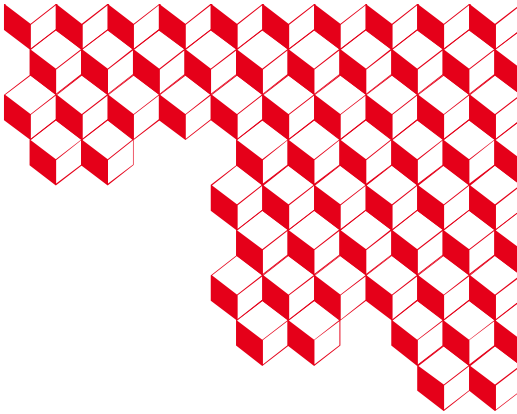

Fast extraction of low-energy QRPA modes

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ESNT Workshop
21/11/2024

Outline

1. Low-energy QRPA-modes
   - QRPA equation and resolution methods
   - Focus on low-energy modes and applications
2. Jacobi-Davidson method for interior eigenvalues equations
   - Jacobi-Davidson in a nutshell
   - Combining JD and FAM : complexity analysis
3. Validation and application with Gogny interaction
   - Benchmark and analysis
   - Application in U238 low-lying spectrum
4. Conclusion

1. Low-energy QRPA modes

QRPA equation and resolution methods

Master QRPA equation

$$\begin{pmatrix} A & B \\ B^+ & A^* \end{pmatrix}\begin{pmatrix} X_i \\ Y_i \end{pmatrix} = \epsilon_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X_i \\ Y_i \end{pmatrix}$$

$$\boldsymbol{Mx_i = \epsilon_i N x_i}$$

Exact resolution

1. Construction of system $O(n^5)/\,O(n^8)$
2. Resolution of eigenvalue equation $O(n^6)$

Matrix-less product?
Alternating between sp and qp basis
Only mean-field like contractions
Can exploit compressed format of H

Arnoldi method

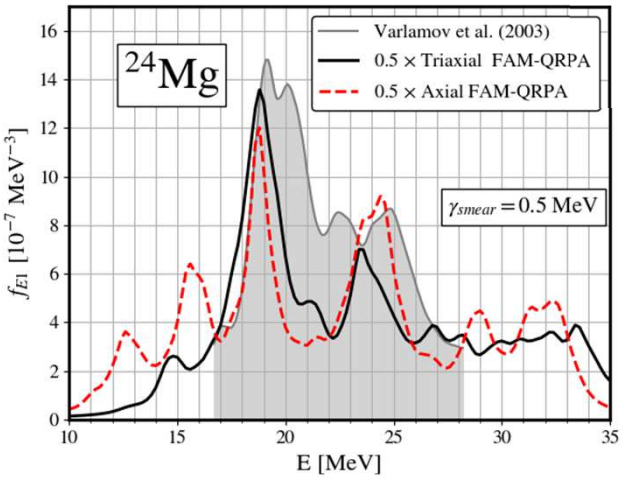
1. Non-symmetric eigenvalue problem

$$NMx_i = \epsilon_i x_i$$

2. Matrix-less Arnoldi resolution

$$O(n^4)$$

Toivanen et al Phys. Rev. C 81 034312 (2010)



Finite Amplitude Method

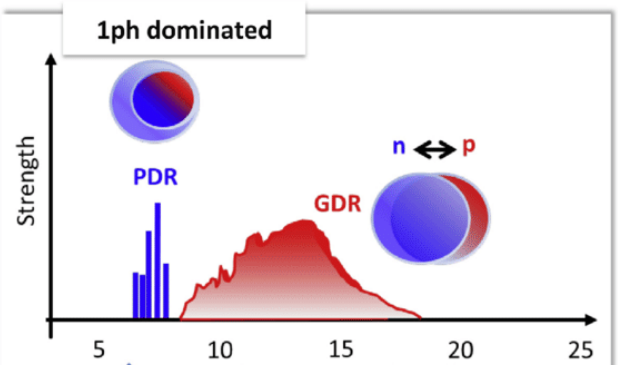
1. Matrix-less matrix inversion

$$(M - \omega N)^{-1} \qquad 30 \cdot O(n^4)$$

2. Strength function calculation

$$PSF(EXL, \omega) \sim \Im\{Q^{L^+} \cdot (M - \omega N)^{-1} \cdot Q^L\}$$

Focus on low-energy modes and applications

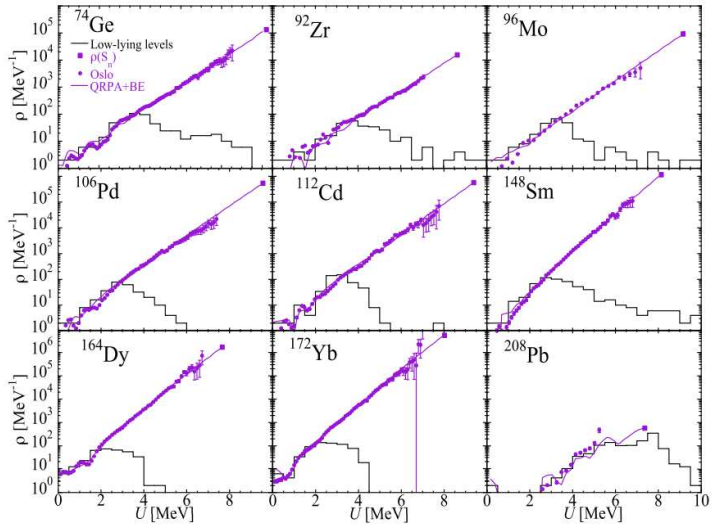


Individual mode study

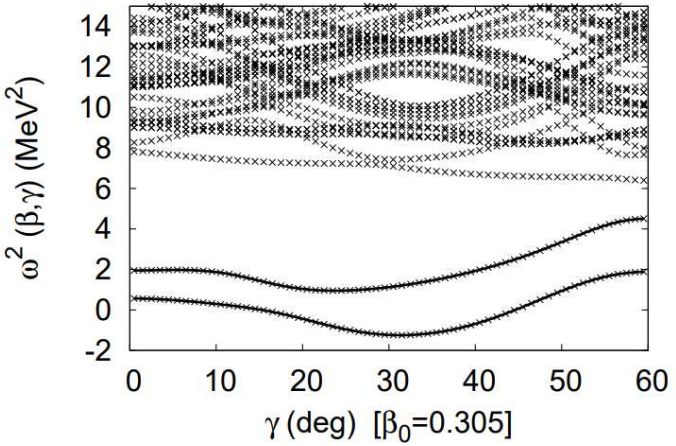
Pygmy resonances
M1 spin-flip / scissor modes
Low Energy Enhancement

Nuclear Level Densities

Combination of low-lying modes
Much better agreement with experiment



Hilaire et al, Physics Letters B 843, 137989 (2023)



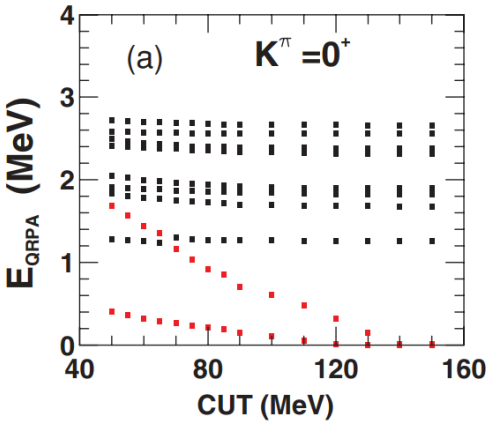
Inertia calculations

TDMF masses
LQRPA : very good description
Very costly as well

Hinohara et al, Phys. Rev. C **82**, 064313 (2010)
Washiyama et al, Phys. Rev. C **109**, L051301 (2024)

2. Jacobi-Davison method for fast calculation of interior eigenvalues

QRPA equation and resolution methods



Master QRPA equation

Exact resolution

$$\begin{pmatrix} A & B \\ B^{+} & A^{*} \end{pmatrix}\begin{pmatrix} X_i \\ Y_i \end{pmatrix} = \epsilon_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X_i \\ Y_i \end{pmatrix}$$

$$Mx_i = \epsilon_i N x_i$$

Full calculation… works but too costly

Martini et al, Phys. Rev. C 83, 014314 (2011)

1. Construction of system $O(n^5)/\,O(n^8)$
2. Resolution of eigenvalue equation $O(n^6)$

Jacobi-Davidson method

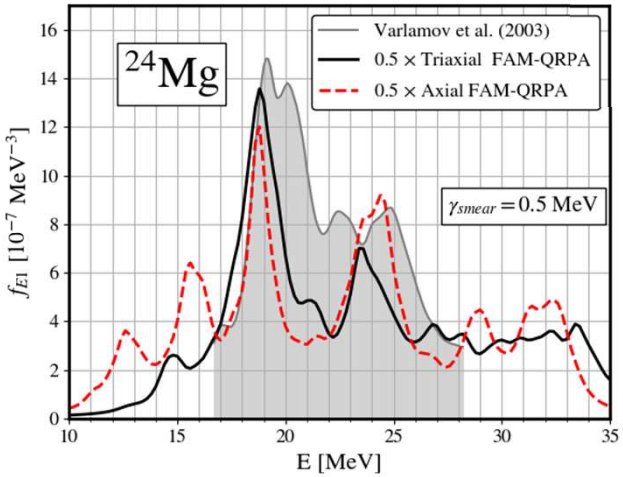
1. Matrix-less matrix product & inverse

   $30 \cdot O(n^4)$
2. Local eigenpair determination

   $n_{iter} \cdot 30 \cdot O(n^4)$

Davidson et al (1975)

Cubic rate of convergence
Efficient determination in isolated region



Arnoldi method

1. Non-symmetric eigenvalue problem

   $NMx_i = \epsilon_i x_i$
2. Matrix-less Arnoldi resolution

   $O(n^4)$

Toivanen et al Phys. Rev. C 81 034312 (2010)

Converges extremal eigenvalues fast…
Significant storage in basic formulation

Finite Amplitude Method

1. Matrix-less matrix inversion

   $(M-\omega N)^{-1}$ $30 \cdot O(n^4)$
2. Strength function calculation

$$PSF(EXL,\omega) \sim \Im\{Q^{L^{+}} \cdot (M-\omega N)^{-1} \cdot Q^{L}\}$$

Complex integration can extract poles
Need prior knowledge of position
Requires separated eigenvalues
Many iterations required

Jacobi-Davidson in a nutshell

Parenthesis : Rayleigh quotient iteration (RQI)

$$\begin{cases} \omega_i = \dfrac{x_i^+ M x_i}{x_i^+ N x_i} (\equiv \rho(x_i)) \\ x_{i+1} \propto (M - \omega_i N)^{-1} x_i \end{cases}$$

- Eigenvector magnified when close to eigenvalue
- *Local cubic convergence* towards ground state
- System solving ⇔ single FAM call

Promising but…

- ❑ One eigenvalue at a time
  - ❑ Deflation could be implemented
  - ❑ Still not fully efficient
- ❑ Instable near true eigenvalue
  - ❑ System becomes singular (more FAM iterations)
  - ❑ Can be stabilized by complex shift

Jacobi Davidson as upgraded RQI

2 steps method to find eigenparis closest to τ

$\mathcal{U} \equiv (u_1 \cdots u_k)$ search space at iteration k

Subspace extraction (find eigenpairs)

Solving eigenvalue equation in reduced space: new $\mathcal{U}$

$$\mathcal{M}c = \omega \mathcal{N}c$$

Accept eigenpairs based on $||Mu_i - \omega_i N u_i|| < \epsilon_{tol}$

Improved RQI : many eigenvalues at once

Subspace expansion (build search space)

Defining residuals $r \equiv (M - \rho(u)N)u$

Correction equation (classic JD) to solve

$$(I - \eta_u N u u^+)(M - \rho(u)N)(I - \eta_u u u^+ N)t = -r$$

Easily generalized with deflation

Can be solve approximately… or exactly (single FAM call !)

- ❑ Tweaked with complex shift for improved stability

cea

3. Validation and application with Gogny interaction

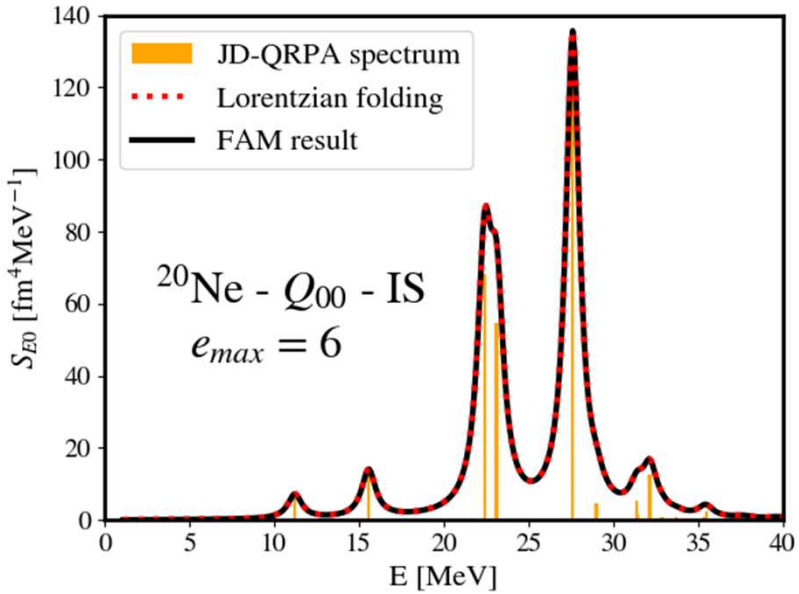
Validation of the method

M-QRPA Benchmark in sd-shell (M1)

K	E (JD) [MeV]	E (SM-QRPA) [MeV]
0	10.406418	10.406417
0	10.949270	10.949270
0	13.298152	13.298153
0	14.525524	14.525526
1	8.898729	8.898731
1	9.536392	9.536393
1	11.172634	11.172633
1	12.586020	12.586019
1	14.835711	14.835712
1	15.163259	15.163258
1	16.503927	16.503927
K	B_{M1} (JD) $[\mu_N^2]$	B_{M1} (SM-QRPA) $[\mu_N^2]$
0	0.000190	0.000190
0	0.096031	0.096031
0	0.000941	0.000941
0	0.334619	0.334622
1	0.783673	0.783673
1	0.000334	0.000334
1	0.028456	0.028456
1	0.000212	0.000212
1	0.014002	0.014002
1	0.000028	0.000028
1	0.025487	0.025487

Very difficult with complex integration

FAM-QRPA Benchmark with chiral Hamiltonian

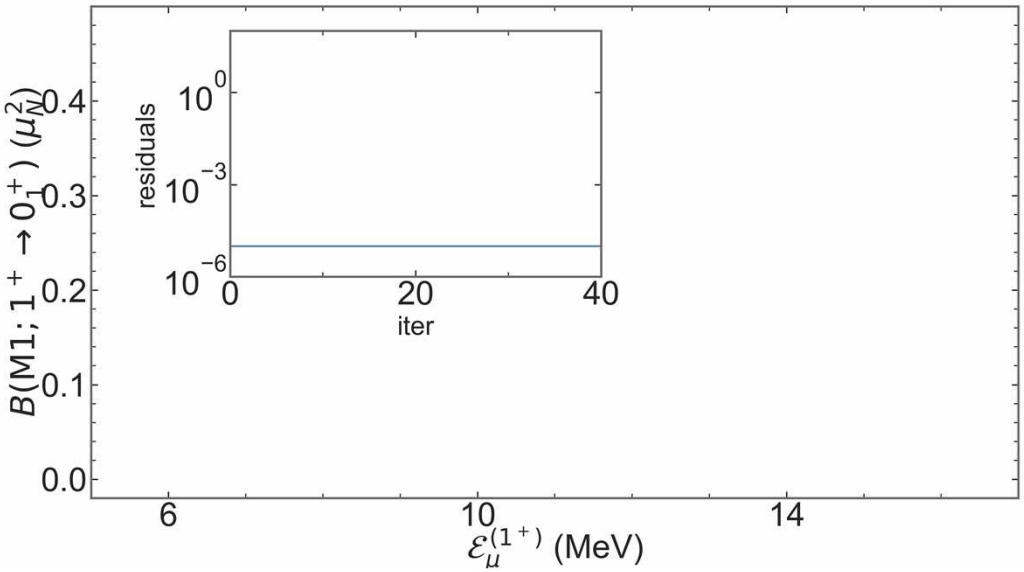


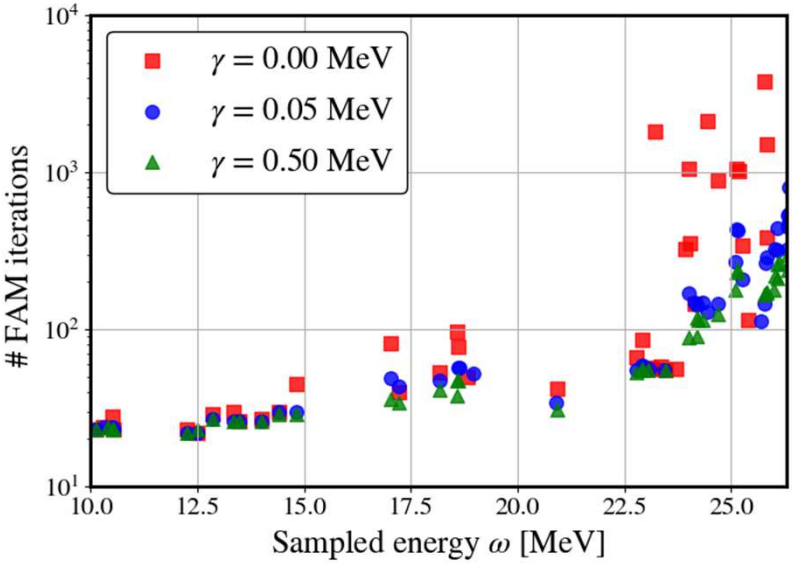
Perfect agreement with M-QRPA / FAM-QRPA
What about performance?

Performance of JD methods

FAM calls can become **too involved in dense regions**
- **Singular system** difficult to invert
- Iterative methods break down

Introduction of **small complex shift** to regularize the system
Greatly reduces the number of HFB-like iterations
No significant impact on number of JD iterations

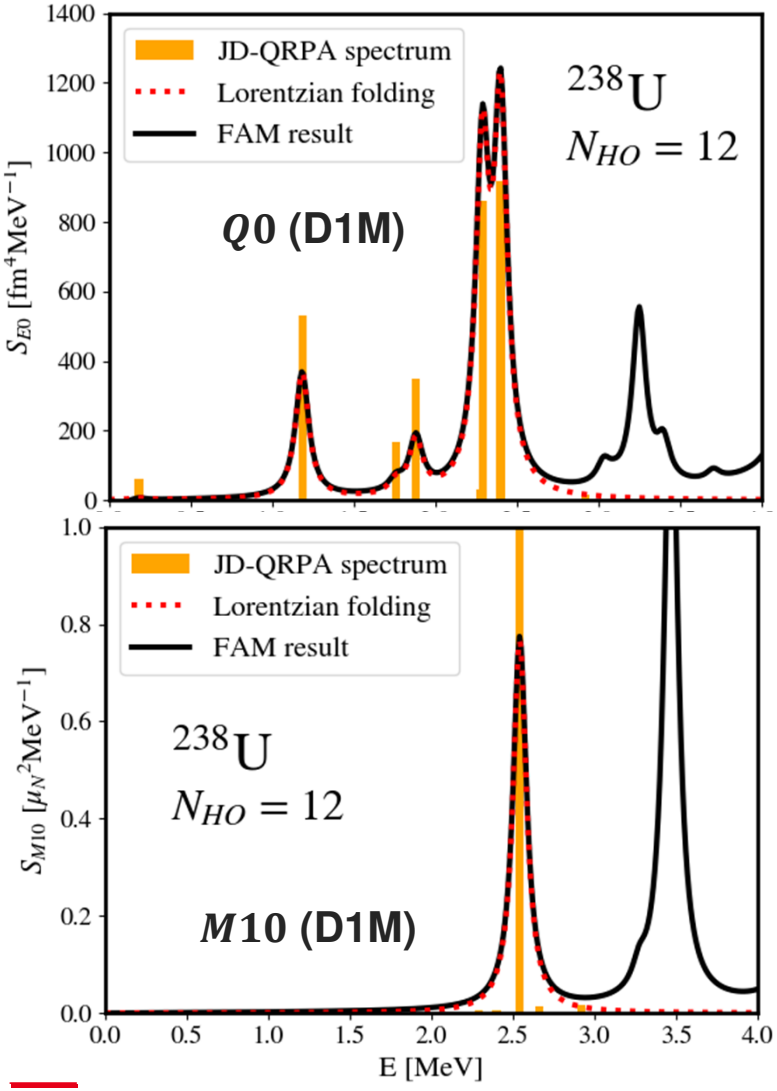




M1,K=0 strength
2 FAM calls per eigenvalue
20-50 HFB-like contractions per iteration

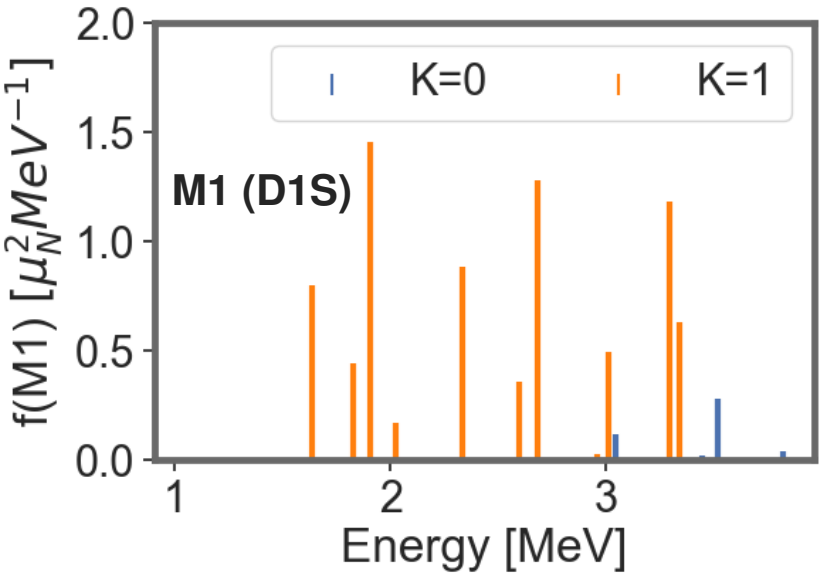
Comparing to complex integration
- Faster
- More accurate
- Not dependent on observable

Example in U8



D1M interaction

7 CPUh on single core for 10 eigenvalues
vs. **5-50k CPUh** for M-QRPA
Fully self-consistent calculation (Coulomb exact)



4. Conclusion

Conclusion

- A new resolution algorithm has been proposed to **extract interior QRPA modes**
  - Combines Arnoldi & QRPA-FAM methods
  - Extract single eigenmode in **few FAM calls**

- This method is improving on the previously proposed complex integration
  - Better numerical stability
  - Requires less FAM evaluations
  - Does not rely on the previous knowledge of modes position

- **Proper benchmark** with valence space / chiral interactions
- **Application with D1M** interaction in realistic calculations

Gonzalez-Miret et al, in preparation

Thanks for your attention

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