Angular Momentum Projected Random Phase Approximation

TECHNISCHE UNIVERSITÄT DARMSTADT

CEA ESNT Workshop

Nuclear energy density functional method: going beyond the minefield

November 23rd, 2023

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EMMI

SFB 1245

Outline

1 Physical introduction

- Giant resonances
- Existing EDF tools

2 Random Phase Approximation

- Theoretical introduction
- Angular momentum projection

3 Results

- Rotation-vibration coupling
- Comparison to *ab initio* PGCM

Conclusions and perspectives

Outline

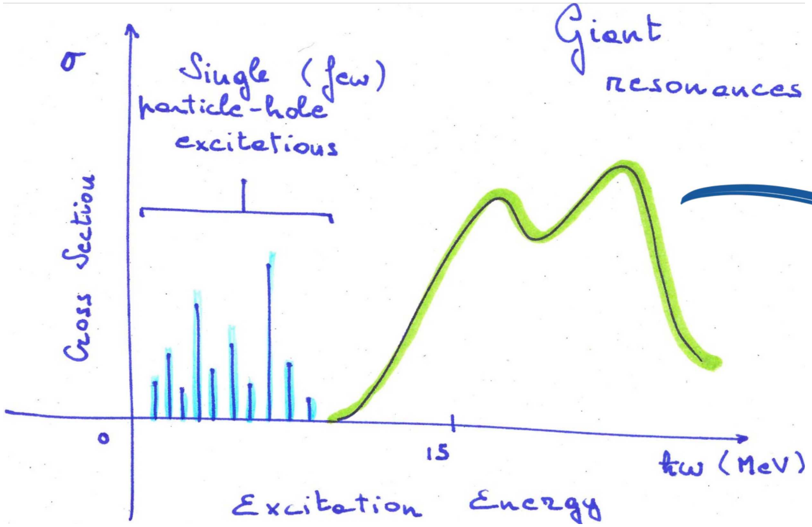
Giant Resonances

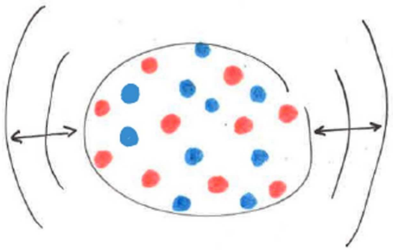
Dual nature of nucleus

- Single-particle features
- Collective behaviour

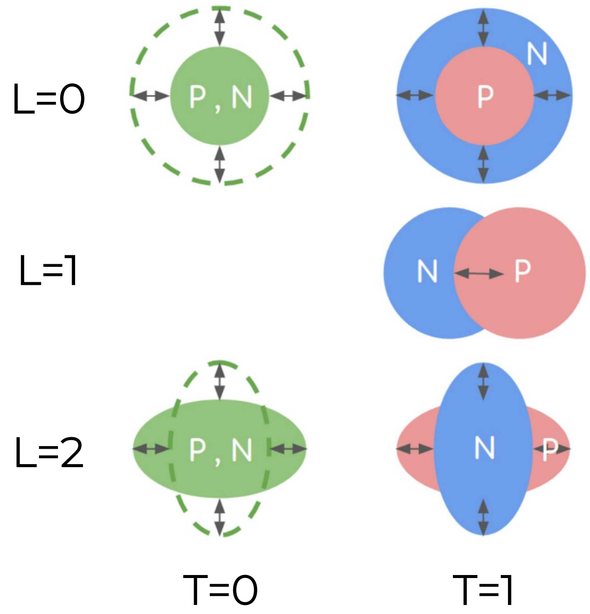
Compression-mode resonances

- Incompressibility of nuclear matter K_∞
- Nuclear Equation of State
- Core-collapse supernova explosion





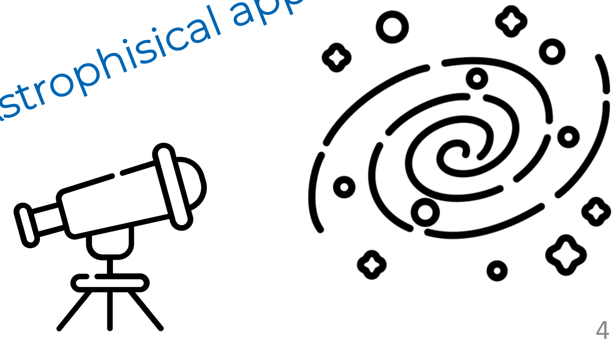
Liquid drop picture
vibrations, oscillations



Giant Resonances (GRs)

clearest manifestation of collective motion

Astrophisical applications !



Theoretical EDF tools

(Q)RPA

- Very popular and systematic: **Gogny**, **Skyrme,** relativistic
- **Deformation** and **coupling** effects
- Many variants: **(Q)FAM**, **2nd-RPA**, **SCRPA**, **PVC**

[Péru, Goutte, PRC, 2008]
[Losa, Pastore, Dossing, Vigezzi, Broglia, PRC, 2010]
[Li, Niu, Colò, PRL, 2023]

TD-HF(B)

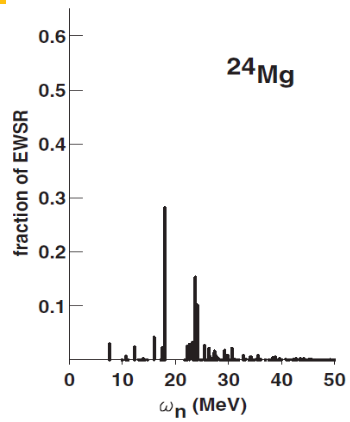
- Equivalent to **(Q)RPA** in the **small-amplitude** limit
- **Systematic** along the nuclear chart
- **Multi-reference** extensions

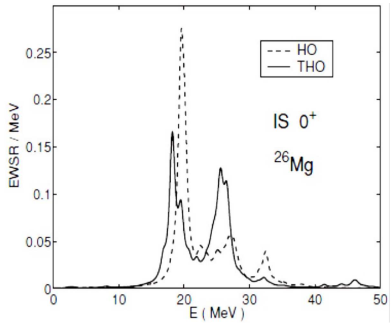
[Avez, Simenel, EPJA, 2013]
[Scamps, Lacroix, PRC, 2014]
[Marevic, Regnier, Lacroix, PRC, 2023]

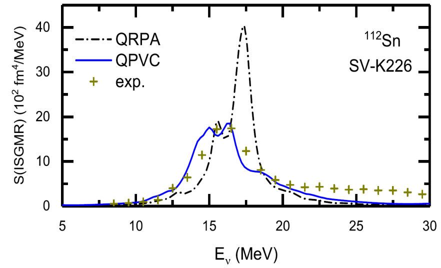
GCM

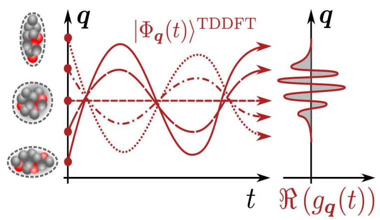
- Early studies of GRs in the GCM frame
- **Anharmonic** effects in **light-** and **medium-mass** systems

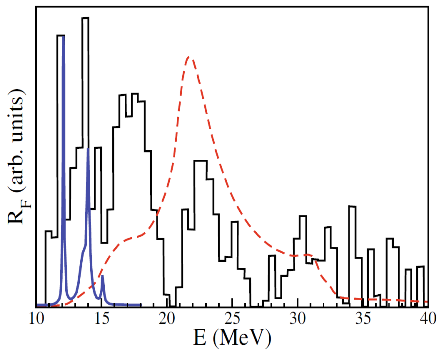
[Flocard, Vautherin, NPA, 1976]
[Blaizot, Berger, Dechargé, Girod, NPA, 1995]

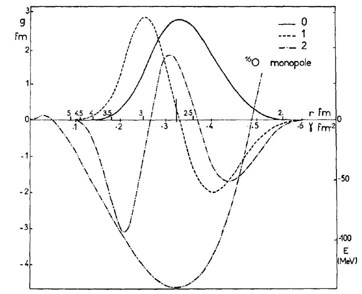












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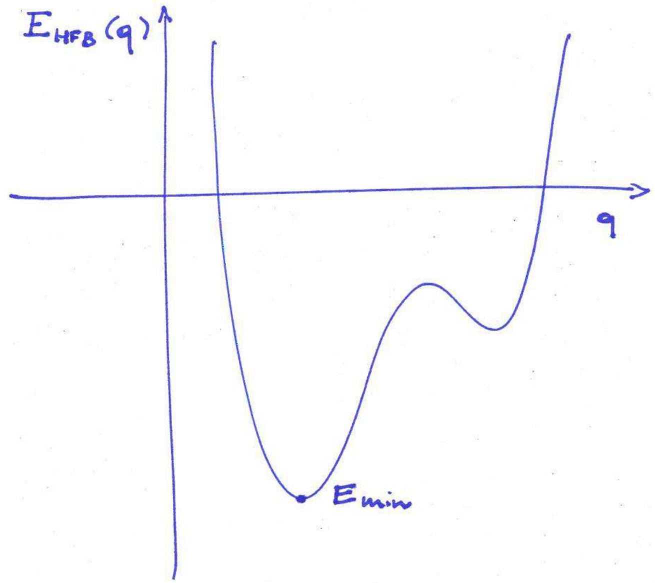
GCM and (Q)RPA

Schrödinger equation $H|\Psi_n\rangle = E_n|\Psi_n\rangle$



Open-shell systems → Strong static correlations → Symmetry-breaking reference states

1 Constrained HFB solutions

$$|\Phi(q)\rangle$$

Generator coordinates

(q can be any coordinate)

Diagonalization in a physically-informed reduced Hilbert space

2 PGCM Ansatz

$$|\Psi_n\rangle = \int \mathrm{d}q\, f_n(q)\, |\Phi(q)\rangle$$

Linear coefficients

Initially developed for large-amplitude collective motion

3 HWG Equation

Variational method

$$\delta \frac{\langle\Psi_n|H|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle} = 0$$

Schrödinger-like equation

$$\int \left[\mathcal{H}(p,q) - E_n \mathcal{N}(p,q)\right] f_n(q)\,\mathrm{d}q = 0$$

Kernels evaluation

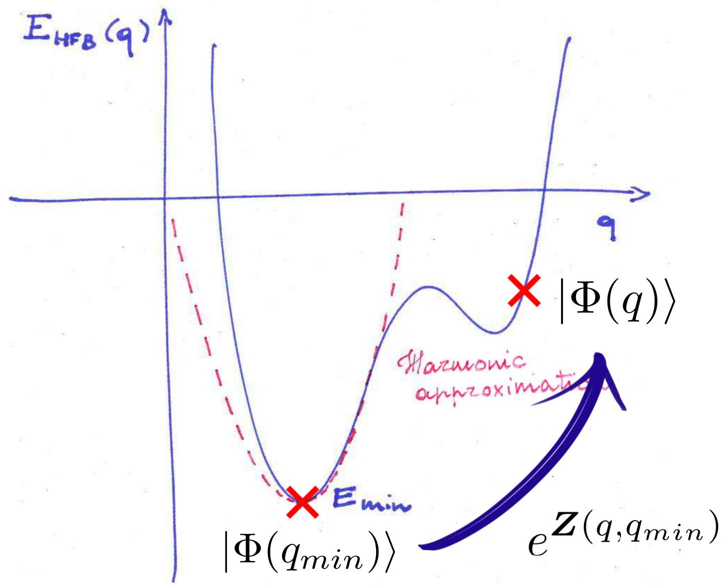
$$\mathcal{H}(p,q) \equiv \langle\Phi(p)|H|\Phi(q)\rangle$$
$$\mathcal{N}(p,q) \equiv \langle\Phi(p)|\Phi(q)\rangle$$

GCM and (Q)RPA

Thouless theorem

$$|\Phi(q)\rangle = \langle\Phi(q_{min})|\Phi(q)\rangle e^{\boldsymbol{Z}(q,q_{min})}|\Phi(q_{min})\rangle$$

Non-unitary transformation



HWG equation

$$\delta\frac{\langle\Psi_n|H|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle} = 0$$

Introduce the Quasi-Boson approximation (QBA)

Expand to the quadratic level in $\boldsymbol{Z}(q,q_{min})$

Harmonic approximation → No coordinates dependency !

All coordinates are explored

(differently from GCM)

Eventually rewrites as (Q)RPA equations

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

Nuclei that are stiff against deformations

(anharmonic effects negligible)

[Jancovici, Schiff, 1964]

Symmetry restoration in QRPA

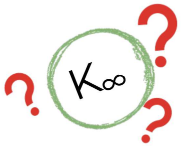
Intrinsic density is the fundamental variable in EDF

Much is learnt from symmetry breaking and restoration

Projection

Intrinsic frame → Laboratory frame

- Common in SR and MR EDF
- Not in linear response on SR EDF (i.e. QRPA)



SYMMETRY-CONSERVING RANDOM PHASE APPROXIMATION†

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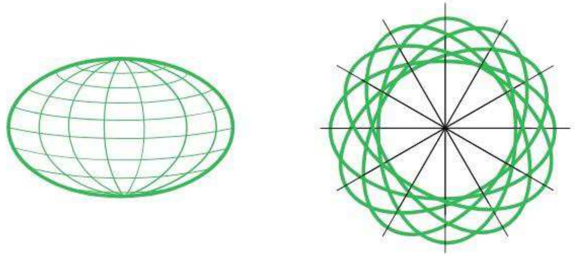
Received 18 July 1984

Abstract: The projected random phase approximation (PRPA) is derived from a generator coordinate ansatz. It allows the calculation of excited states in the region of phase transitions, where conventional RPA breaks down. The theory is applied for an approximate solution of the R(8) model which shows a pairing collapse at large angular momenta.



Projection before solving QRPA

VAP QRPA

Computationally expensive, no realistic application

What about PAV QRPA ?

Can we treat projection a posteriori ?

PAV RPA

[Erler, PhD Thesis, TUD, 2012]

Standard assumptions

- Needle approximation for AMP
- RPA reinstates the missing symmetries to some extent

The Random Phase Approximation: Its Role in Restoring Symmetries Lacking in the Hartree–Fock Approximation

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AND

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Fisica Atomica y Nuclear, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain

Received April 1, 1980

Hartree–Fock wave-functions often lack symmetries possessed by the Hamiltonian. It is often said that the Random Phase Approximation (RPA) restores the missing symmetries. Since the RPA does not readily lead to explicit wave-functions, it is not a trivial matter to verify this assertion. We analyse the situation, and show that, while RPA restores symmetry in some respects, it does not do so completely. Besides the normal RPA, we discuss the generalisation of RPA that describes modes in isobars of the given nucleus. This is needed to enable us to discuss the case of isospin symmetry, which is analysed in detail.

Present work

- Exact Angular Momentum Projection (RPA)
- Focus on **K=0** (monopole and quadrupole)

Theoretical challenge !

$$Q_n^\dagger \,|\mathrm{RPA}\rangle = |n\rangle \qquad Q_n \,|\mathrm{RPA}\rangle = 0 \quad \forall n$$

$$Q_n^\dagger = \sum_{ph} \left\{ X^n_{ph} c_p^\dagger c_h - Y^n_{ph} c_h^\dagger c_p \right\}$$

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

- Symmetry-breaking solutions $|\mathrm{RPA}\rangle$ $|n\rangle$
- Implicit wave-functions
- Correlations encoded in 1B transition amplitudes

Projected states $|n^J\rangle \equiv N_n^J P^J \,|n\rangle$

Angular Momentum Projection

Reminder

For integer J

$$P^J_{MK} = \frac{2J+1}{8\pi^2} \int d\Omega \; \mathcal{D}^{J*}_{MK}(\Omega)\mathcal{R}(\Omega)$$

(α, β, γ)

Wigner D matrices

Rotation operator

In axial systems (good K) equivalent to

$$P^J_{MK} = \frac{2J+1}{2} \int_{-1}^{+1} d\,(cos\beta) \;\; d^J_{MK}(\beta) e^{-i\beta \hat{J}_y}$$

Wigner small-d matrices

1d rotation

Remark

For J=0 projection is a pure rotation

Introduce a rotational state

$$|\mathrm{ROT}\rangle \equiv N_{\mathrm{ROT}} P^0_{00} |\mathrm{HF}\rangle$$

$$= N_{\mathrm{ROT}} \frac{1}{2} \int_{-1}^{+1} d\,(cos\beta) \;\; e^{-i\beta \hat{J}_y} |\mathrm{HF}\rangle$$

Outline

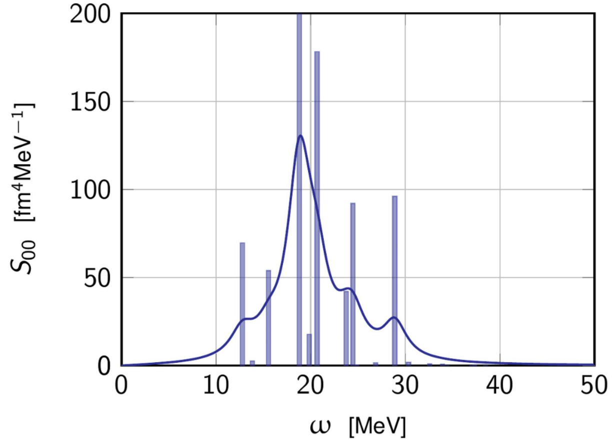
Setting

Studied quantity: monopole (quadrupole) strength

- Transition amplitudes: height of peaks
- Energy difference: position of peaks

$$S_{00}(\omega) \equiv \sum_{\nu} |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

JM=00



Numerical details

- QRPA code based on HFBTHO v1.66
- SkM* parametrisation

N_{sh}	E_{HF} [MeV]	r [fm]	β
7	-195.65	2.991	0.378
9	-196.21	3.009	0.392
11	-196.93	3.011	0.383
13	-197.15	3.016	0.390

Systematic study for ^{24}Mg

- Non-superfluid solutions found for all studied HO basis dimensions
- HF ground state used for deformed RPA calculations

$$\beta \equiv \sqrt{\frac{\pi}{5}} \frac{\langle Q_{20} \rangle_\pi + \langle Q_{20} \rangle_\nu}{\langle r^2 \rangle_\pi + \langle r^2 \rangle_\nu}$$

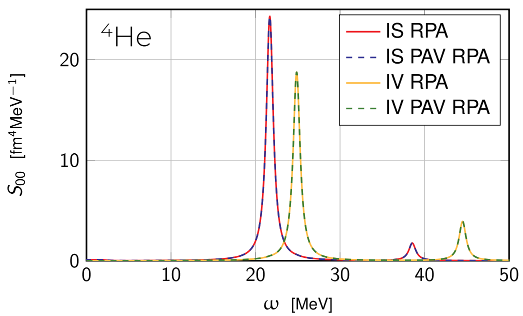
Setting

RPA response stability wrt basis variations

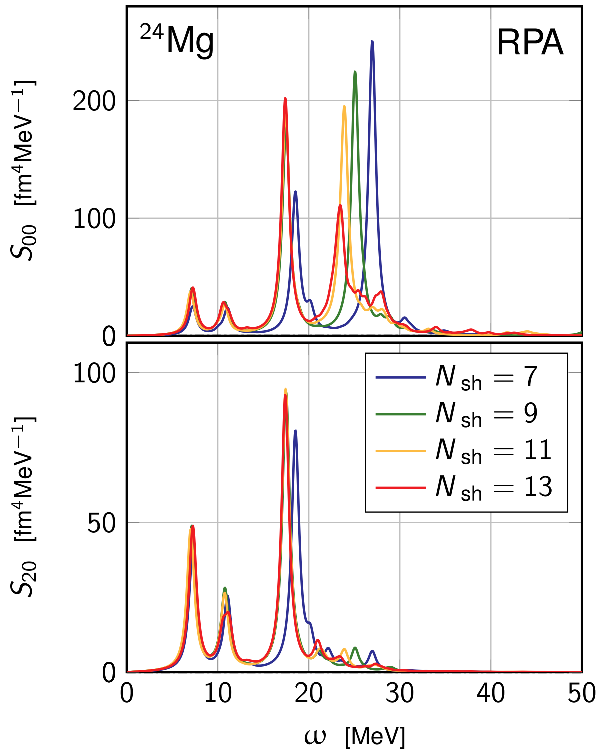
- HO basis convergence
  - Global stability
  - High-energy fragmentation (continuum)
- 1p1h RPA basis
  - Rapid convergence
  - Ecut=100 MeV

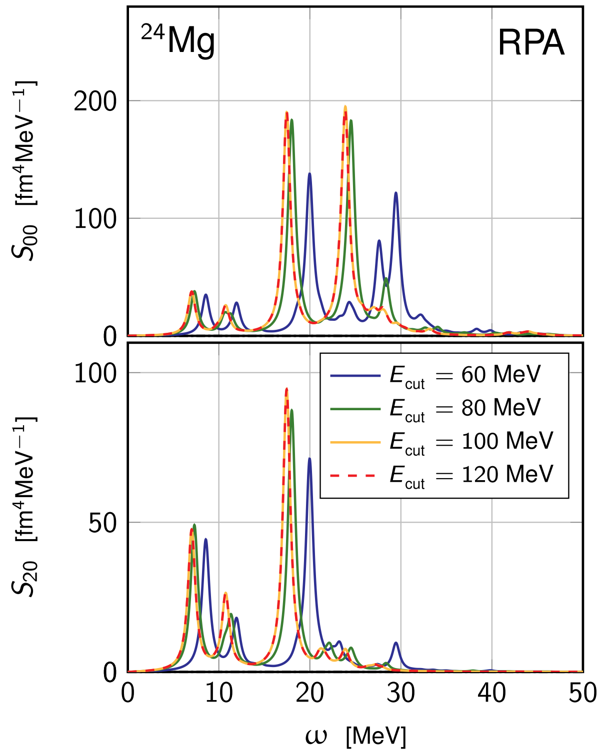
AMP Benchmarks

- Test on a spherical system (^{4}He)
- AMP identity resolution accurately satisfied

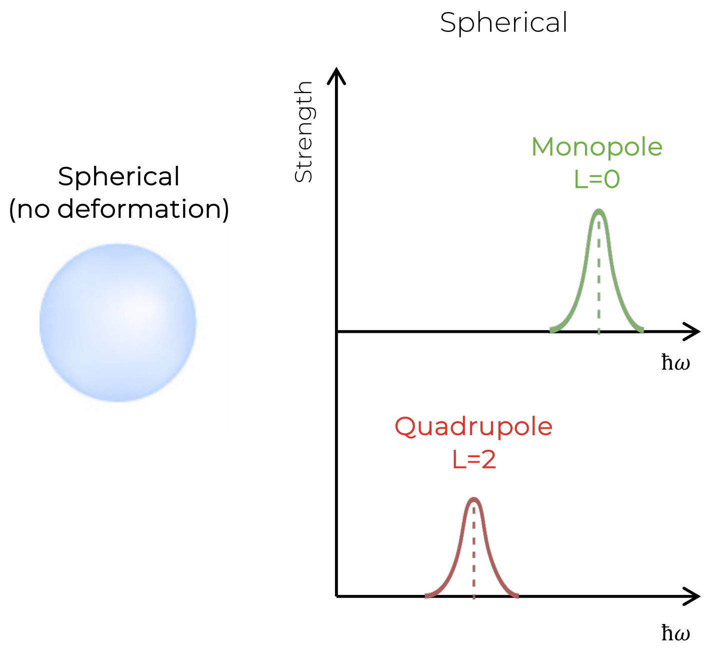


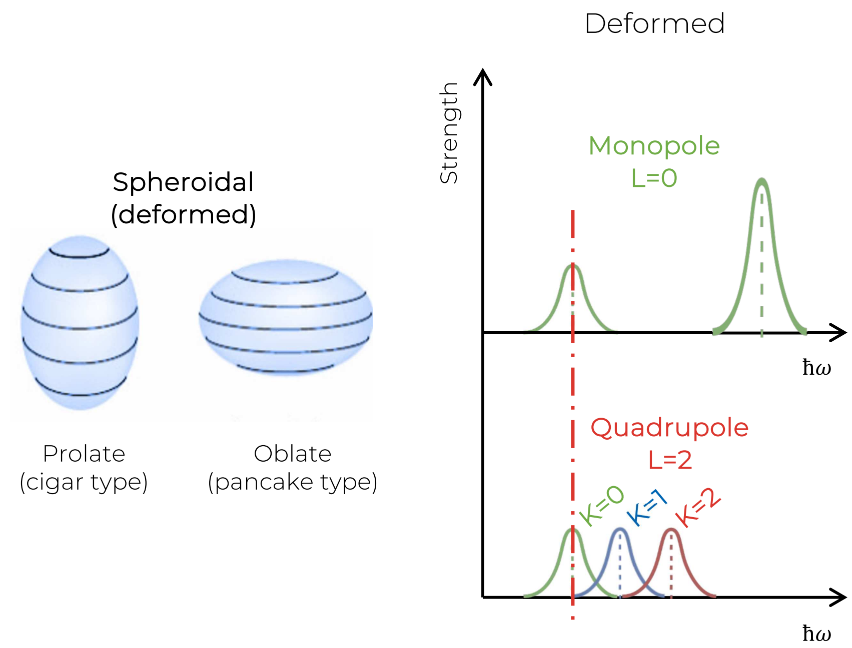
$$\mathbb{1} = \sum_{JM\alpha} |JM\alpha\rangle\langle JM\alpha| = \sum_{JM} P^J_{MM}$$





AMP RPA results

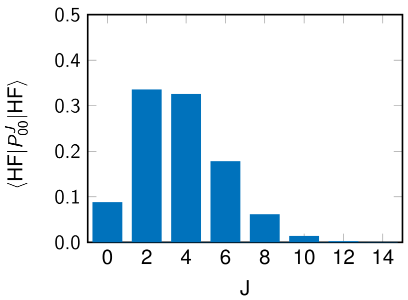




AMP RPA results

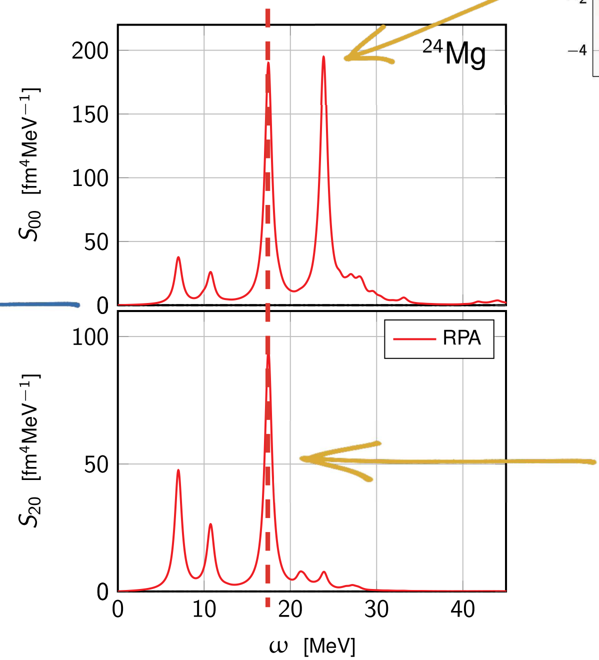
Intrinsic frame (deformed)

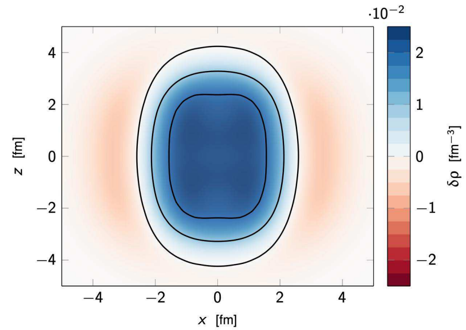
Laboratory frame (projected)



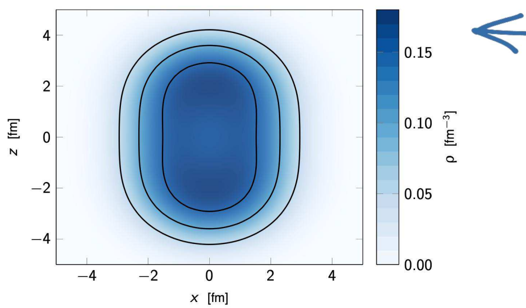
Spread over several J's

GMR-GQR coupling

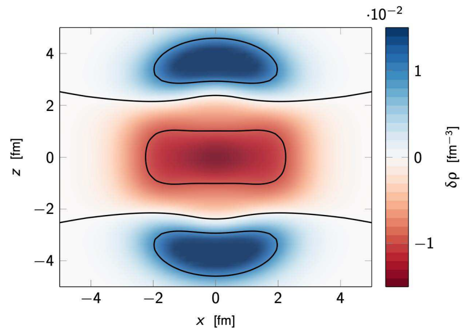




Monopolar vibration (shape-conserving)



Well-deformed HF ground state

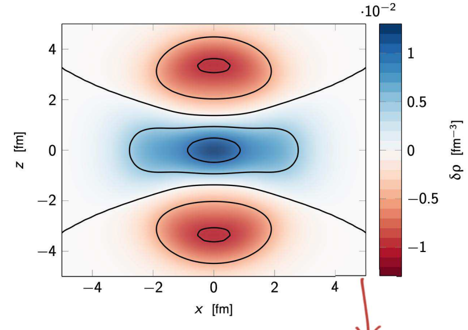


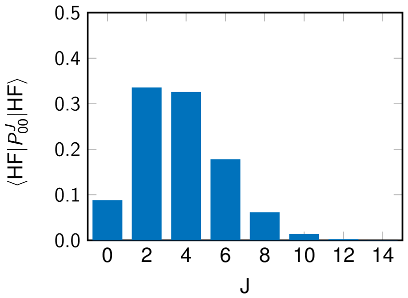
Quadrupolar vibration (clear Y_{20} signature)

AMP RPA results

Intrinsic frame (deformed)

Laboratory frame (projected)





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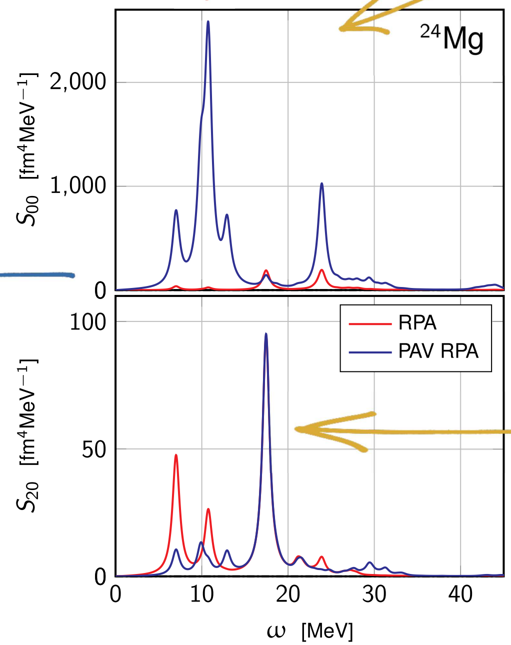
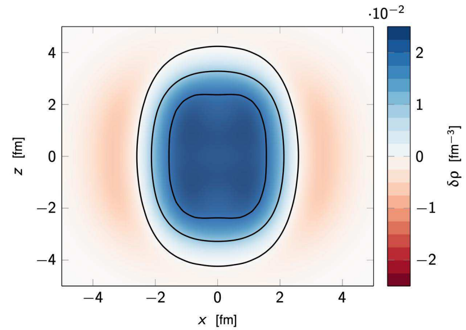
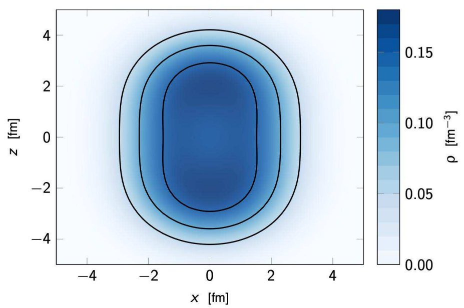




Monopolar vibration
(shape-conserving)



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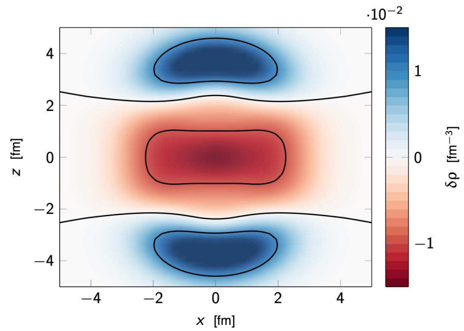
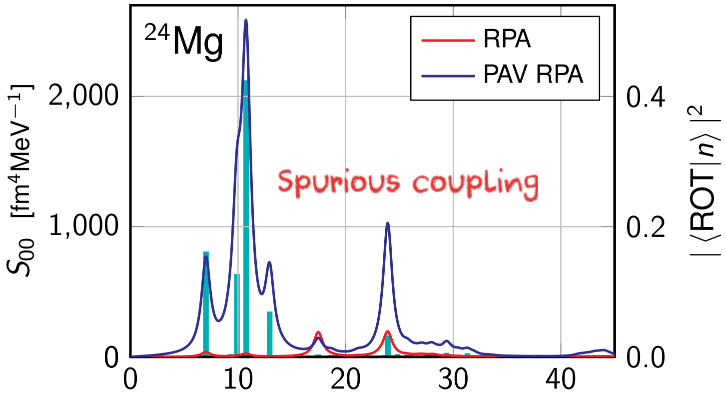


Quadrupolar vibration
(clear Y_{20} signature)

Rotation-vibration coupling

Where does the strength come from ?



RPA : symmetry-breaking solutions $|n\rangle_{\mathrm{def}}$ (vibrational)

Non-vanishing overlap with the rotational state !

$$\langle \mathrm{ROT}|n\rangle_{\mathrm{def}}$$

RPA states have vibrational and rotational (spurious) content

$$|n\rangle_{\mathrm{def}} = a_{\mathrm{rot}}\,|\mathrm{ROT}\rangle + b_{\mathrm{vib}}\,|\mathrm{VIB}\rangle$$

Can be subtracted !

$$|\tilde{n}\rangle \equiv N_{\tilde{n}}\,(|n\rangle - a_n|\mathrm{ROT}\rangle)$$

$$\langle \mathrm{ROT}|\tilde{n}\rangle = 0 \quad \rightarrow \quad a_n = \langle \mathrm{ROT}|n\rangle$$

Subtraction + Projection

Rotation-vibration coupling

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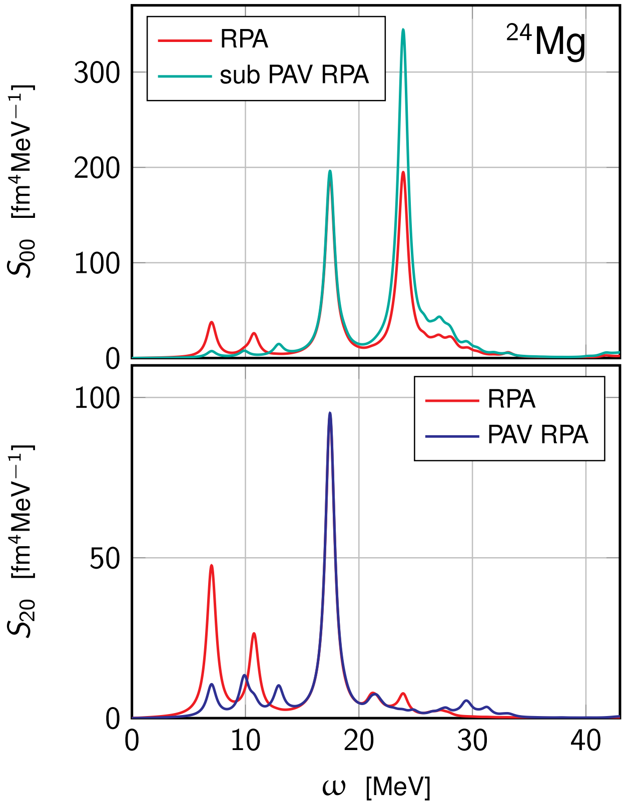

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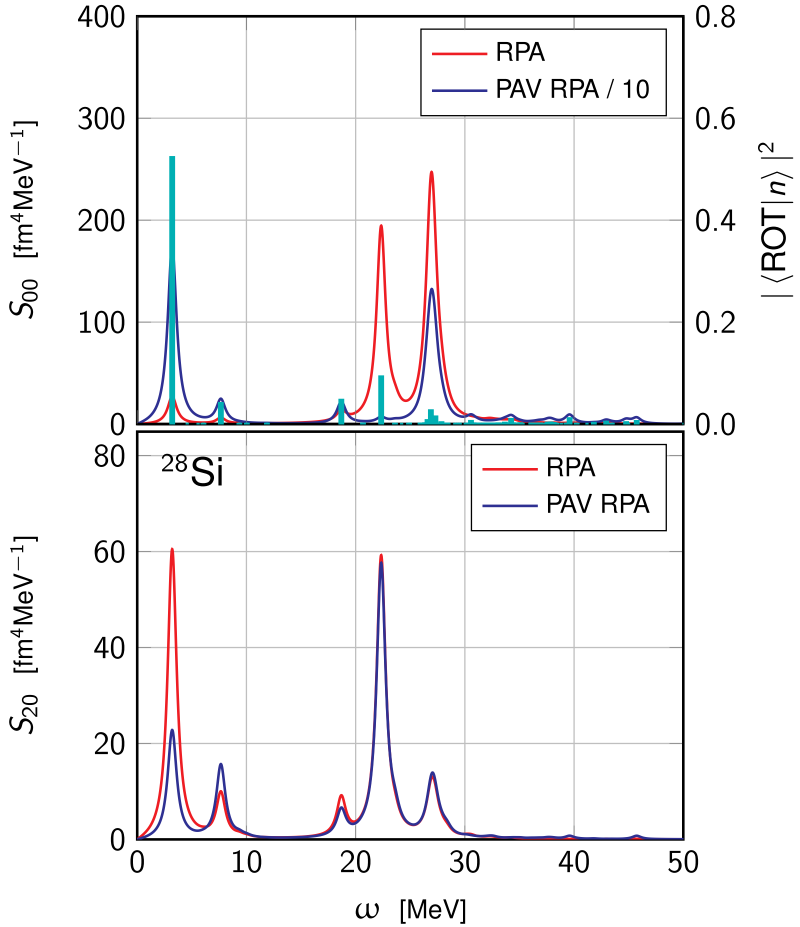
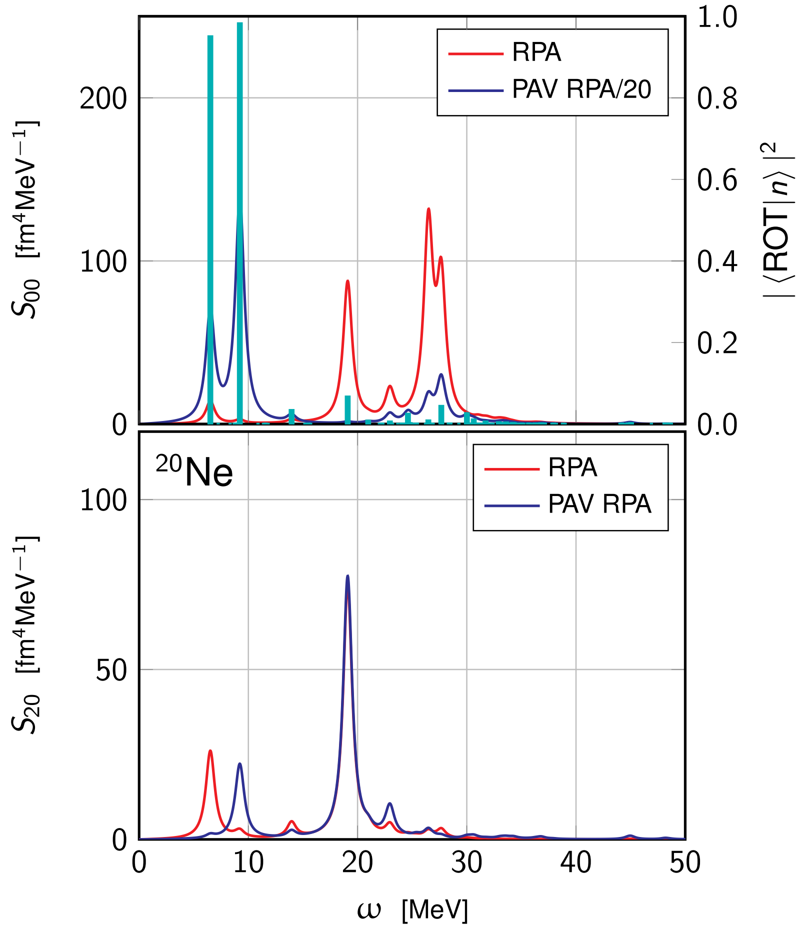
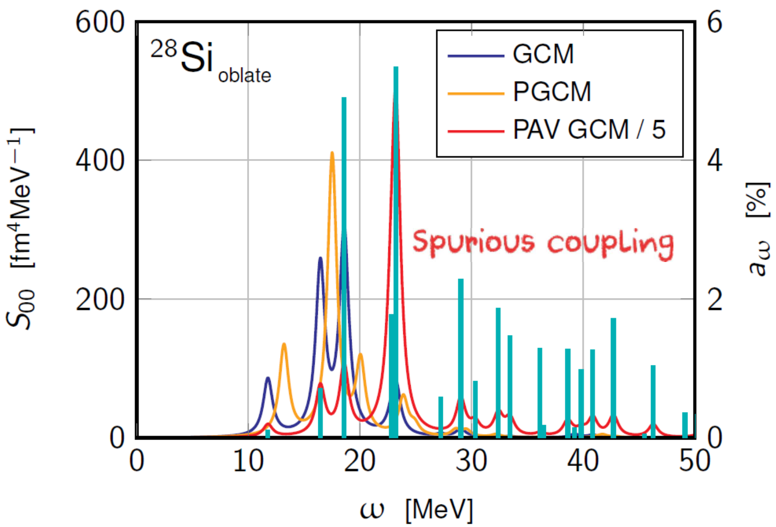
Subtraction + Projection

Observation in other systems





Comparison to *ab initio* PGCM



GCM : symmetry-breaking solutions $|\mathrm{GS}\rangle_{\mathrm{def}}$ $|\omega\rangle_{\mathrm{def}}$

PGCM : symmetry-conserving solutions $|\mathrm{GS}\rangle_{\mathrm{sym}}$ $|\omega\rangle_{\mathrm{sym}}$

Variational treatment of rotations in PGCM !

PAV GCM: projection of symmetry-breaking solution

- Anomalous spectrum
- Zero-frequency rotations (Goldstone modes)
- Born-Oppenheimer-like approximation

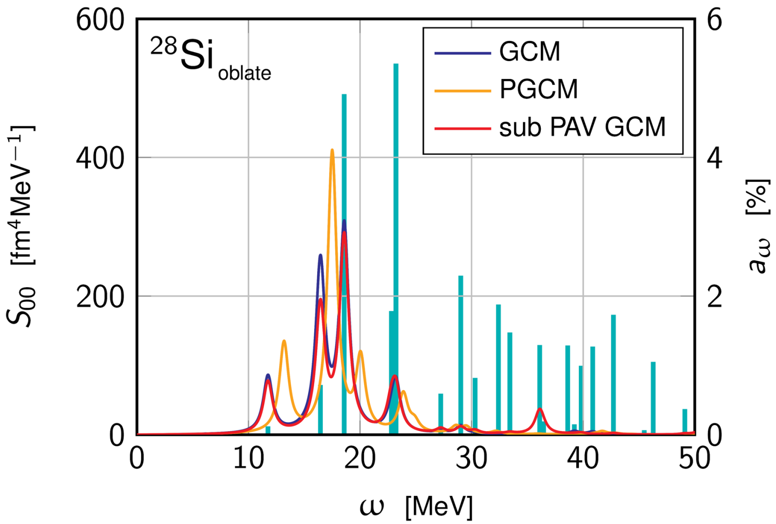
Similar results in GCM and RPA

- Does not depend on the many-body method
- Consequence of deformed ground state

Rotations must be treated variationally !

- PGCM already does
- Projected QRPA needed

Comparison to *ab initio* PGCM



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Summary

DIFFERENT FLAVOURS OF SYMMETRY BREAKING AND RESTORATION

Symmetry breaking

(Q)RPA			GCM
Harmonic fluctuations around deformed HF(B)	✓	✓	Large amplitudes superposition of def. HF(B) states
PROJECTION AFTER DIAGONALIZATION ⚠ Spurious coupling PAV RPA [1] *New implementation*	✓	✓	**PROJECTION AFTER DIAGONALIZATION** ⚠ Spurious coupling PAV GCM *New implementation*
PROJECTION BEFORE DIAGONALIZATION P(Q)RPA [2]	✗	✓	**PROJECTION BEFORE DIAGONALIZATION** PGCM

Needed for proper comparison with experiments !

Symmetry conserving

(1) [Erler, PhD Thesis, TUD, 2012]

(2) [Federschmidt and Ring, NucPhysA, 1985]

Thanks for the attention