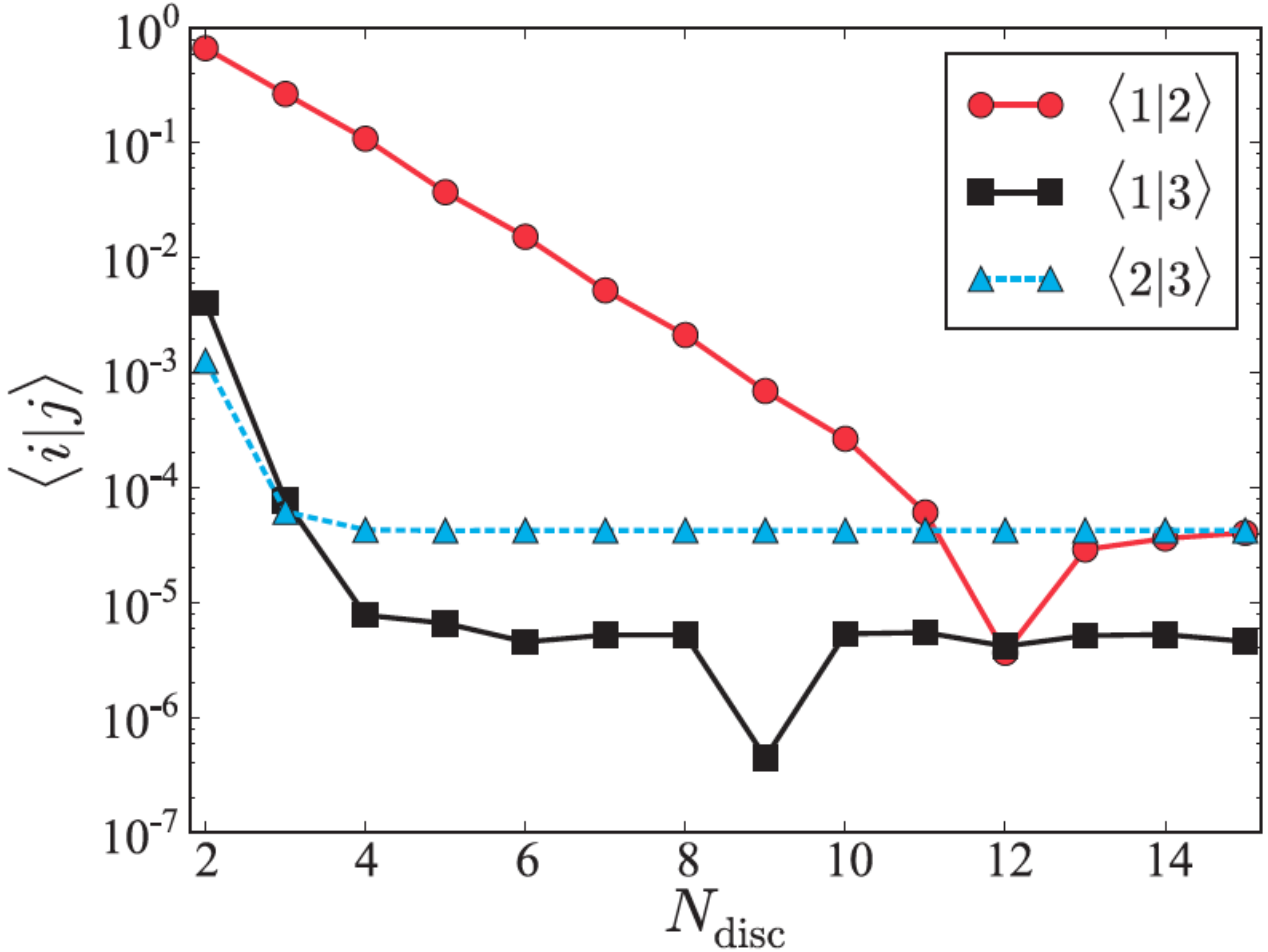
Ω_i (MeV)		isovector monopole strength (e^2fm^4)			
MQRPA	FAM	MQRPA	FAM-A	FAM-C	FAM-D
1.3185	1.3183	1.557(−3)	1.547(−3)	1.547(−3)	1.547(−3)
1.3731	1.3731	5.771(−5)	5.810(−5)	5.827(−5)	5.824(−5)
2.4582	2.4581	1.968(−6)	1.643(−6)	2.188(−6)	2.047(−6)
2.5998	2.5975	8.978(−5)	8.870(−5)	8.919(−5)	8.907(−5)
3.6687	3.6657	1.555(−5)	8.681(−6)	1.498(−5)	1.515(−5)
5.1185	5.1212	3.907(−2)	3.885(−2)	3.914(−2)	3.914(−2)
7.4108	7.4084	1.388(−5)	2.926(−5)	1.697(−5)	1.622(−5)

FAM-A: directly from the contour integration

FAM-C: from QRPA X_i and Y_i amplitudes
calculated from isovector monopole FAM

FAM-D: from QRPA X_i and Y_i amplitudes
calculated from isoscalar monopole FAM

orthogonality of first three QRPA modes



1: 1.32 MeV, 2: 1.37 MeV, 3: 2.46 MeV

Stoitsov et al., PRC84, 041305 (2011)

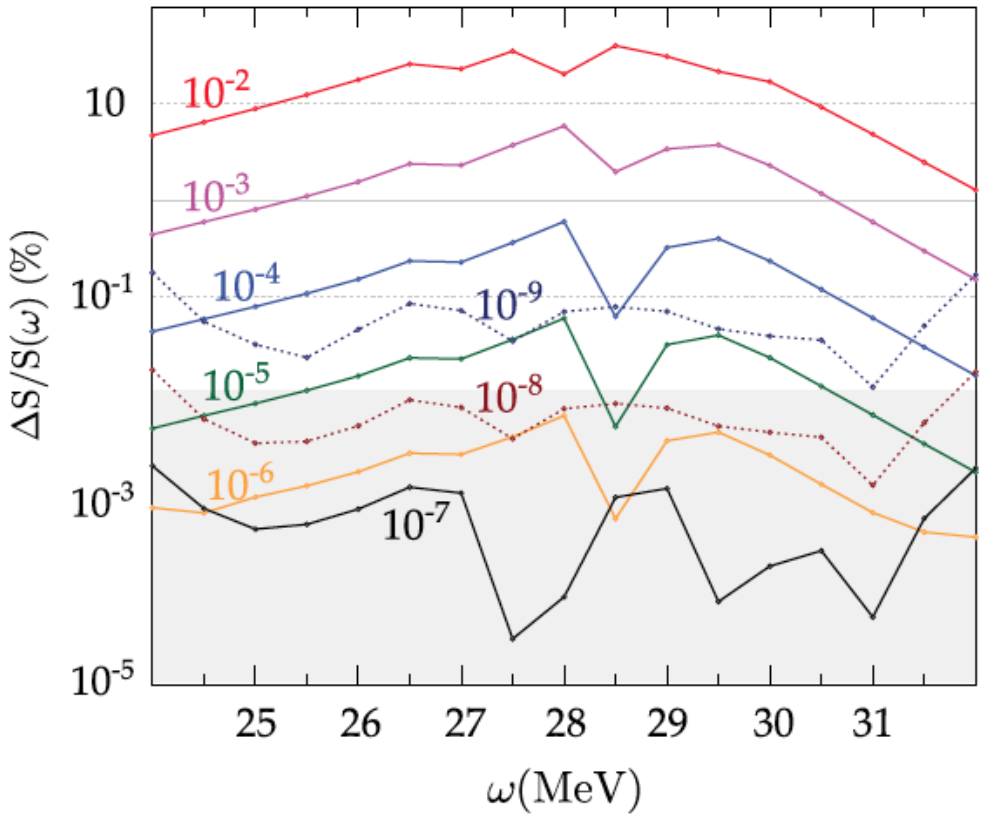
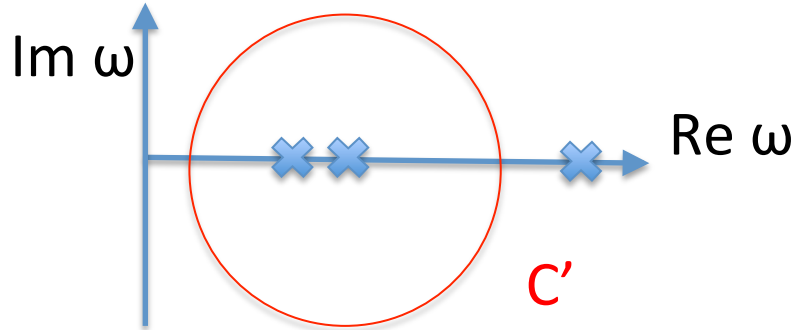
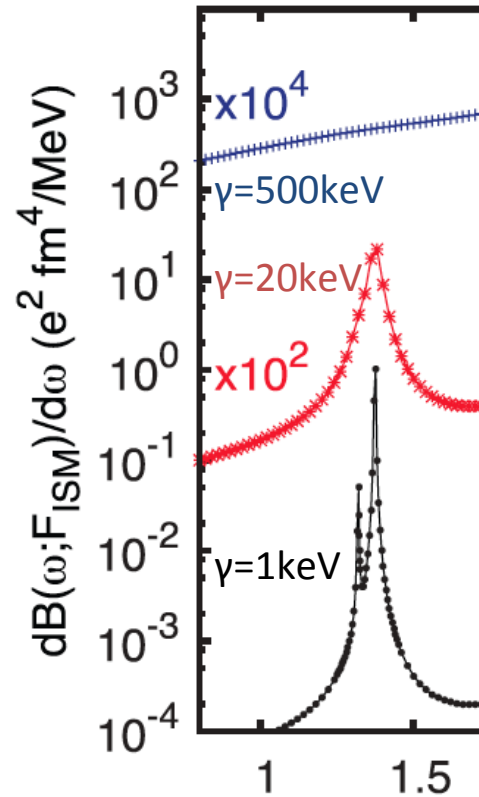


FIG. 2. (Color online) The performance of the FAM-QRPA algorithm applied to the case of Fig. 1 for different values of η in the frequency range of $24 < \omega < 32$ MeV. The relative accuracy is defined as $\Delta S/S$, where $\Delta S(\eta) = |S(10\eta) - S(\eta)|$.

FAM accuracy ~ 4 digits in the strength function

When the contour includes multiple poles





FAM-A: strength from contour integration

$$\sum_{\mu<\nu}\left\{\left|\frac{1}{2\pi i}\oint_{C'} X_{\mu\nu}(\omega)d\omega\right|^2-\left|\frac{1}{2\pi i}\oint_{C'} Y_{\mu\nu}(\omega)d\omega\right|^2\right\}=\sum_{i\in C'}|\langle i|\hat{F}|0\rangle|^2$$

FAM-C: strength through QRPA X and Y amplitudes

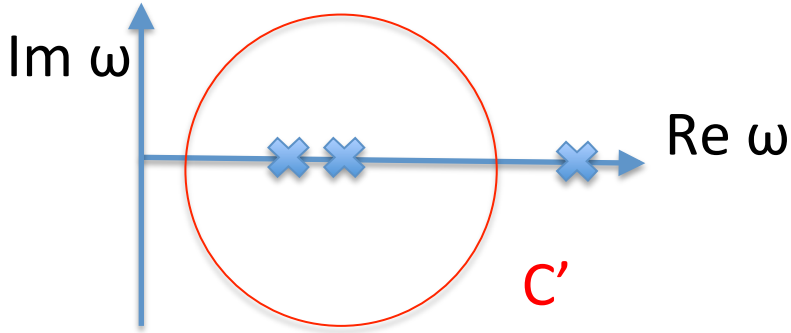
$$B(C';F)=\sum_{i\in C'}|\langle i|\hat{F}|0\rangle|^2$$

FAM-D: strength of F through QRPA X and Y from FAM using F'

$$B_D(C';F)=\frac{|\sum_{i\in C'}\langle i|\hat{F}'|0\rangle\langle i|\hat{F}|0\rangle^*|^2}{\sum_{i\in C'}|\langle i|\hat{F}|0\rangle|^2}$$

multiple pole can be detected
from the FAM with two kinds of external fields.

When the contour includes multiple poles



QRPA energy:

$$\Omega^2_{C'} = \sum_{i \in C'} \left\{ |\langle i|\hat{F}|0\rangle|^2 \Omega_i^2 \right\} / \sum_{i \in C'} |\langle i|\hat{F}|0\rangle|^2$$

when two poles (collective and non-collective) are included,
this expression tells the approximate position of the collective pole.

Example

contour which includes the two poles at 1.32MeV and 1.37MeV (circle, 1.3MeV centered, 0.2MeV radius)

FAM-A,C
ISM: 1.57×10^{-2}
IVM: 1.61×10^{-3}

FAM-D
ISM: 6×10^{-8}
IVM: 3×10^{-9} ($e^2 fm^4$)

isoscalar monopole

MQRPA Ω	FAM Ω	MQRPA ISM
1.3185	1.3183	5.729(-4)
1.3731	1.3731	1.539(-2)

isovector monopole

MQRPA Ω	FAM Ω	MQRPA IVM
1.3185	1.3183	1.557(-3)
1.3731	1.3731	5.771(-5)

energy:
from ISM field: 1.371 MeV
from IVM field: 1.320 MeV

Rare-earth nuclei (^{166,168,172}Yb,^{170}Er)

comparison with Vanderbilt code (SkM*)

MQRPA: Terasaki and Engel, PRC82, 034326 (2010), PRC84 014332 (2011)

TABLE III. FAM-QRPA energies and $B(E2)$ values of the low-lying $K = 0$ states in ^{166}Yb, ^{168}Yb, ^{172}Yb, and ^{170}Er at $E_{\rm cut} = 200$ MeV compared to the MQRPA results of Ref. [13]. The additional result for ^{172}Yb corresponding to $E_{\rm cut} = 60$ MeV is compared to the MQRPA values obtained in Ref. [12].

Nucleus	Ω_i (MeV)		$B(E2)$ (e^2 b^2)	
	MQRPA	FAM	MQRPA	FAM
^{166}Yb	1.802	1.422	0.0398	0.0327
^{168}Yb	2.039	1.747	0.0343	0.0186
^{172}Yb	1.605	1.306	0.0049	0.0088
^{170}Er	1.596	1.322	0.0030	0.0047
^{172}Yb[a]	1.390	1.319	0.0050	0.0092

[a] $E_{\rm cut} = 60$ MeV.

radius: 0.1MeV, 0.02 MeV(168Yb)
center:1.40, 1.76, 1.30, 1.30MeV
166Yb, 168Yb,172Yb,170Er

	HFBTHO FAM	Vanderbilt MQRPA
HFB model space	N=20, 60, 200MeV cutoff	20fmx 20fm box, 60,200MeV cutoff
QRPA model space	full	cutoff associated with the occupation probabilities

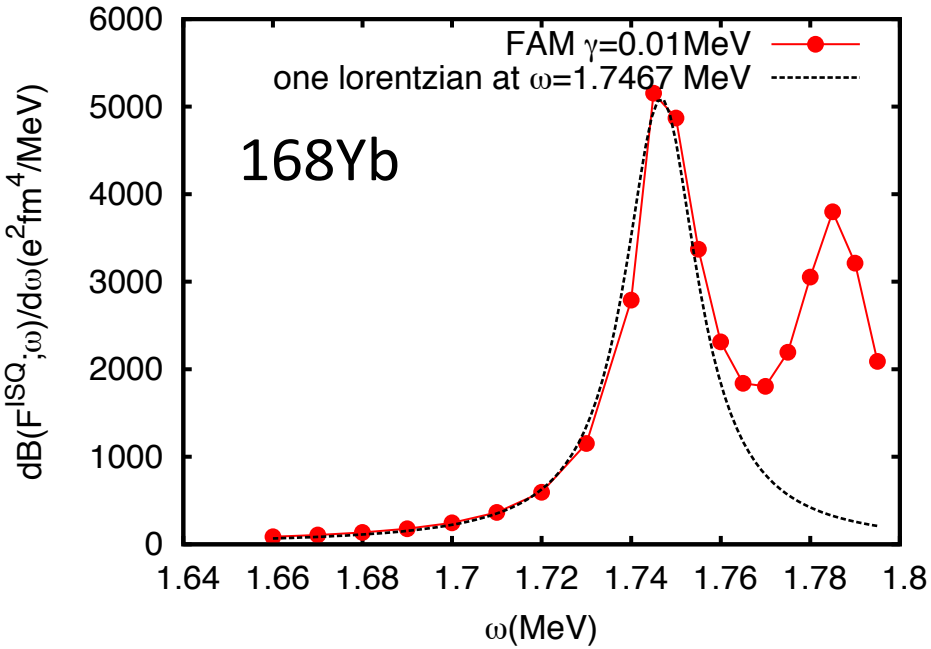
Quadrupole strengths (^{166,168,172}Yb, ^{170}Er)

Nucleus	ISQ		IVQ	
	FAM-C	FAM-D	FAM-C	FAM-D
^{166}Yb	299.854	299.856	0.585519	0.585520
^{168}Yb	160.126	160.127	0.969114	0.969124
^{172}Yb	93.2710	93.2735	0.081406	0.081404
^{170}Er	56.2932	56.2913	0.460285	0.460254

e^2fm^4

ISQ (IVQ) FAM-C: from FAM using isoscalar (isovector) quadrupole field
ISQ (IVQ) FAM-D: from FAM using isovector (isoscalar) quadrupole field

radius: 0.1MeV, 0.02 MeV(168Yb)
center:1.40, 1.76, 1.30, 1.30MeV
166Yb, 168Yb,172Yb,170Er



Sum rule

sum rule $$m_k(\hat{F}) = \sum_{\nu>0} \Omega_\nu^k |\langle \nu | \hat{F} | 0 \rangle|^2$$

- information of energy of giant resonances

$$E_k = \sqrt{\frac{m_k}{m_{k-2}}} \qquad E_{-1} \leq E_0 \leq E_1 \leq \bar{E} \equiv \frac{m_1}{m_0} \leq E_2$$

- giant resonance width

$$\rho^2 \equiv E_2^2 - \bar{E}^2 \leq \frac{1}{4}(E_3^2 - E_1^2)$$

- contributions from all the excited states
  - QRPA: computationally demanding
  - efficient technique for sum rule is desired for
    - mass table calculation of giant resonances
    - new functional parameter fitting

Sum rule from HFB

Thouless Theorem

D.J. Thouless, Nucl. Phys. 22 (1961) 78

QRPA sum rule can be computed from HFB values

energy-weighted sum rule (EWSR) $m_1 = \sum_{\nu>0} \Omega_\nu |\langle \nu|\hat{F}|0\rangle|^2 = \frac{1}{2}\langle \mathrm{HFB}|[\hat{F},[\hat{H},\hat{F}]]\mathrm{HFB}\rangle$

cubic energy-weighted sum rule (CEWSR)

$$m_3 = \sum_{\nu>0} \Omega_\nu^3 |\langle \nu|\hat{F}|0\rangle|^2 = -\frac{1}{2}\left(\frac{2\hbar^2}{m}\right)^2 \langle \mathrm{HFB}|[\hat{G},[\hat{H},\hat{G}]]\mathrm{HFB}\rangle \qquad \hat{G} = -\left(\frac{m}{2\hbar^2}\right)[\hat{H},\hat{F}]$$

- no momentum dependence in the interaction [H, F] = [T, F]
- based on Hamiltonian formalism.

  DFT: correspondence with the effective interaction is necessary

  cannot be justified for Skyrme+ simple (volume/mixed) pairing functionals.

In DFT, alternative approach for (C)EWSR is necessary.

Dielectric theorem for inverse energy-weighted sum rule (IEWSR)

QRPA value can be computed from constrained HFB

$$m_{-1} = \frac{1}{2}\frac{\partial^2}{\partial\lambda^2}\langle \phi(\lambda)|\hat{H}|\phi(\lambda)\rangle_{\lambda=0} \qquad \delta\langle \phi(\lambda)|\hat{H} - \lambda\hat{F}|\phi(\lambda)\rangle = 0$$

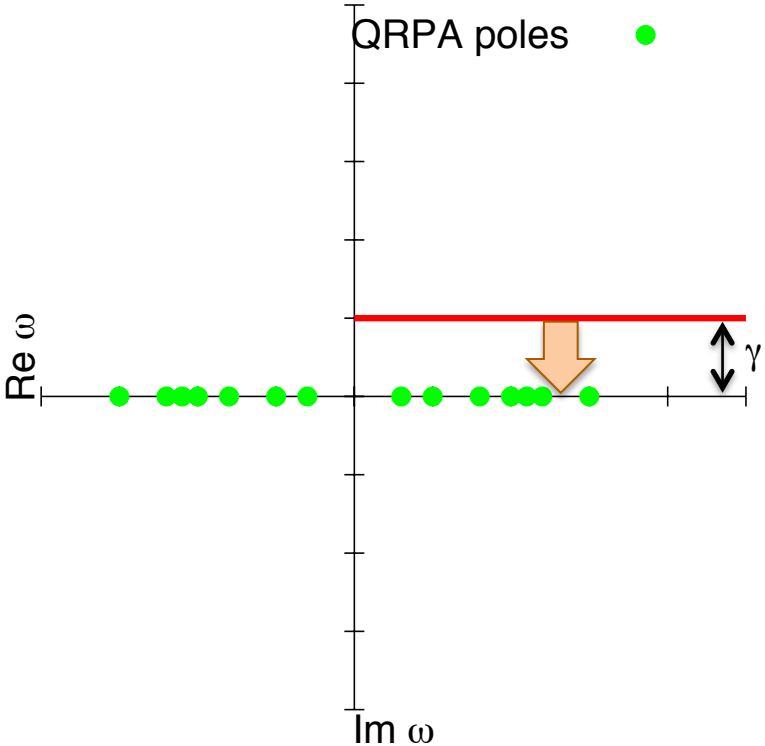
Capelli et al. Phys. Rev. C79, 054329 (2009)

IEWSR formula can be applied to any density functional

Sum rule from linear response theory

- QRPA sum rule

$$m_k(\hat{F}) = \sum_{\nu>0} \Omega_\nu^k |\langle \nu|\hat{F}|0\rangle|^2$$



$$m_k(\hat{F}) = -\lim_{\gamma\to 0} \frac{1}{\pi} \int_0^\infty \omega^k \mathrm{Im} S(\hat{F}, \omega_\gamma) d\omega$$

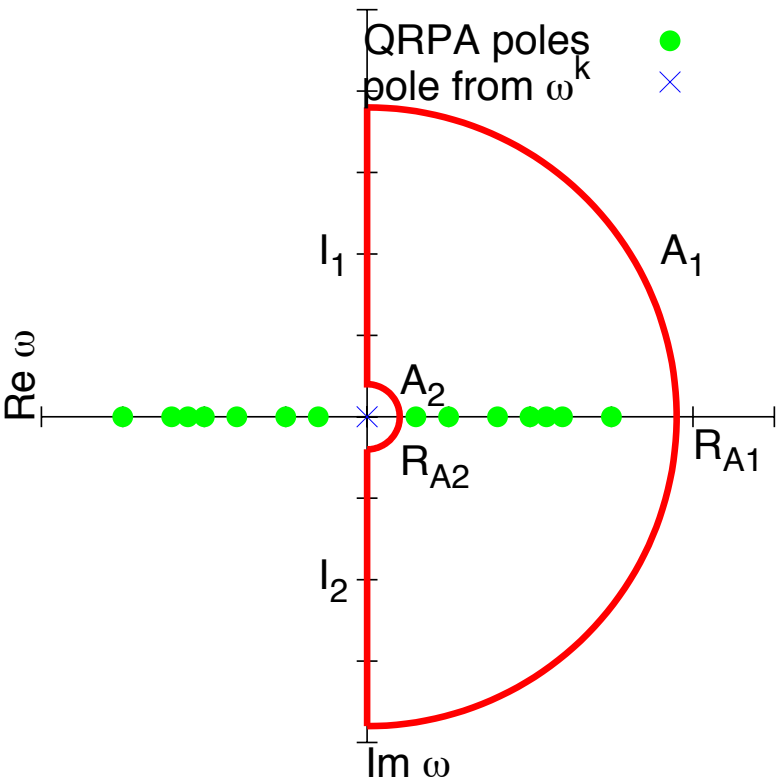
$$S(\hat{F}, \omega_\gamma) = -\sum_\nu \left\{ \frac{|\langle \nu|\hat{F}|0\rangle|^2}{\Omega_\nu - \omega_\gamma} + \frac{|\langle 0|\hat{F}|\nu\rangle|^2}{\Omega_\nu + \omega_\gamma} \right\}$$

$$\frac{1}{\omega + i\gamma} = P(\frac{1}{\omega}) - i\pi\delta(\omega)$$

Complex-energy FAM to QRPA sum rule

- QRPA sum rule

$$m_k(\hat{F}) = \sum_{\nu>0} \Omega_\nu^k |\langle\nu|\hat{F}|0\rangle|^2$$



$$S(\hat{F},\omega_\gamma) = -\sum_\nu \left\{ \frac{|\langle\nu|\hat{F}|0\rangle|^2}{\Omega_\nu - \omega_\gamma} + \frac{|\langle 0|\hat{F}|\nu\rangle|^2}{\Omega_\nu + \omega_\gamma} \right\}$$

$$m_k = \frac{1}{2\pi i} \oint_D \omega_\gamma^k S(\hat{F},\omega_\gamma) d\omega_\gamma$$

D = A1 + I1 + A2 + I2

note: S(F, ω) is an even function of ω
for Hermite operator F

I1 + I2 vanishes for odd k
I1 = I2 for even k

pole at ω=0 present for k<0:
need to exclude it using A2

A1/A2 integral convergence (real part)

isoscalar monopole operator, 24Mg oblate configuration, SLy4, Nsh=5

R_A1 = 200 MeV, N: number of discretized points

A1

N_{A_1}	$k=-4$	$k=-3$	$k=-2$	$k=-1$	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
2	-9.0(-9)	-2.6(-6)	-3.8(-4)	-2.7(-3)	14.4512	4195.39	608586	4318622	-23121955103
3	8.9(-9)	6.8(-8)	-1.7(-4)	1.1(-4)	13.8330	4199.86	574158	4338883	-10598231322
4	3.3(-9)	-2.6(-9)	-1.4(-4)	-5.7(-6)	13.5754	4199.47	562640	4336658	-8503069979
5	2.5(-9)	2.1(-10)	-1.3(-4)	4.1(-6)	13.4602	4199.52	557432	4336742	-7722929569
7	2.0(-9)	7.1(-12)	-1.2(-4)	2.9(-6)	13.3596	4199.52	552948	4336831	-7119897520
9	1.9(-9)	2.2(-12)	-1.1(-4)	2.9(-6)	13.3183	4199.52	551117	4336843	-6889900293
10	1.8(-9)	1.7(-12)	-1.1(-4)	2.9(-6)	13.3063	4199.52	550586	4336838	-6824833562
11	1.8(-9)	1.9(-12)	-1.1(-4)	2.9(-6)	13.2975	4199.52	550193	4336836	-6777210535
12	1.8(-9)	1.9(-12)	-1.1(-4)	2.9(-6)	13.2907	4199.52	549895	4336839	-6741282496
101	1.6(-9)	1.9(-12)	-1.1(-4)	2.9(-6)	13.2558	4199.52	548351	4336840	-6558892890
201	1.6(-9)	1.9(-12)	-1.1(-4)	2.9(-6)	13.2554	4199.52	548335	4336840	-6556976091
301	1.6(-9)	1.9(-12)	-1.1(-4)	2.9(-6)	13.2554	4199.52	548332	4336841	-6556616988

equivalent to sum rule value

A2

N_{A_2}	$k=-4$	$k=-3$	$k=-2$	$k=-1$	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
5	-1.20929	0.0372665	3.26165	5.00438	3.23108	1.0(-3)	-1.22915	2.2(-3)	0.996929
11	-1.06784	0.0369931	3.21891	5.00387	3.18902	2.7(-5)	-1.09039	4.1(-5)	0.691153
21	-1.04368	0.0369883	3.21098	5.00385	3.18127	6.1(-6)	-1.06646	-5.8(-7)	0.649057
31	-1.03883	0.0369871	3.20937	5.00385	3.17969	6.0(-6)	-1.06164	9.8(-7)	0.640899
51	-1.03625	0.0369867	3.20850	5.00385	3.17884	5.5(-6)	-1.05908	1.1(-6)	0.636595
101	-1.03512	0.0369871	3.20812	5.00385	3.17847	5.9(-6)	-1.05797	7.3(-7)	0.634729

R_A2 = 1 MeV, lowest QRPA energy, 1.34 MeV

note: convergence of FAM calculation at A1 path is very fast (5-6 iterations)

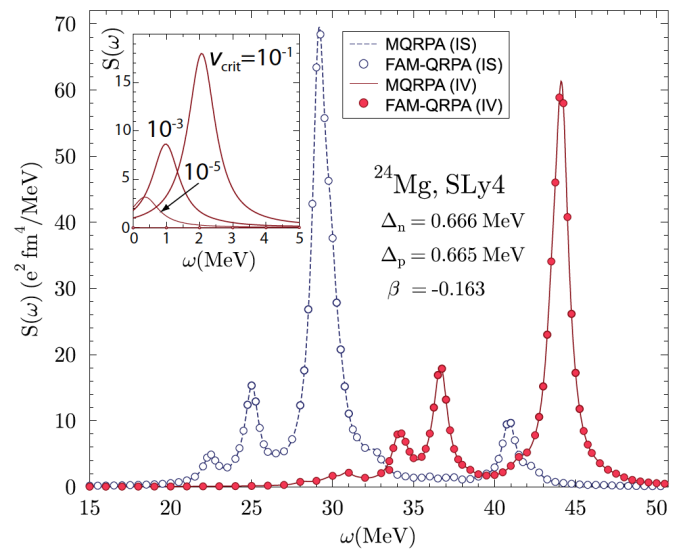
Sum rule

isoscalar/isovector monopole operator unit: MeV and fm

	$k=-4$	$k=-3$	$k=-2$	$k=-1$	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
HFB(ISM)	-	-	-	5.00997	-	4303.67	-	-	-
MQRPA(ISM)	0.013077	0.037185	0.253118	5.00072	139.825	4200.82	131368	4342358	157906069
FAM(ISM)	0.0125818	0.0369871	0.253127	5.00385	139.850	4199.52	131278	4336841	157087148
MQRPA(IVM)	0.00063616	0.00273872	0.07120949	2.78540	113.908	4735.03	199525	8527358	370625216
FAM(IVM)	0.00043113	0.00275064	0.0713296	2.78615	113.908	4734.37	199520	8525896	368719245

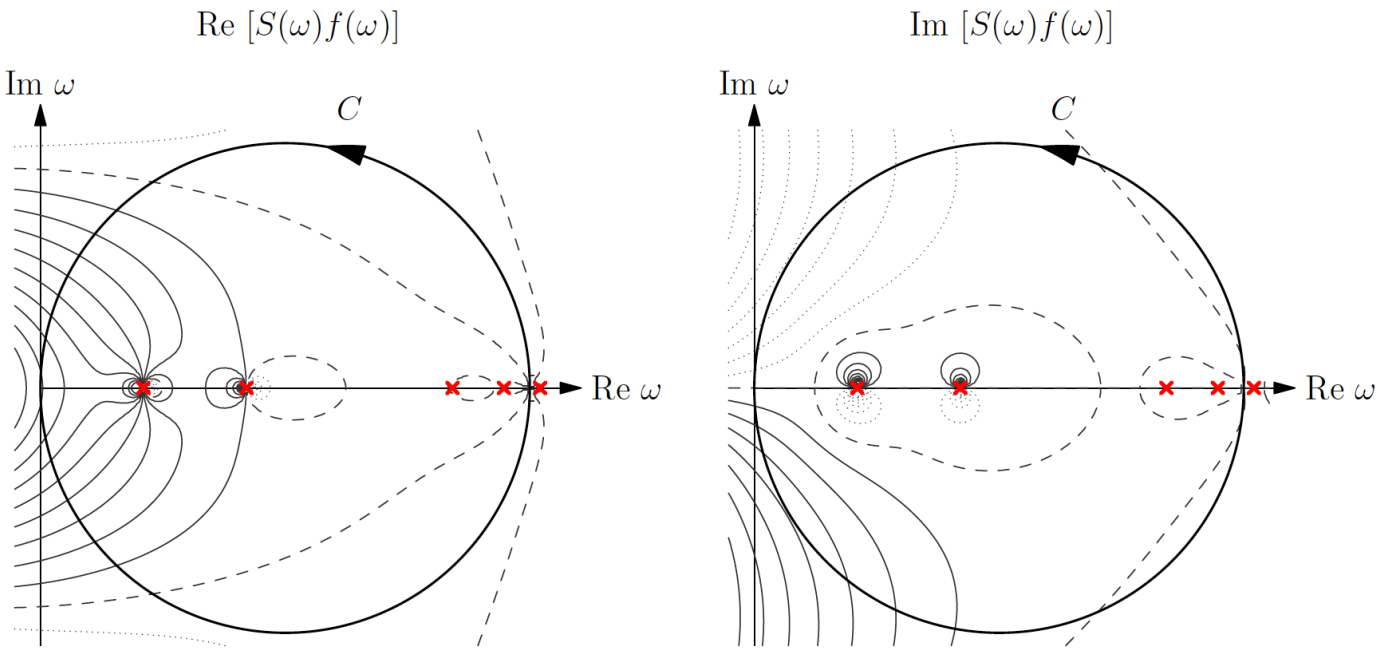
MQRPA: matrix diagonalization of the QRPA
HFB: commutation / dielectric theorem

E1 = 28.97 MeV (ISM), E = 30.03 MeV (ISM)
rho = 9.97 MeV (ISM)
E1 = 41.22 MeV (IVM), E = 41.56 MeV (IVM)
rho = 7.23 MeV (IVM)



m1: complex-energy FAM is very efficient
m-1: dielectric theorem

beta-decay rate



$$\lambda_{1+} = \frac{\ln 2}{\kappa} \sum_n f(\Omega_n) B_n^{(\mathrm{GT})}$$

$$\approx -\frac{\ln 2}{\kappa} \sum_n f_{\mathrm{poly}}(\Omega_n)\, \mathrm{Res}[S(\sigma\tau_-), \Omega_n]$$

$$= -\frac{\ln 2}{\kappa} \sum_n \mathrm{Res}[f_{\mathrm{poly}} S(\sigma\tau_-), \Omega_n]$$

$$= -\frac{\ln 2}{\kappa} \frac{1}{2\pi i} \oint_C \mathrm{d}\omega\, f_{\mathrm{poly}}(\omega) S(\sigma\tau_-; \omega),$$

Mustonen et al., arXiv:1405.0245

Summary

- FAM for low-lying collective states is formulated using contour integration and tested.

- The complex-energy FAM provides the QRPA solution of a specific energy. A approximate information of the QRPA energy (pole in the response function) is necessary in advance. The conventional FAM calculation can be used to find the poles.

- Incorrect assignment of the contour will give the summed strengths, but one can numerically detect it.

- The method is especially powerful for isolated collective states, but not suitable for non-collective states with small strengths.

- QRPA sum rules can be computed from contour integration very efficiently.