Effects of angular momentum projection in RPA and GCM calculations

SSNET'24 - Shapes and Symmetries in Nuclei: from Experiment to Theory

IJCLab, Orsay, November 6th, 2024

Andrea Porro
Technische Universität Darmstadt

[PRC (2024) 109, 044315]

Based on

PHYSICAL REVIEW C **109**, 044315 (2024)

Symmetry-restored Skyrme-random-phase-approximation calculations of the monopole strength in deformed nuclei

A. Porro,[1,2,3,*] G. Colò,[4,5,†] T. Duguet,[1,6,‡] D. Gambacurta,[7,§] and V. Somà[1,‖]

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[2]*Department of Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany*
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[7]*INFN-LNS, Laboratori Nazionali del Sud, 95123 Catania, Italy*

(Received 16 December 2023; accepted 12 March 2024; published 9 April 2024)

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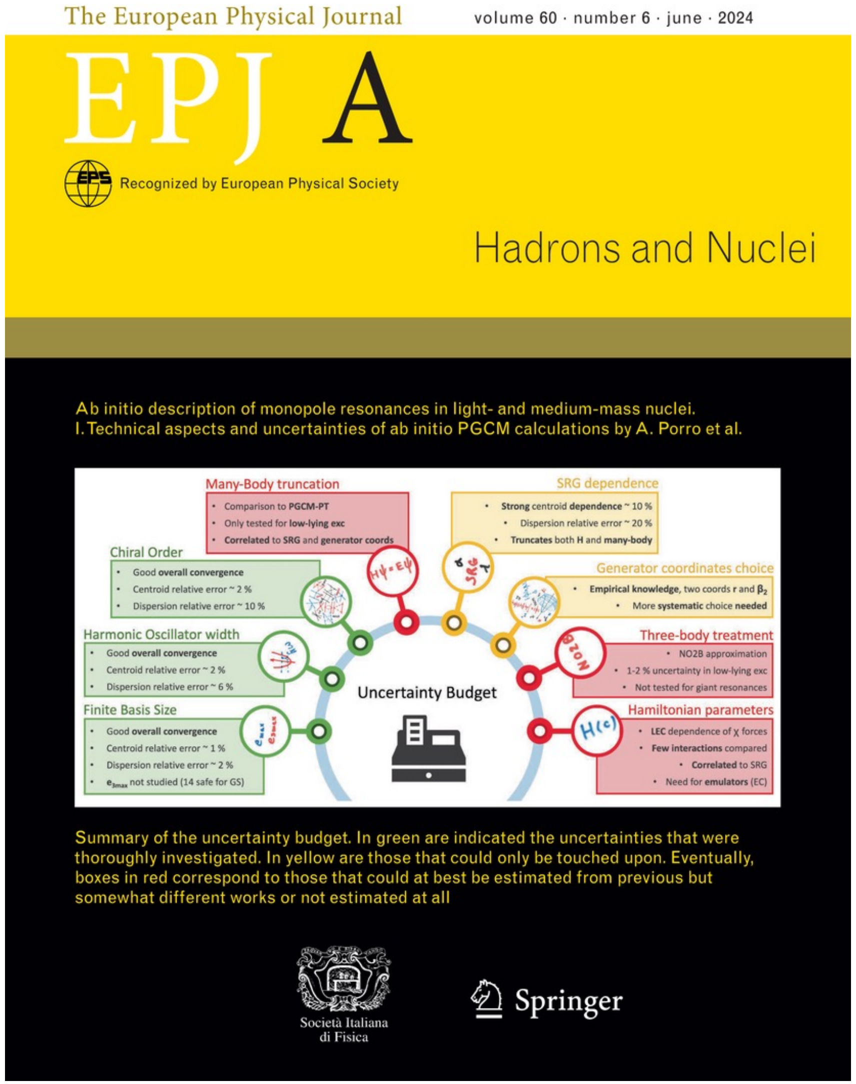
arXiv > nucl-th > arXiv:2407.01325

Nuclear Theory

[Submitted on 1 Jul 2024]

Ab initio description of monopole resonances in light- and medium-mass nuclei: IV. Angular momentum projection and rotation-vibration coupling

Andrea Porro, Thomas Duguet, Jean-Paul Ebran, Mikael Frosini, Robert Roth, Vittorio Somà



I. [EPJA (2024) 60, 133]
II. [EPJA (2024) 60, 134]
III. [EPJA (2024) 60, 155]
IV. [arXiv:2407.01325]

Outline

Introduction

- Giant Resonances
- GCM and RPA

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Random Phase Approximation

- Theoretical introduction
- Angular Momentum Projection

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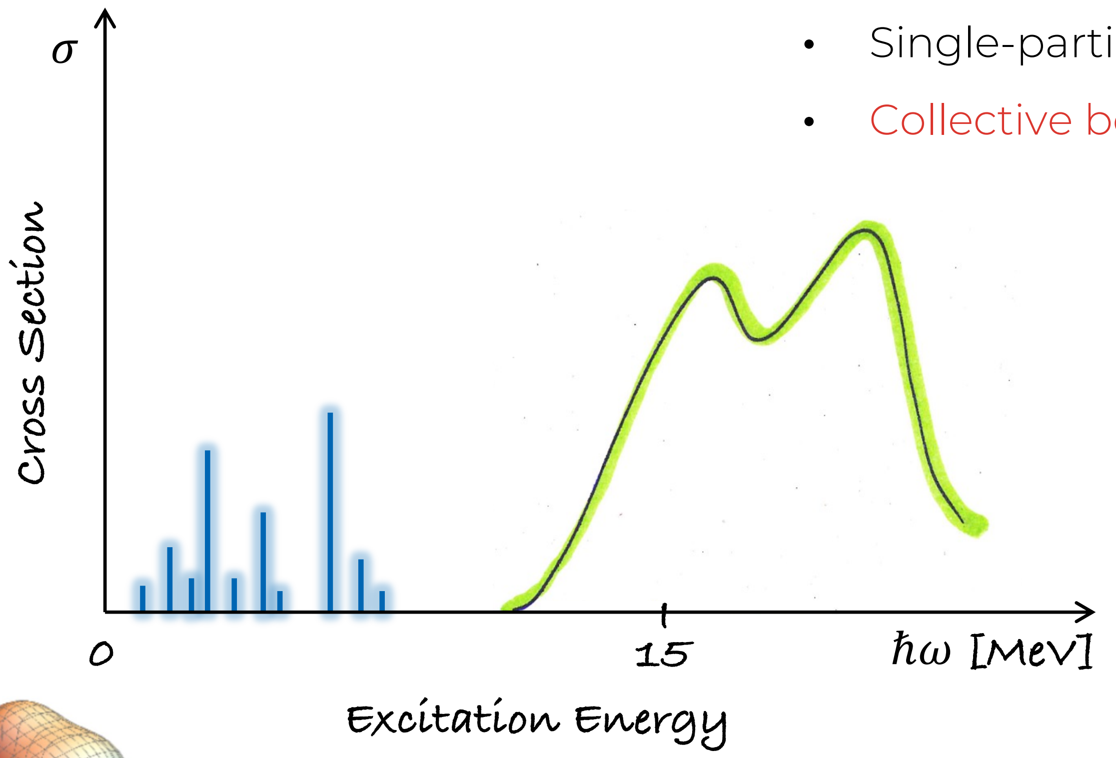
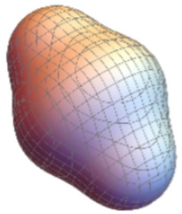
Giant Resonances



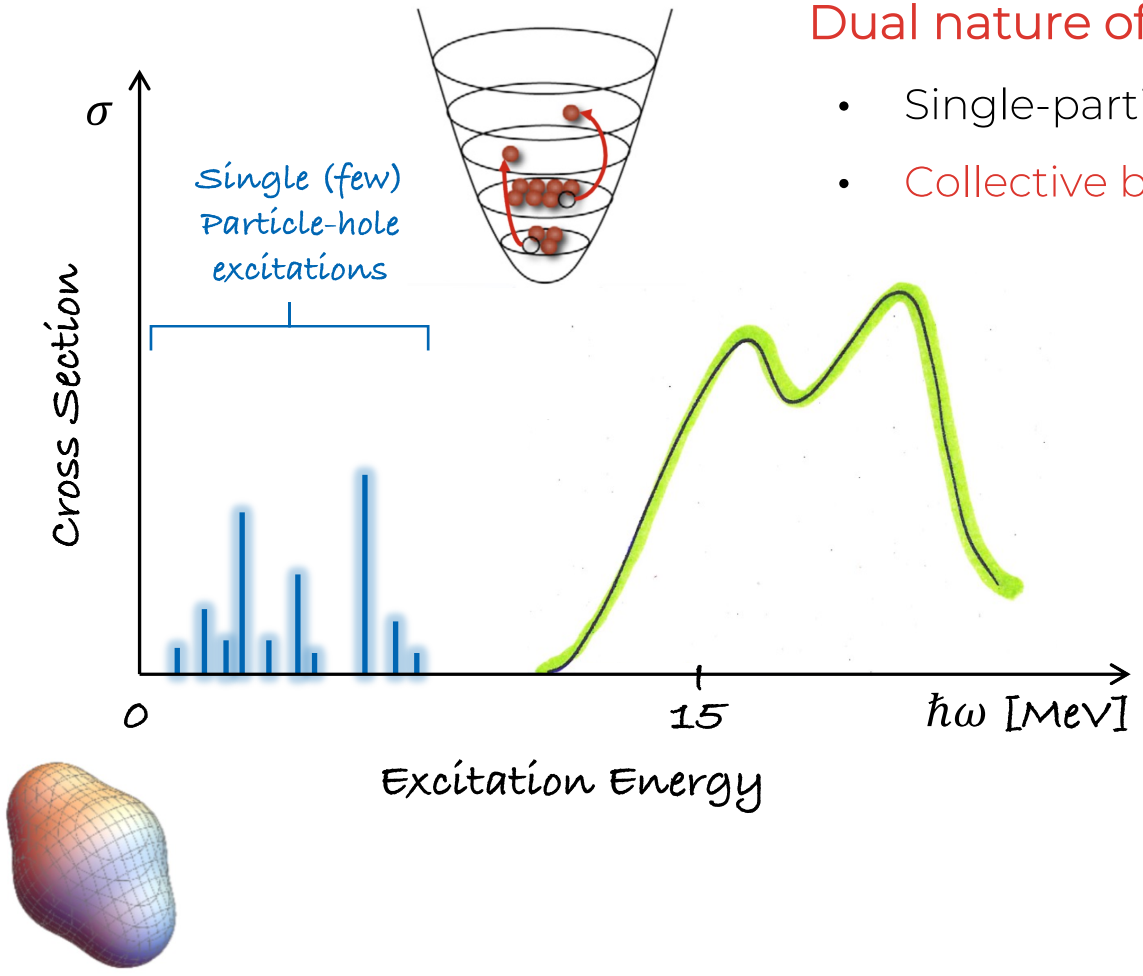


Dual nature of nucleus

- Single-particle features
- Collective behaviour

[Pictures from Dytrych et al., PRL, 2020]

Giant Resonances



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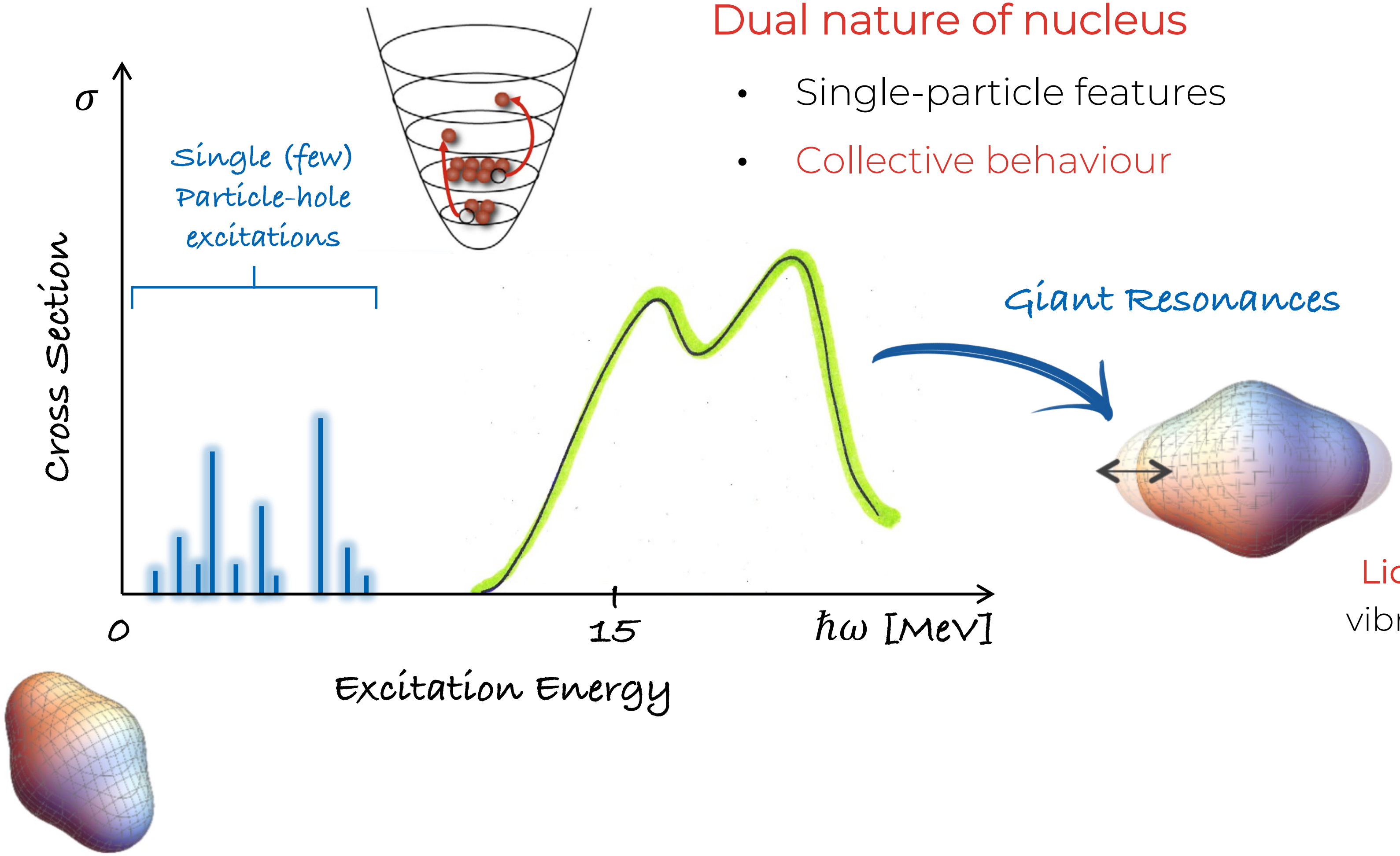

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Liquid drop picture
vibrations, oscillations

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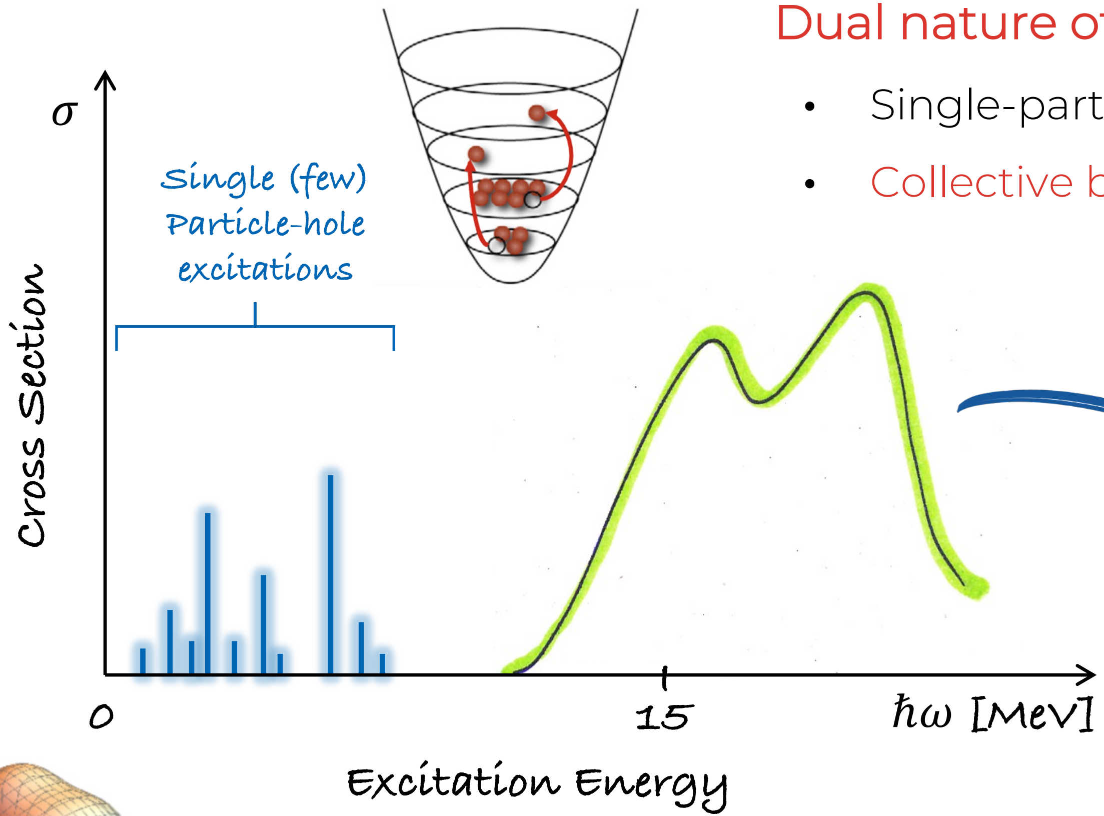

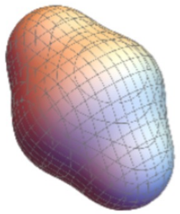

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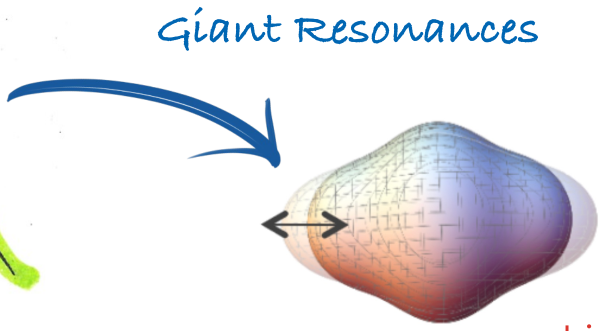

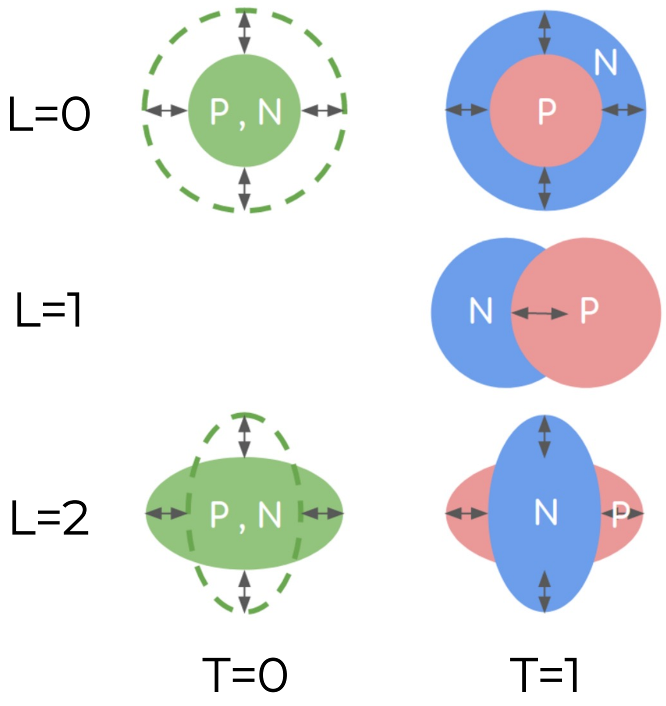

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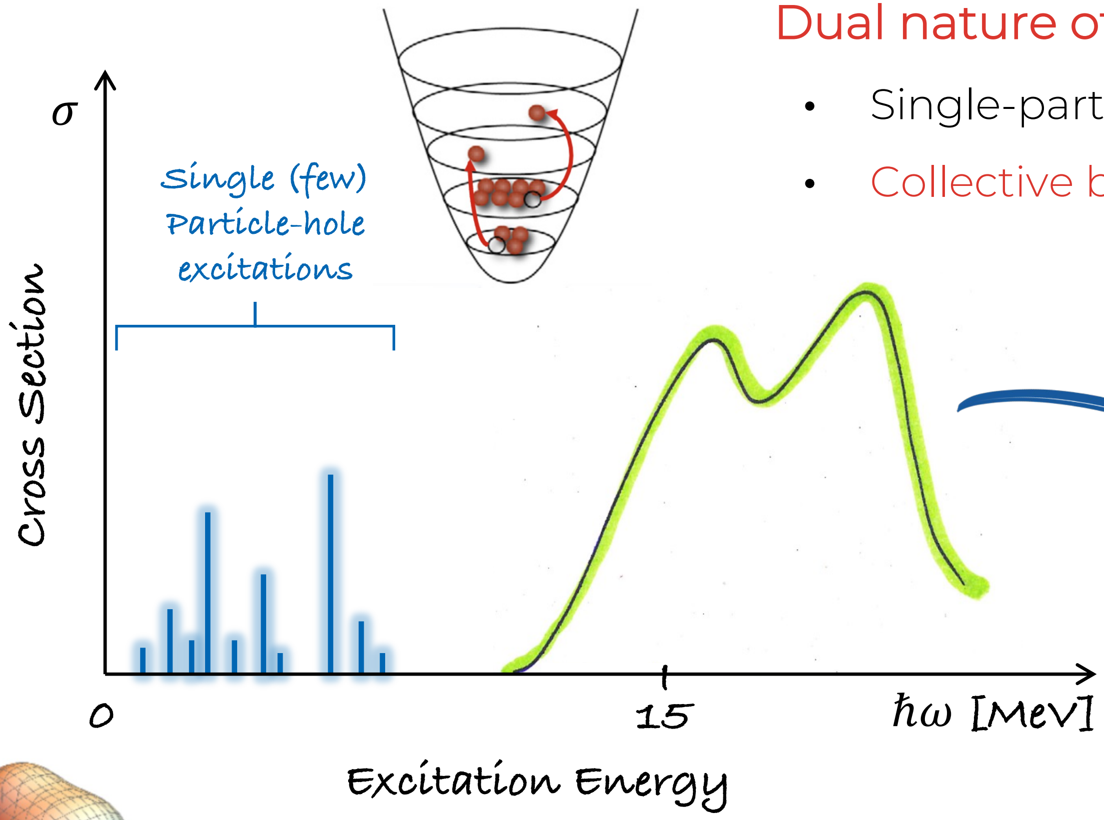

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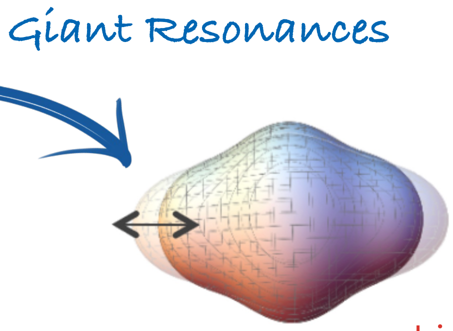

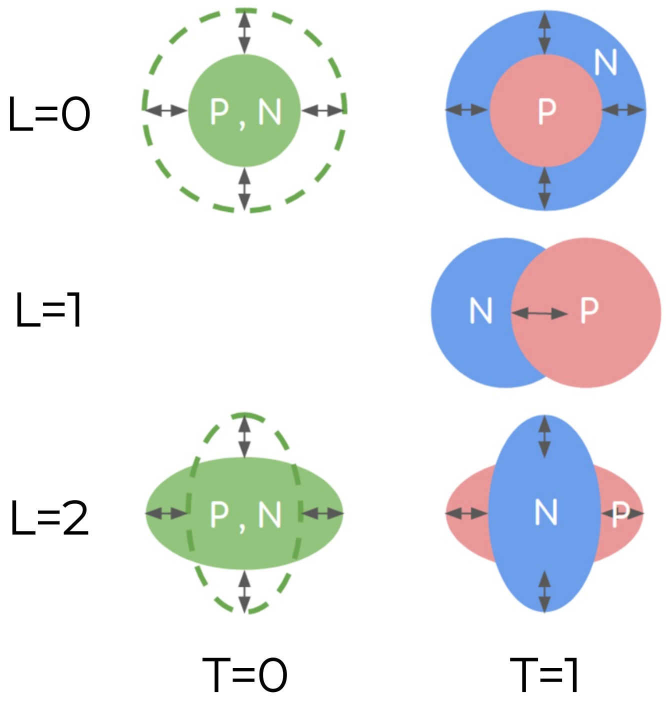

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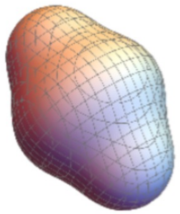
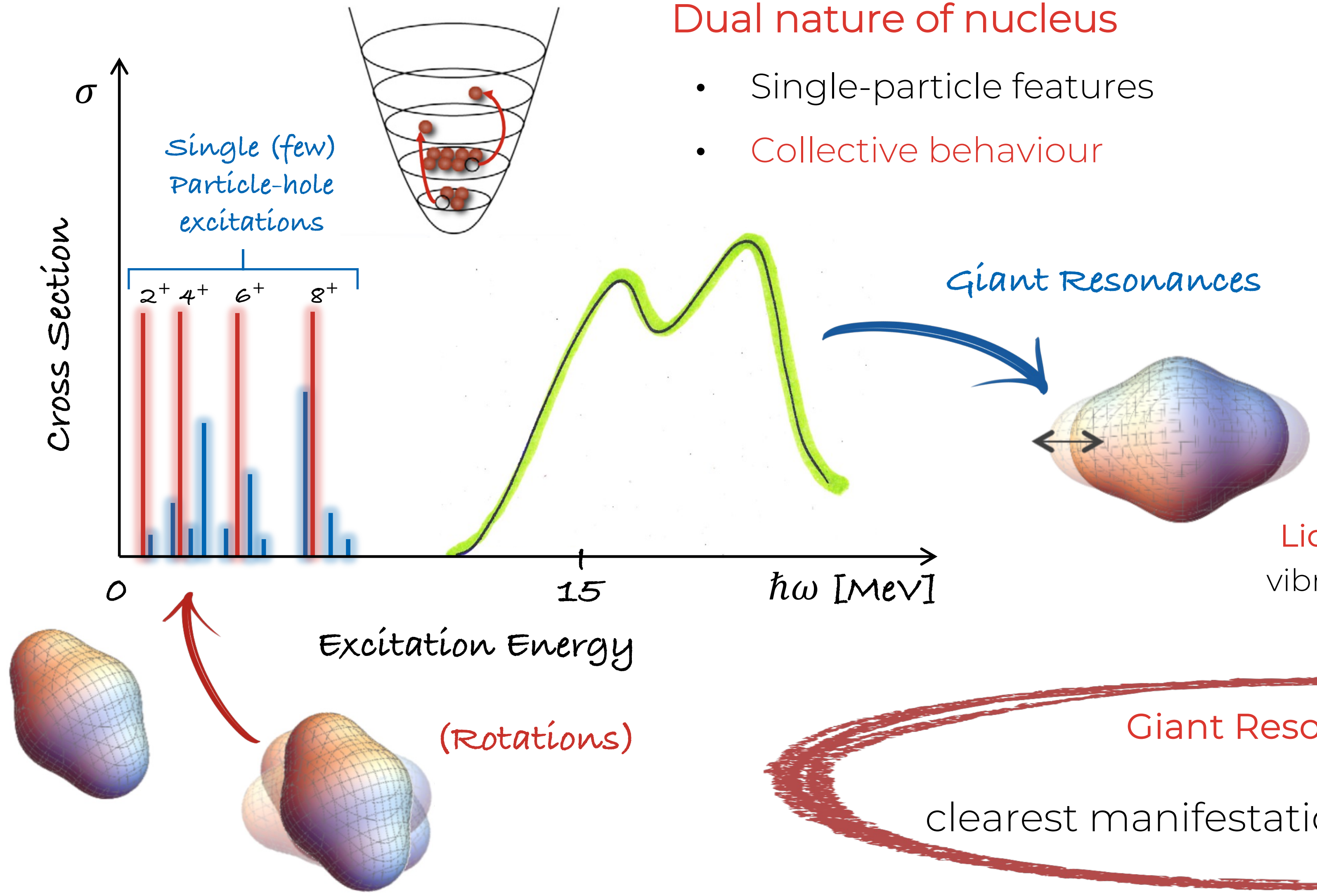


Giant Resonances (GRs)

clearest manifestation of collective motion

[Pictures from Dytrych et al., PRL, 2020]

Giant Resonances



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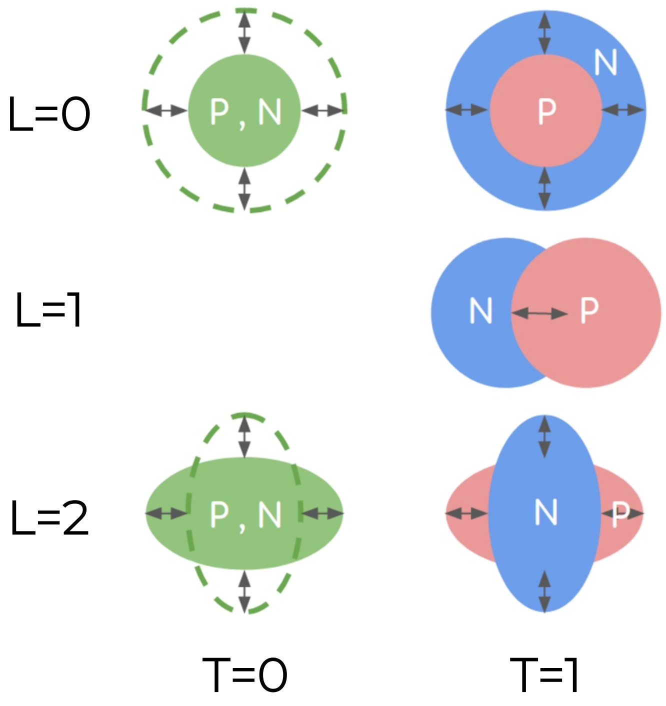

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GCM and (Q)RPA

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

GCM and (Q)RPA

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Open-shell systems

GCM and (Q)RPA

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Open-shell systems

→ Strong static correlations

GCM and (Q)RPA

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

Open-shell systems

Symmetry-breaking reference states

Strong static correlations

GCM and (Q)RPA

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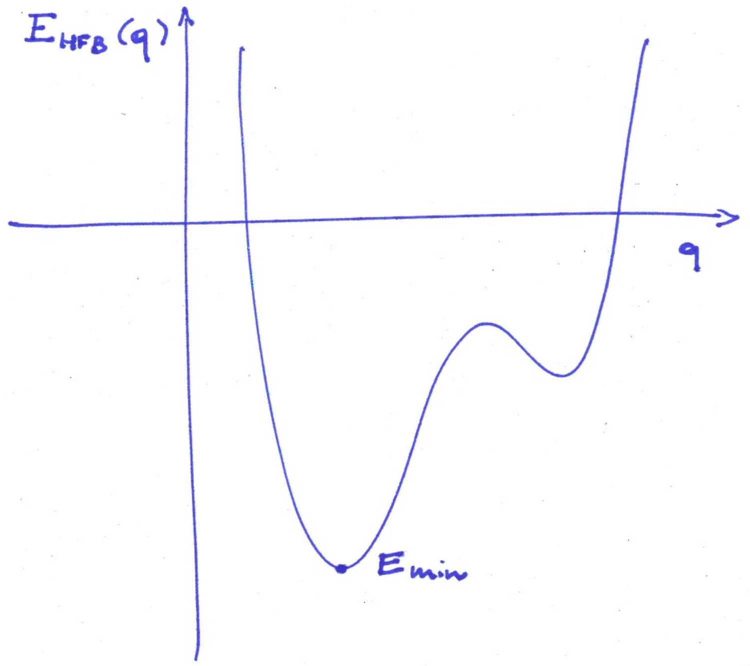
Open-shell systems → Strong static correlations → Symmetry-breaking reference states

1 *Constrained HFB solutions*

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



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Open-shell systems

Symmetry-breaking reference states

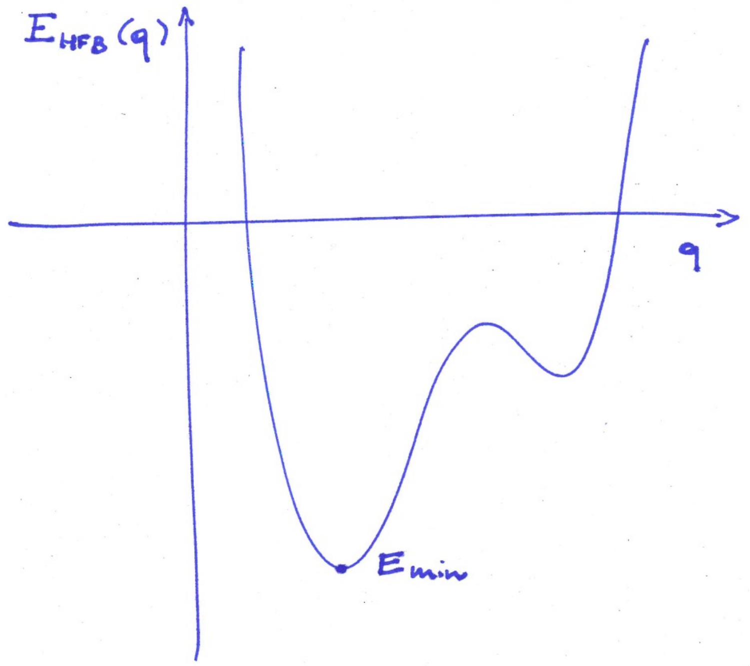
Strong static correlations

1 *Constrained HFB solutions*

$|\Phi(q)\rangle$

Generator coordinates

(q can be any coordinate)



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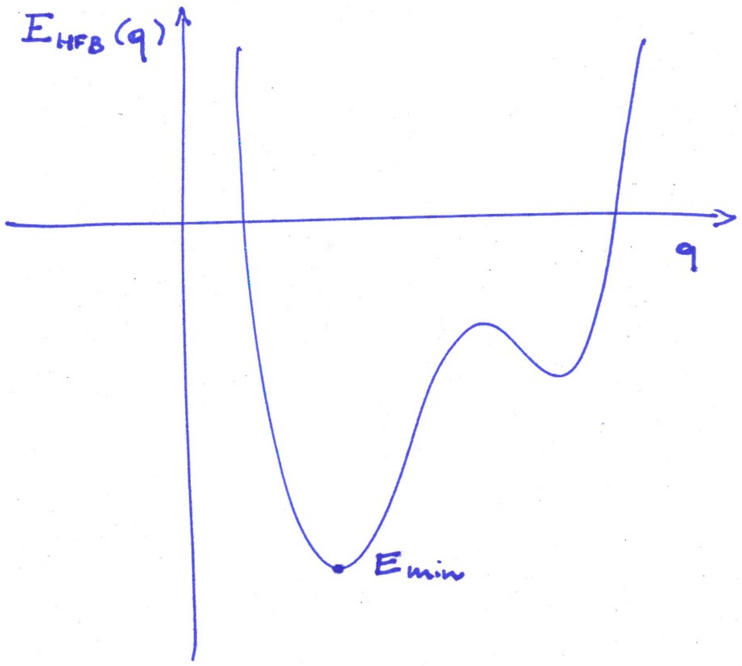
2 PGCM Ansatz

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



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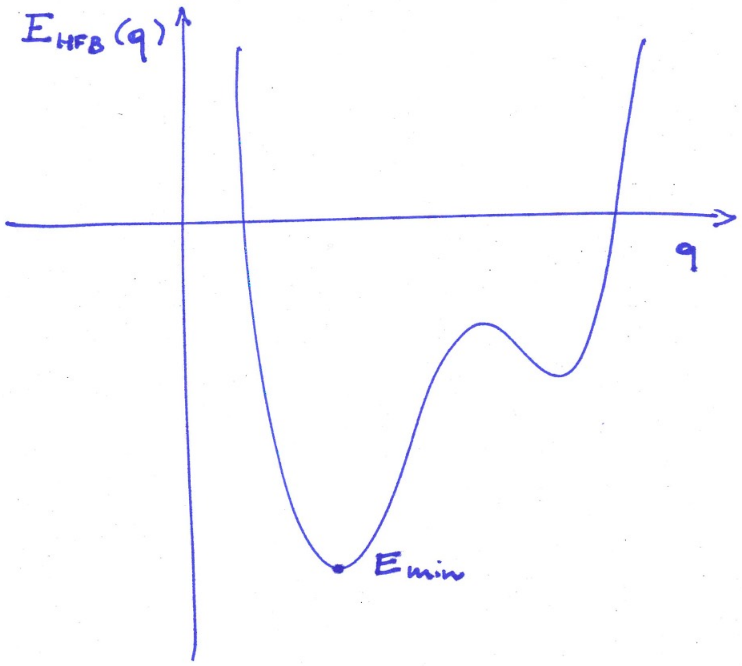

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$$|\Psi_n\rangle = \int \mathrm{d}q\, f_n(q)\, |\Phi(q)\rangle$$

Initially developed for large-amplitude collective motion

GCM and (Q)RPA

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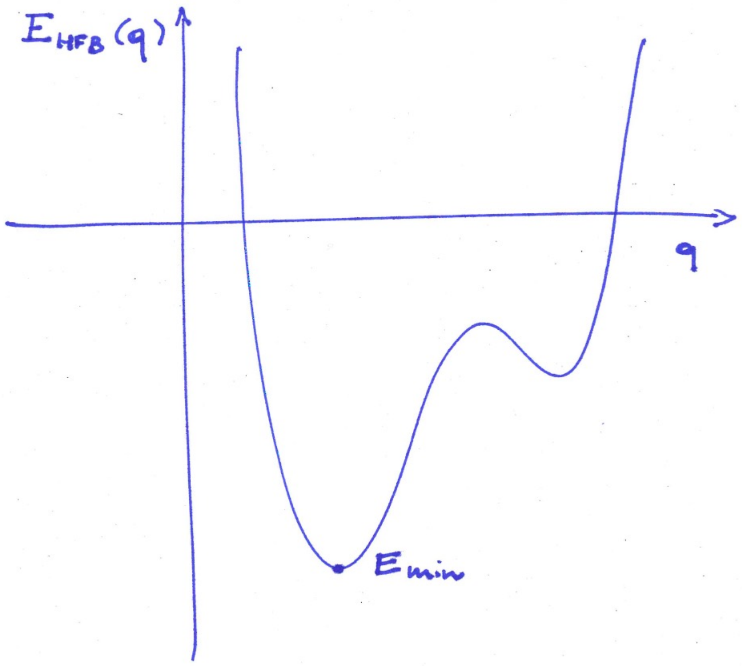
Linear coefficients



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

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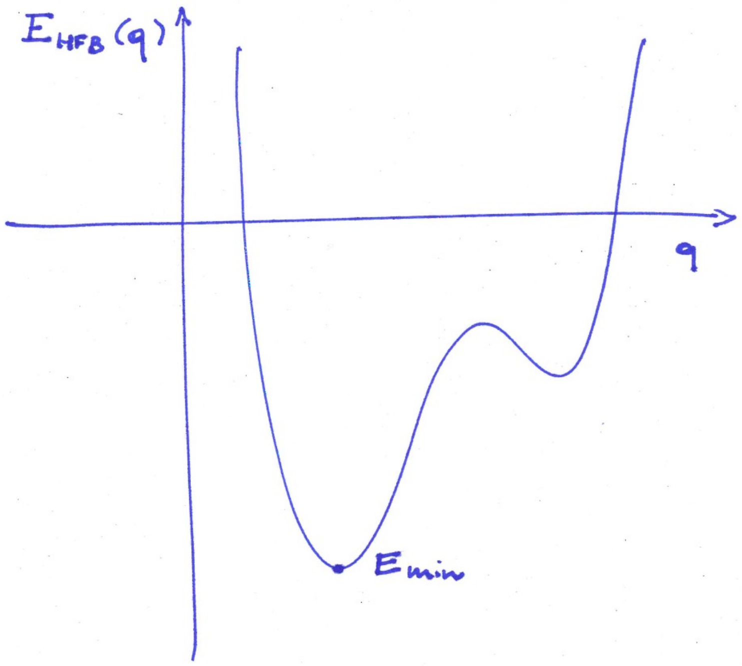

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Linear coefficients

3 HWG Equation

Variational method

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

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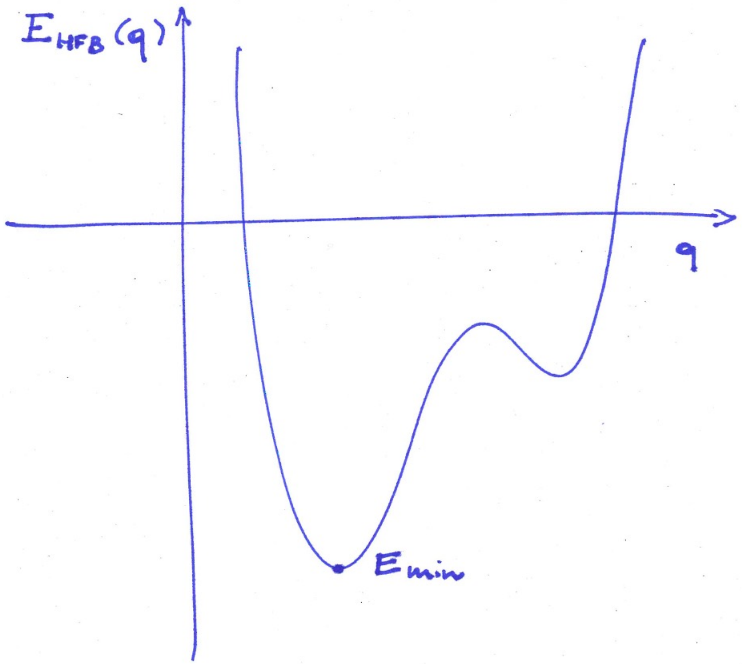

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Schrödinger-like equation

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

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

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

Diagonalization in a physically-informed reduced Hilbert space

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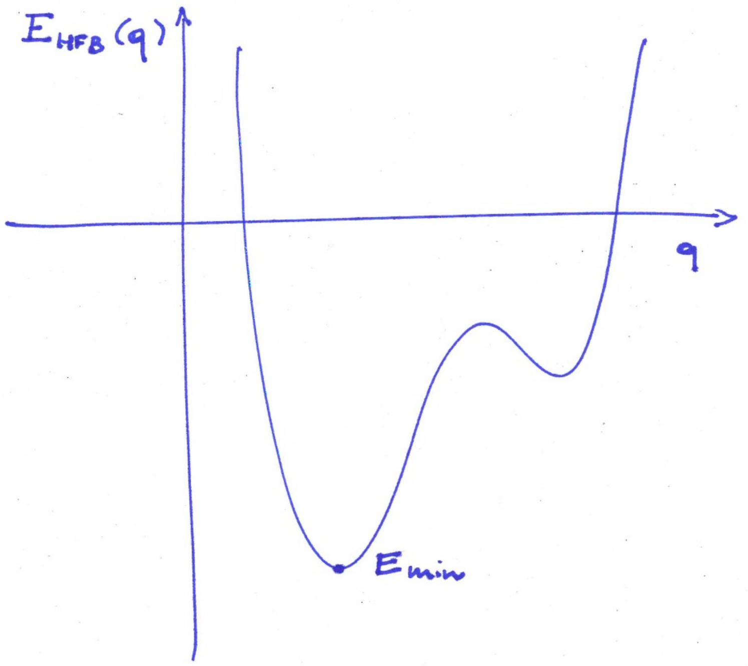

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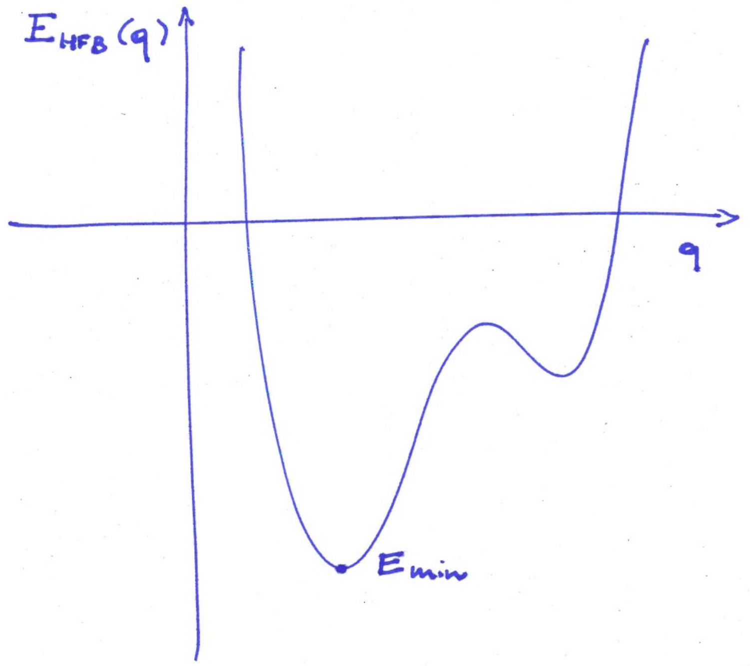
Thouless theorem

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



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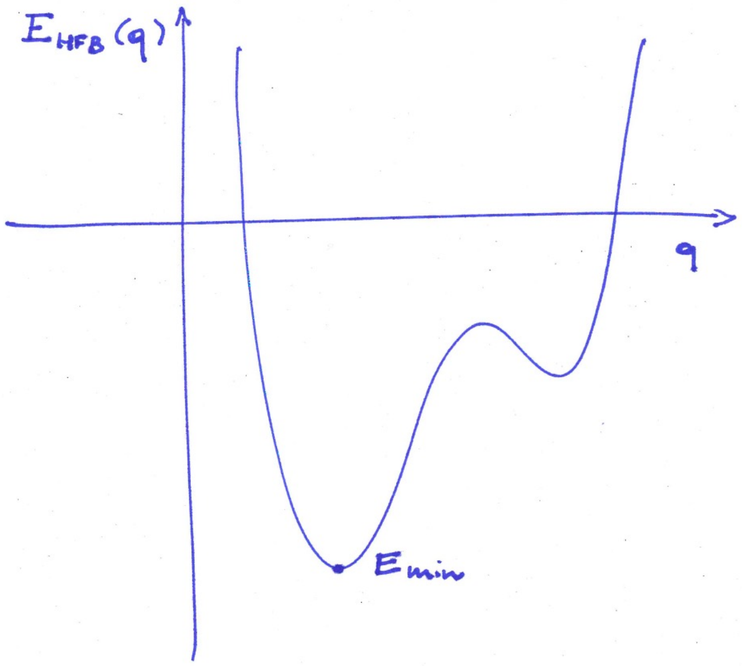
Non-unitary transformation



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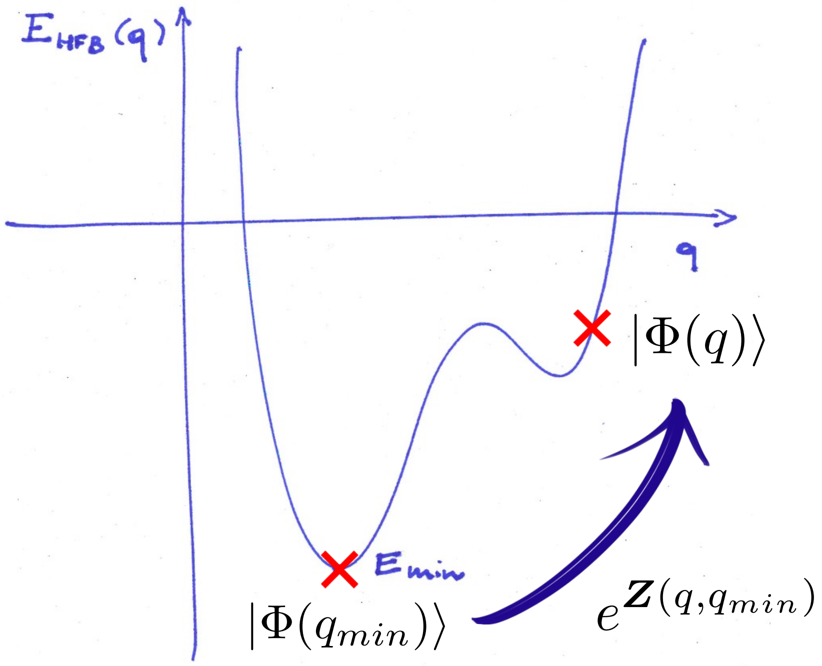

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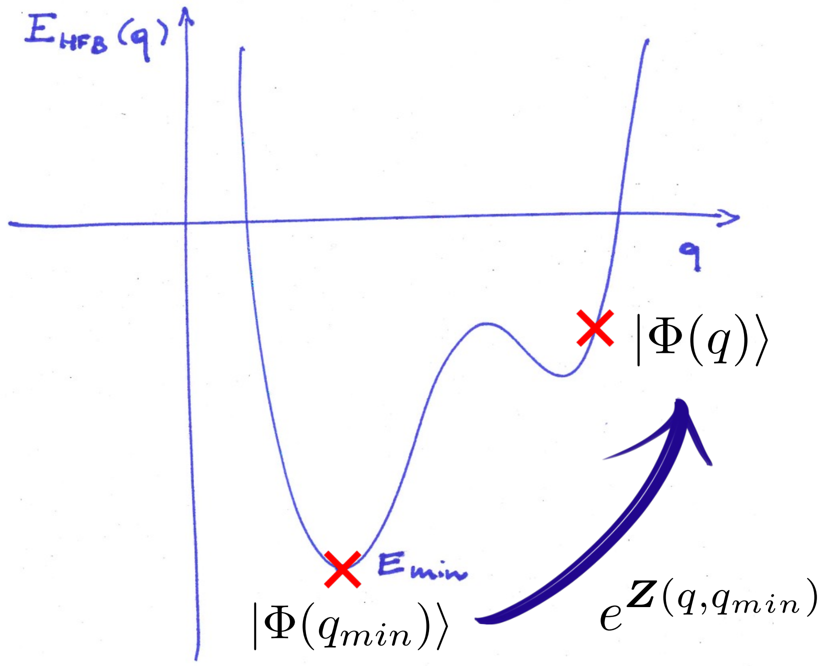

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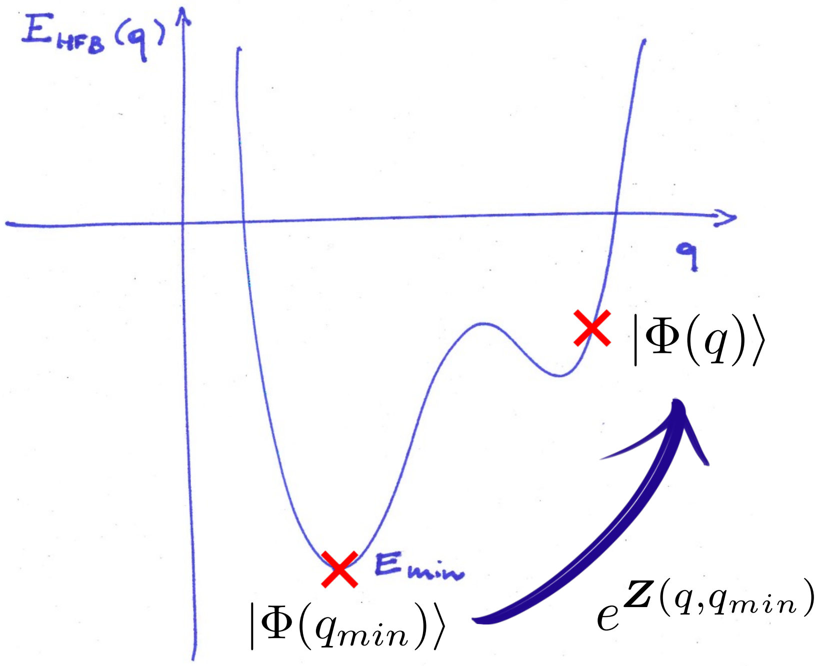
Introduce the Quasi-Boson approximation (QBA)



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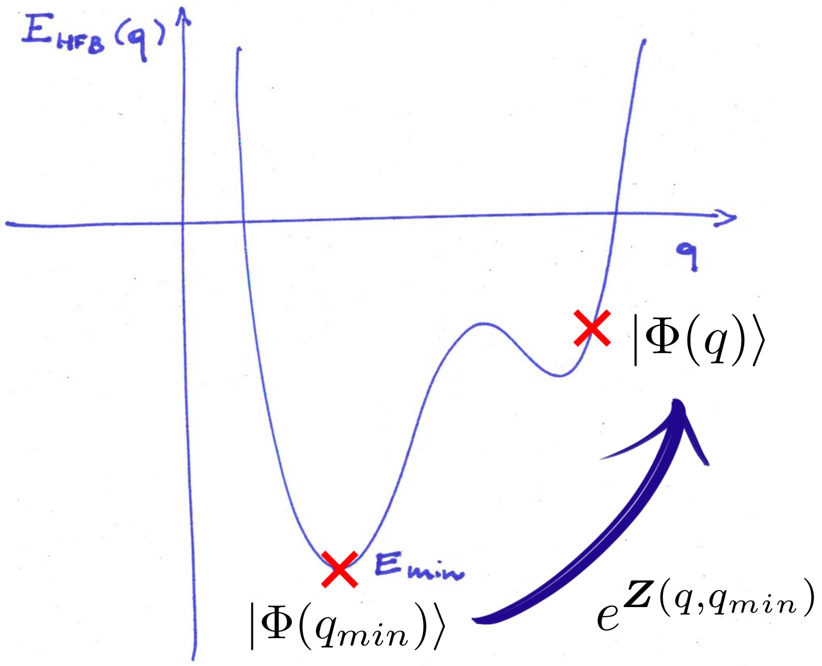
Introduce the Quasi-Boson approximation (QBA)

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



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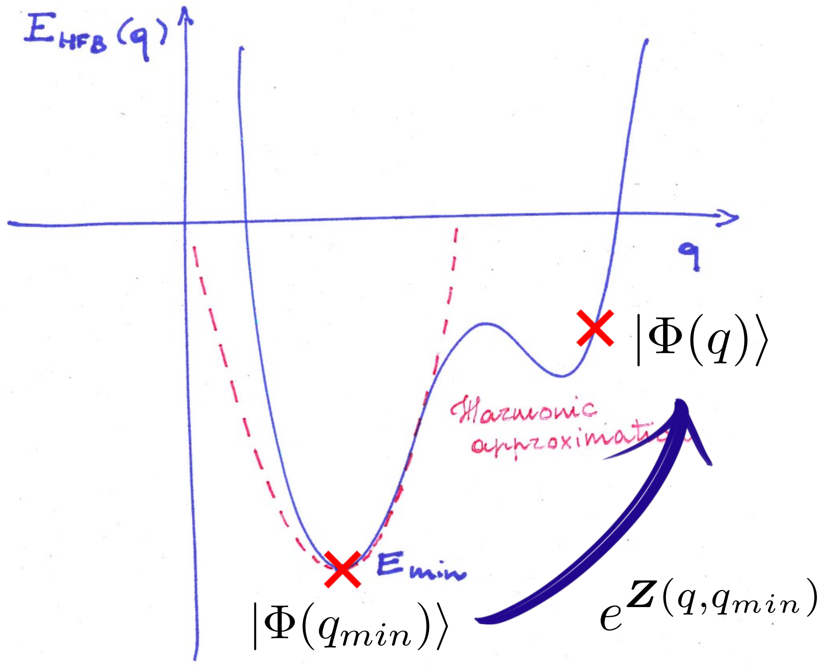

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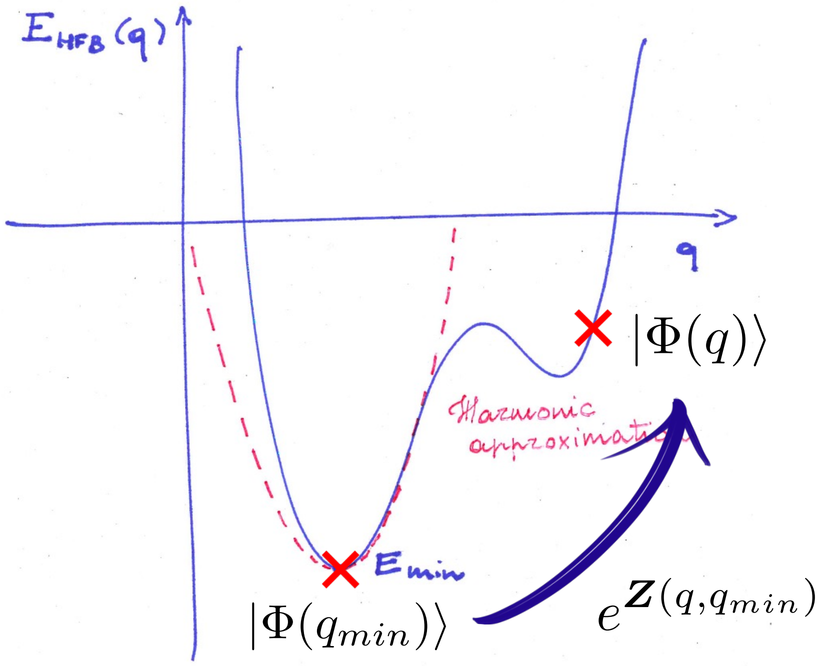

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→ Expand to the quadratic level in $\boldsymbol{Z}(q, q_{min})$

→ Harmonic approximation → No coordinates dependency !

All coordinates are explored (differently from GCM)

GCM and (Q)RPA

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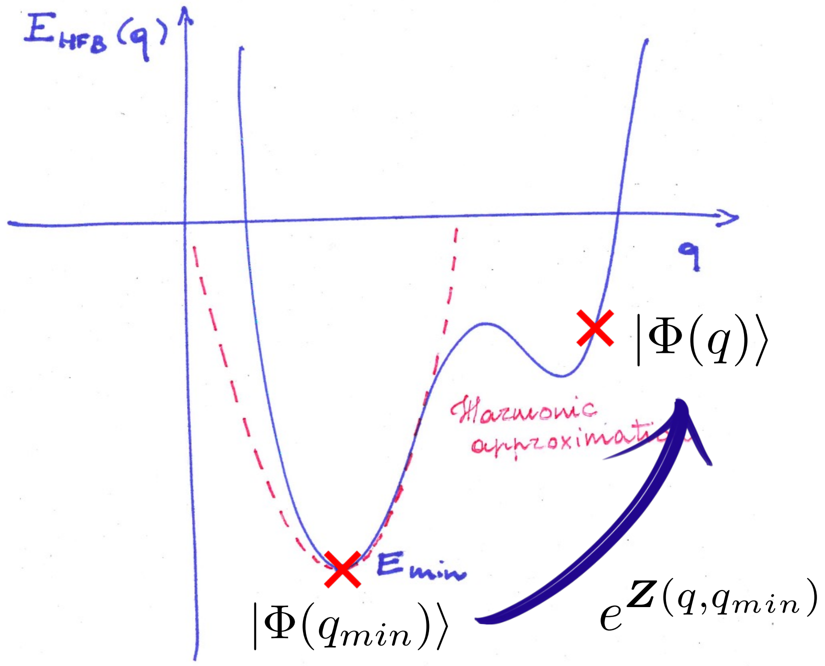

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Eventually rewrites as (Q)RPA equations

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

[Jancovici, Schiff, 1964]

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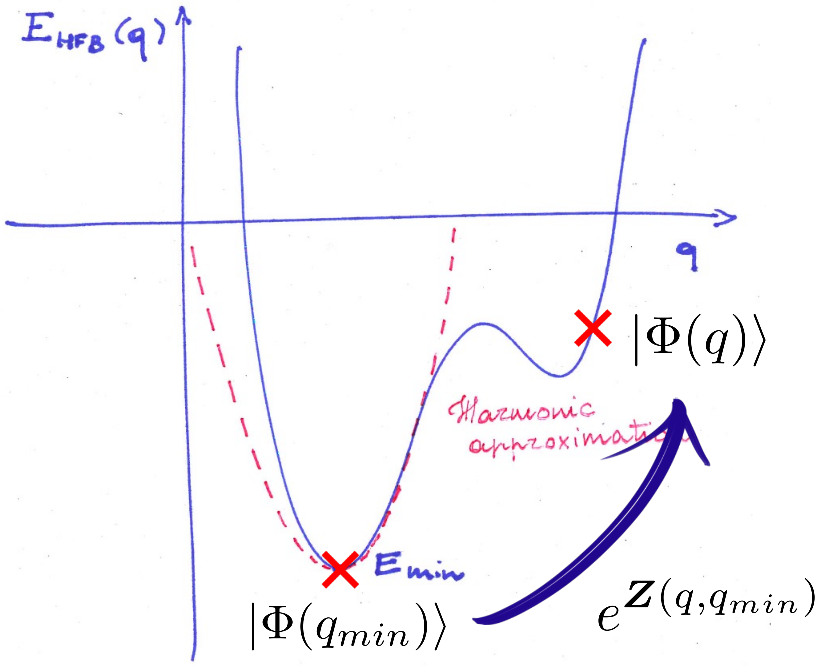

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Nuclei that are stiff against deformations

(anharmonic effects negligible)

[Jancovici, Schiff, 1964]

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Symmetry restoration in the QRPA

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Intrinsic density is the fundamental variable in EDF

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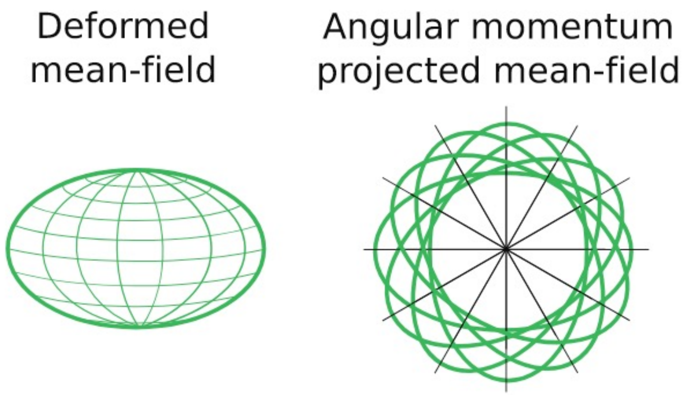
Much is learnt from symmetry breaking and restoration

Symmetry restoration in the QRPA

Intrinsic density is the fundamental variable in EDF

Much is learnt from symmetry breaking and restoration

Intrinsic frame —Projection→ Laboratory frame



Symmetry restoration in the QRPA

Intrinsic density is the fundamental variable in EDF

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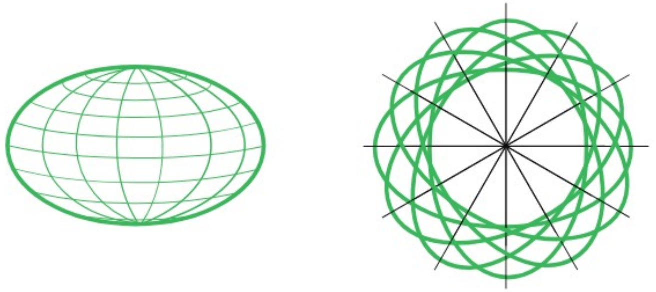
- Common in SR and MR EDF
- Not in linear response on SR EDF (i.e. QRPA)

Deformed mean-field | Angular momentum projected mean-field



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SYMMETRY-CONSERVING RANDOM PHASE APPROXIMATION†

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Physik-Department der Technischen Universität München, D-8046 Garching, West Germany

Received 18 July 1984

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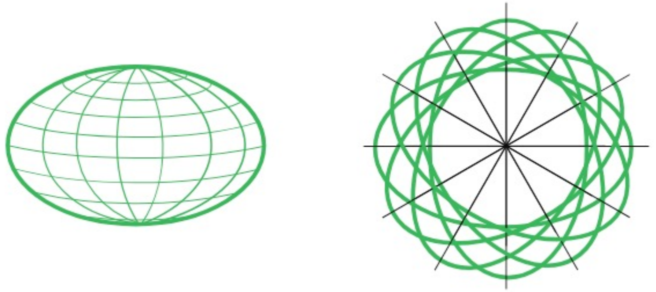

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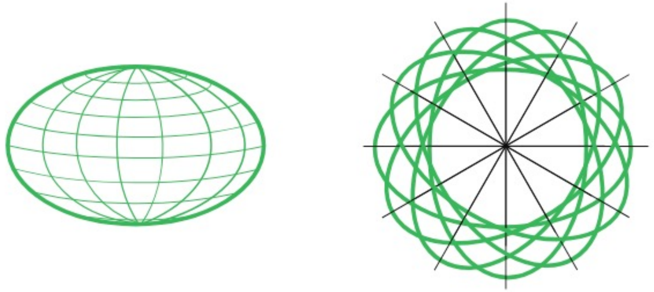

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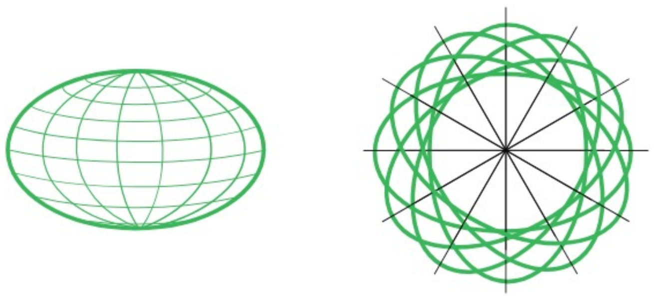

Projection before solving QRPA

VAP QRPA

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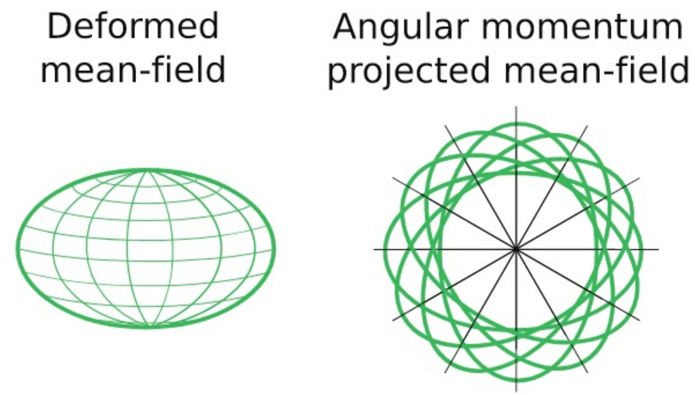

Projection before solving QRPA

VAP QRPA

Computationally expensive, no realistic application

[Gambacurta, Lacroix, PRC (2012) 86, 064320]

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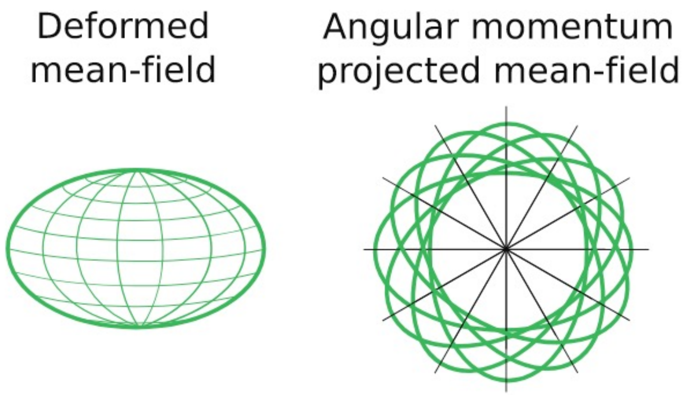

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What about PAV QRPA ?

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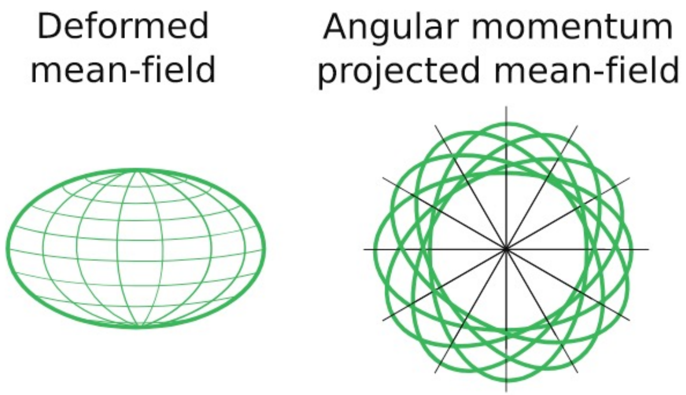

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What about PAV QRPA ?

Can we treat projection a posteriori ?

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Wigner small-d matrices

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Remark

For J=0 projection is a pure rotation $|\mathrm{ROT}\rangle \equiv N_{\mathrm{ROT}} P^0_{00} |\mathrm{HF}\rangle$

Outline

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- Giant Resonances
- GCM and RPA

Random Phase Approximation

- Theoretical introduction
- Angular Momentum Projection

Results

- Rotation-Vibration coupling
- Comparison to ab initio PGCM

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SkM* parametrisation

Systematic study for ^{24}Mg

AMP RPA results

[PRC (2024) 109, 044315]

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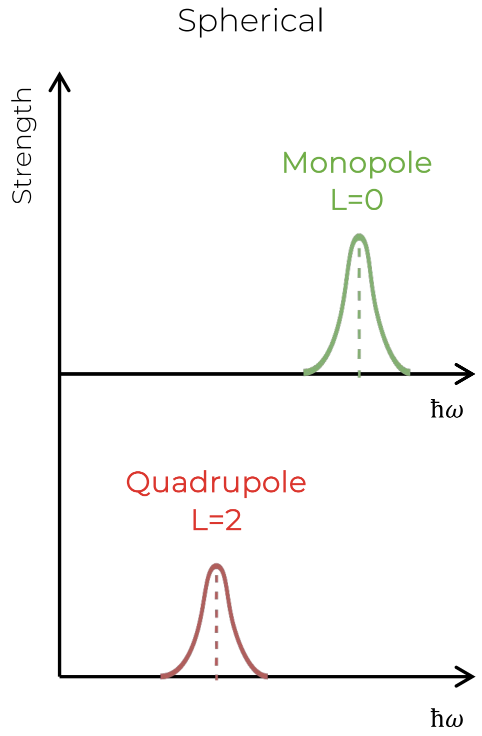
AMP RPA results

Spherical
(no deformation)



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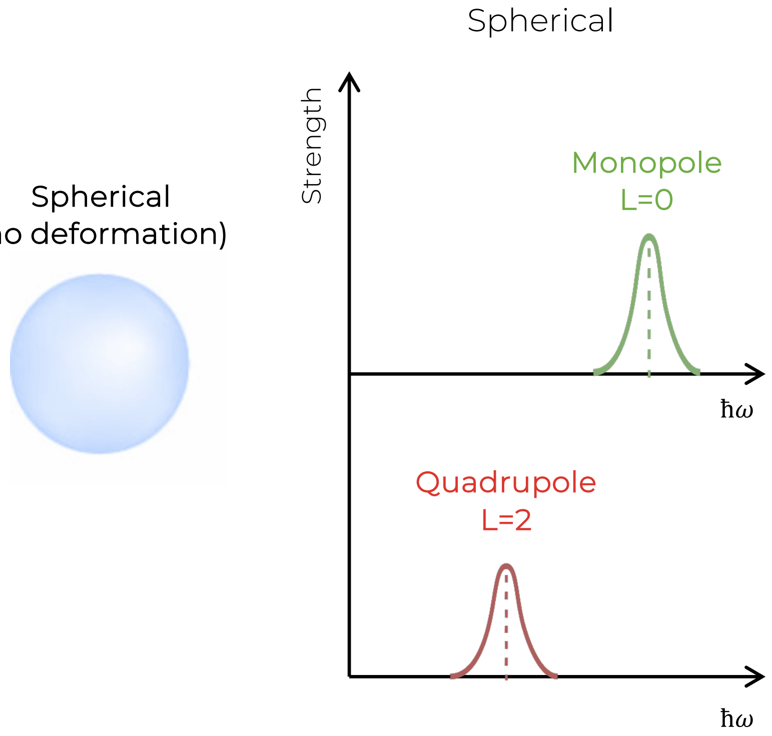

Spheroidal
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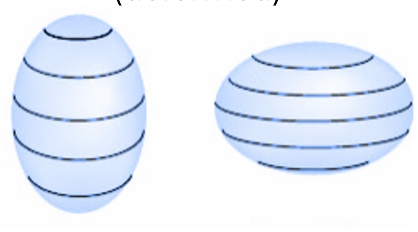
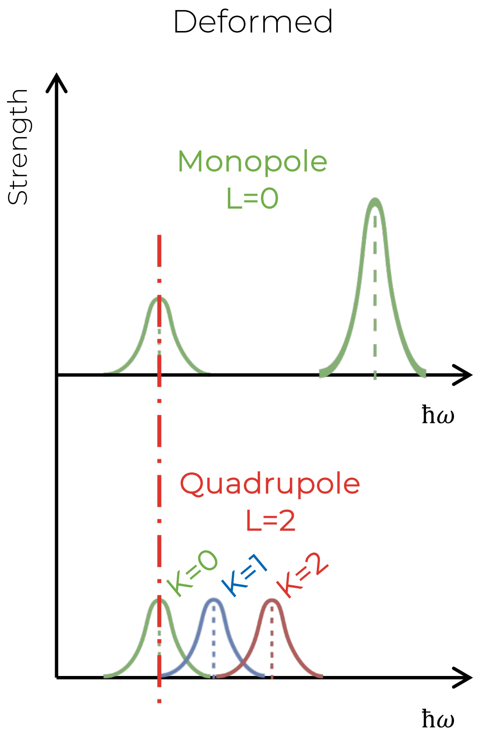


Prolate
(cigar type)

Oblate
(pancake type)



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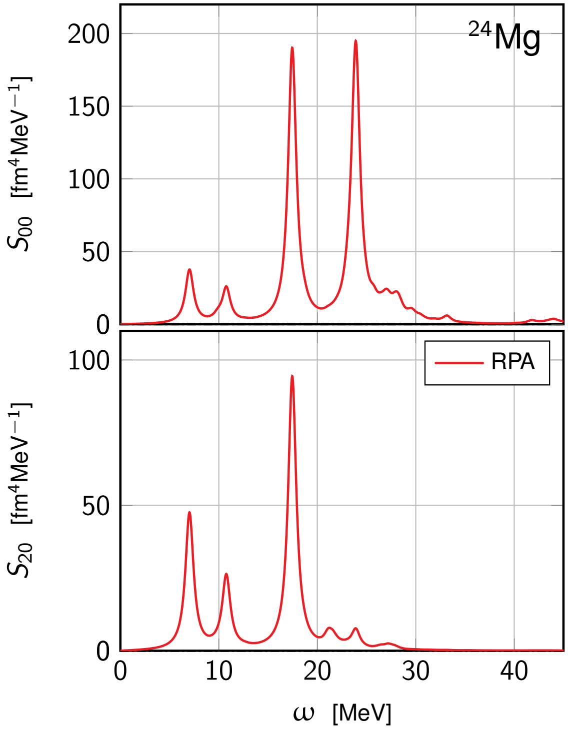
Intrinsic frame (deformed)

[PRC (2024) 109, 044315]



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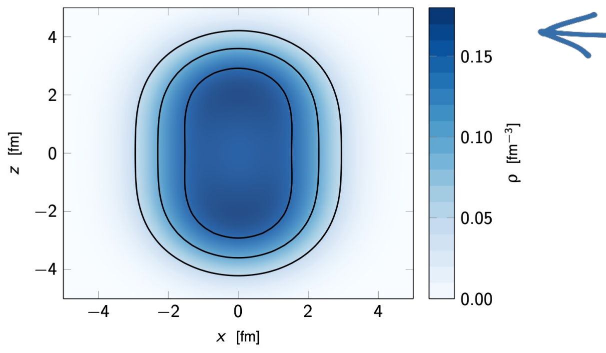
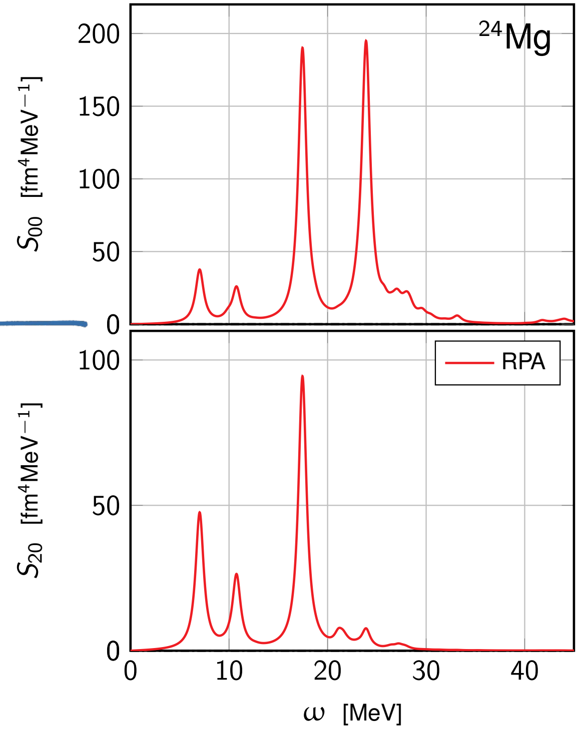


Well-deformed HF ground state



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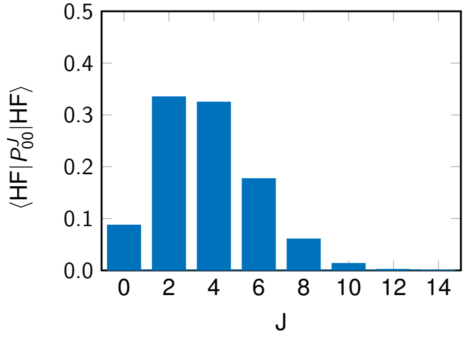
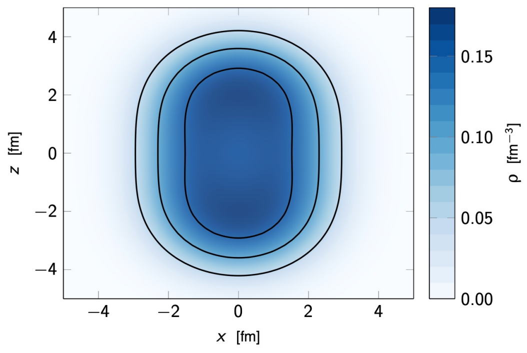


Spread over several J's



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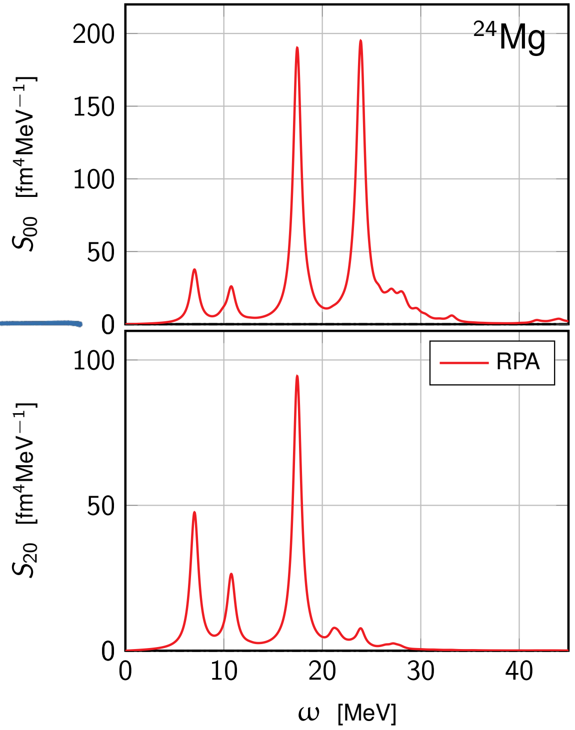

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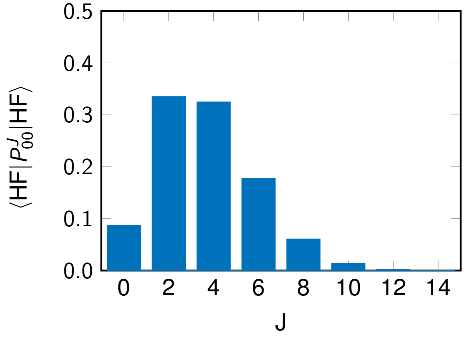

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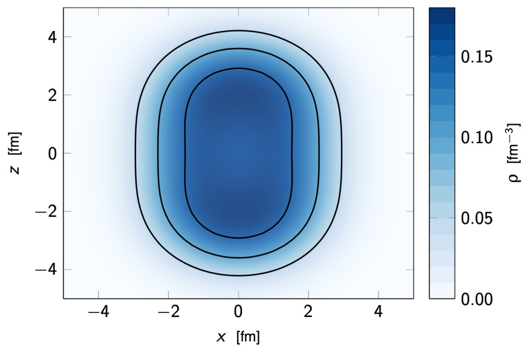
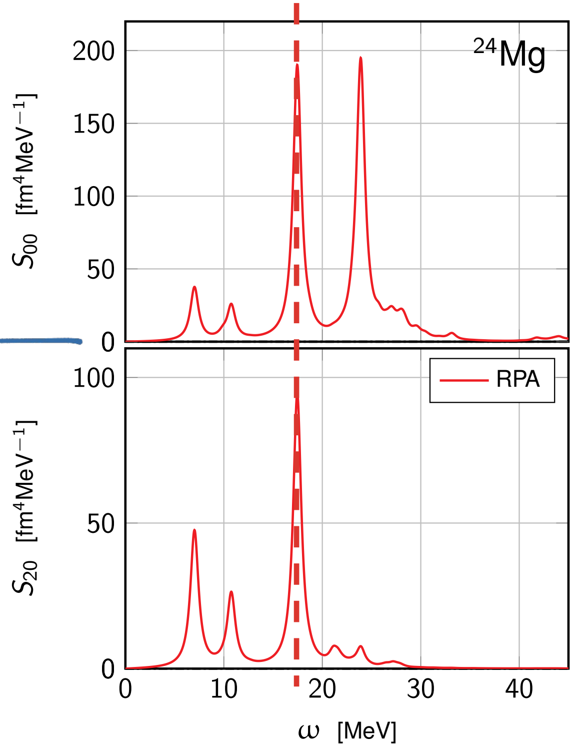


Well-deformed HF ground state

GMR-GQR coupling



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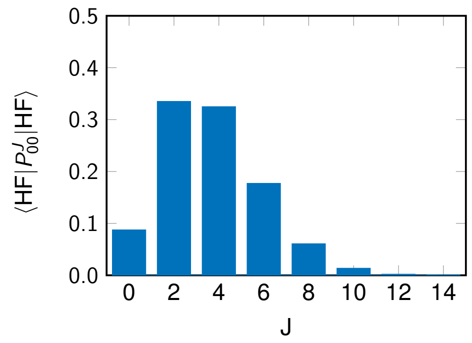

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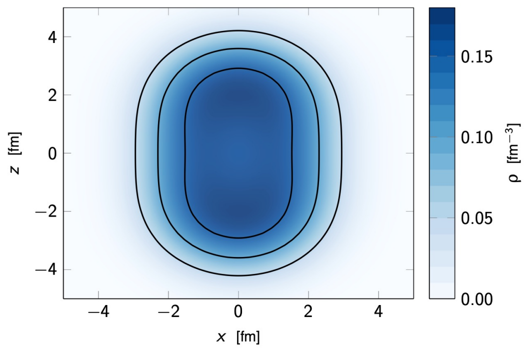

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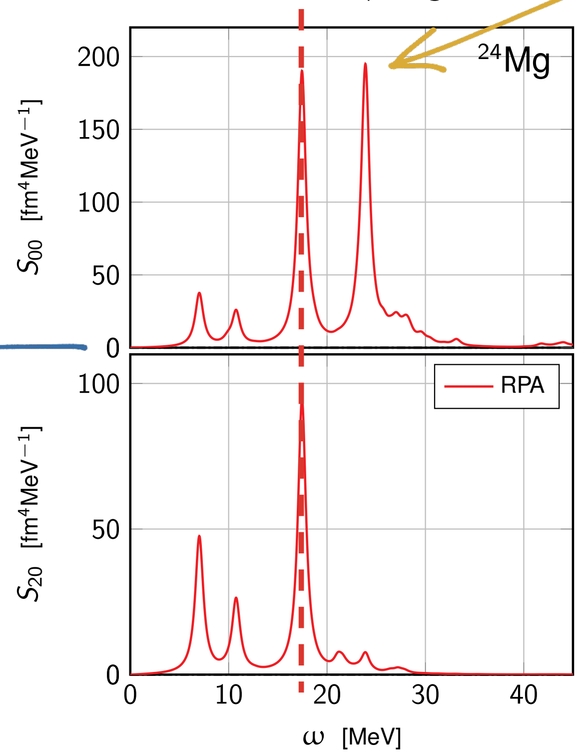
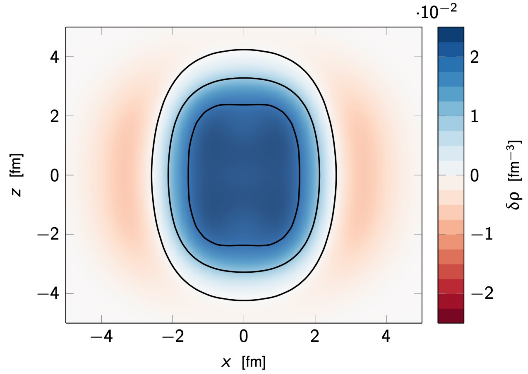


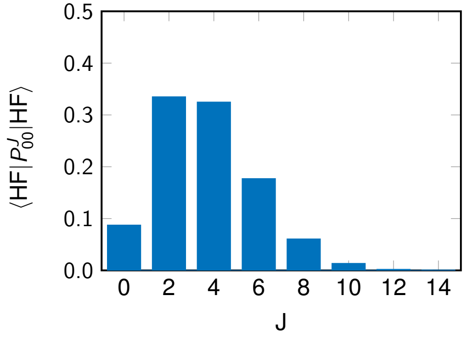


Monopolar vibration
(shape-conserving)

AMP RPA results

Intrinsic frame (deformed)

[PRC (2024) 109, 044315]



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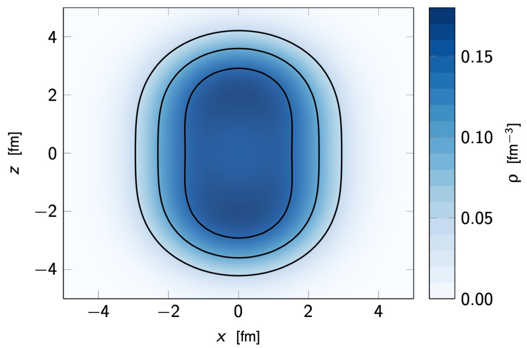
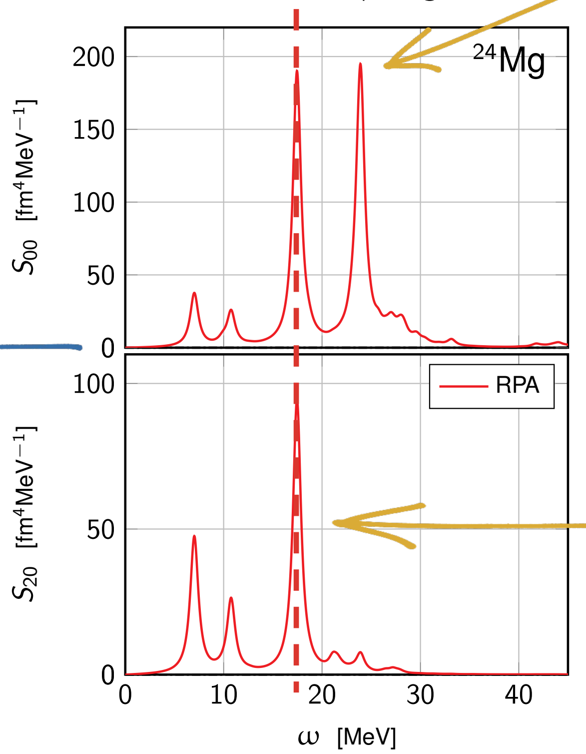
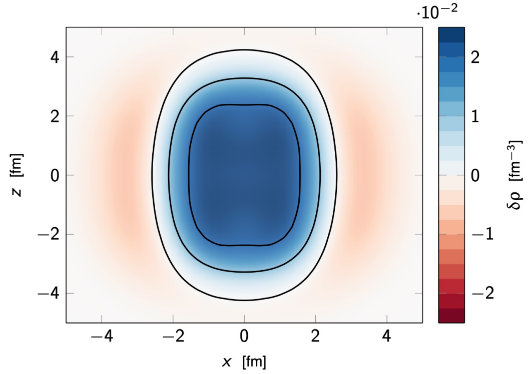


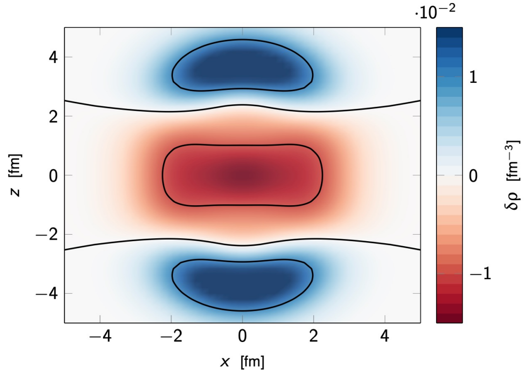
Well-deformed HF ground state

GMR-GQR coupling





Monopolar vibration (shape-conserving)



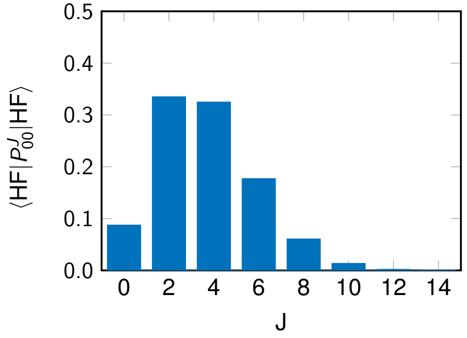
Quadrupolar vibration (clear Y_{20} signature)

AMP RPA results

Intrinsic frame (deformed)

Laboratory frame (projected)

[PRC (2024) 109, 044315]



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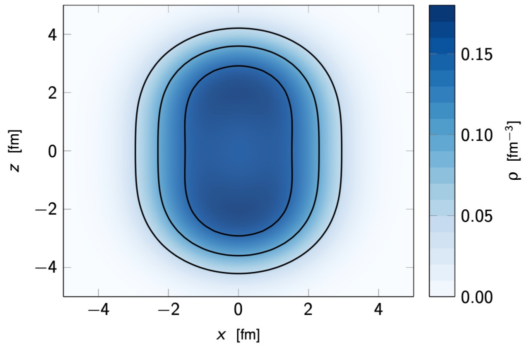

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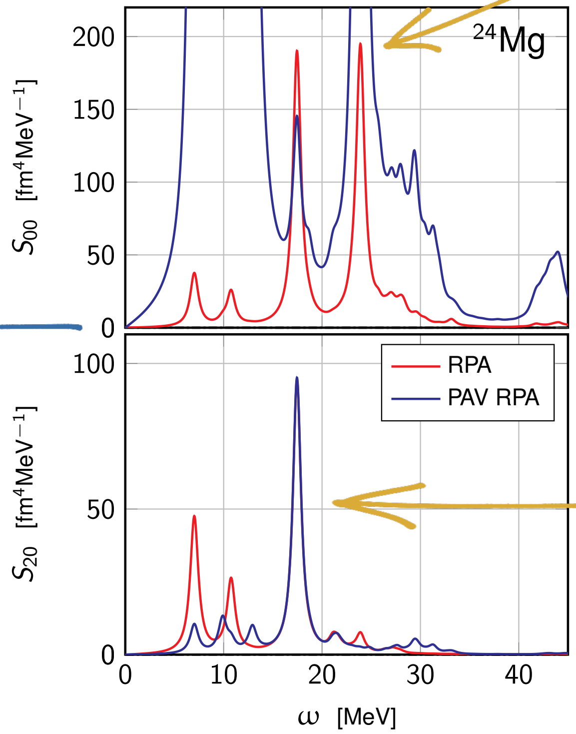

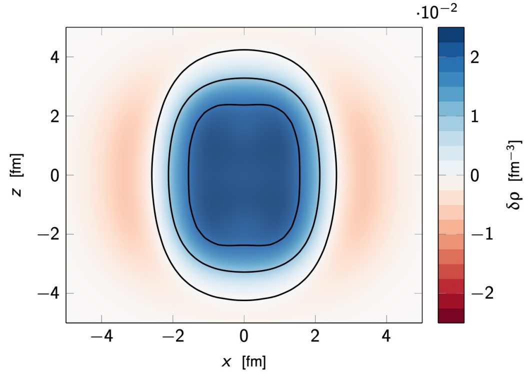

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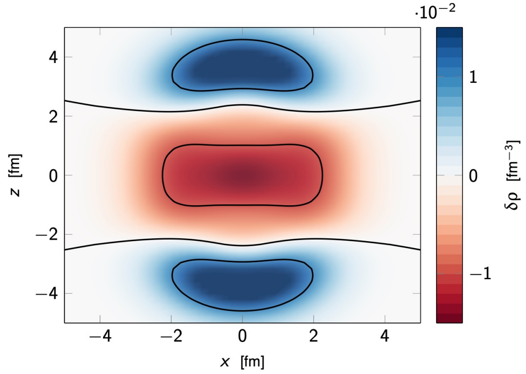

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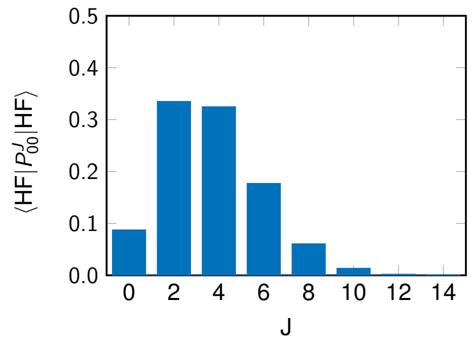

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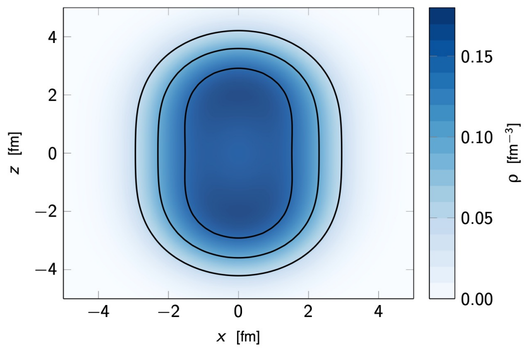

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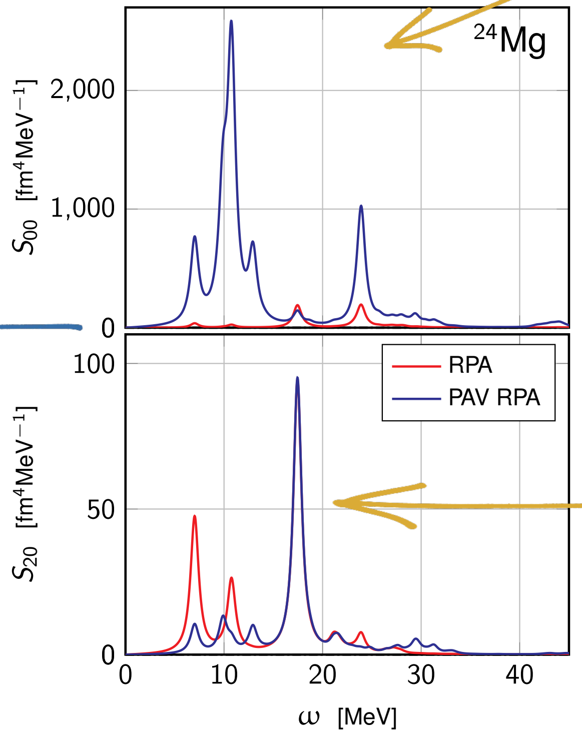

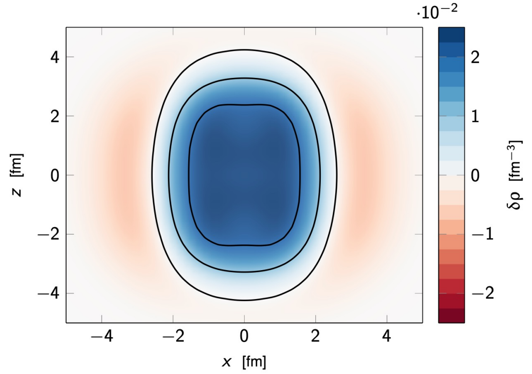

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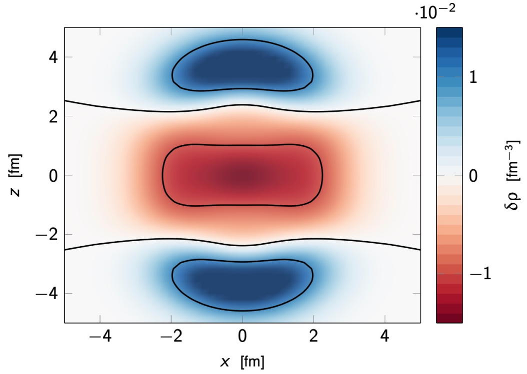

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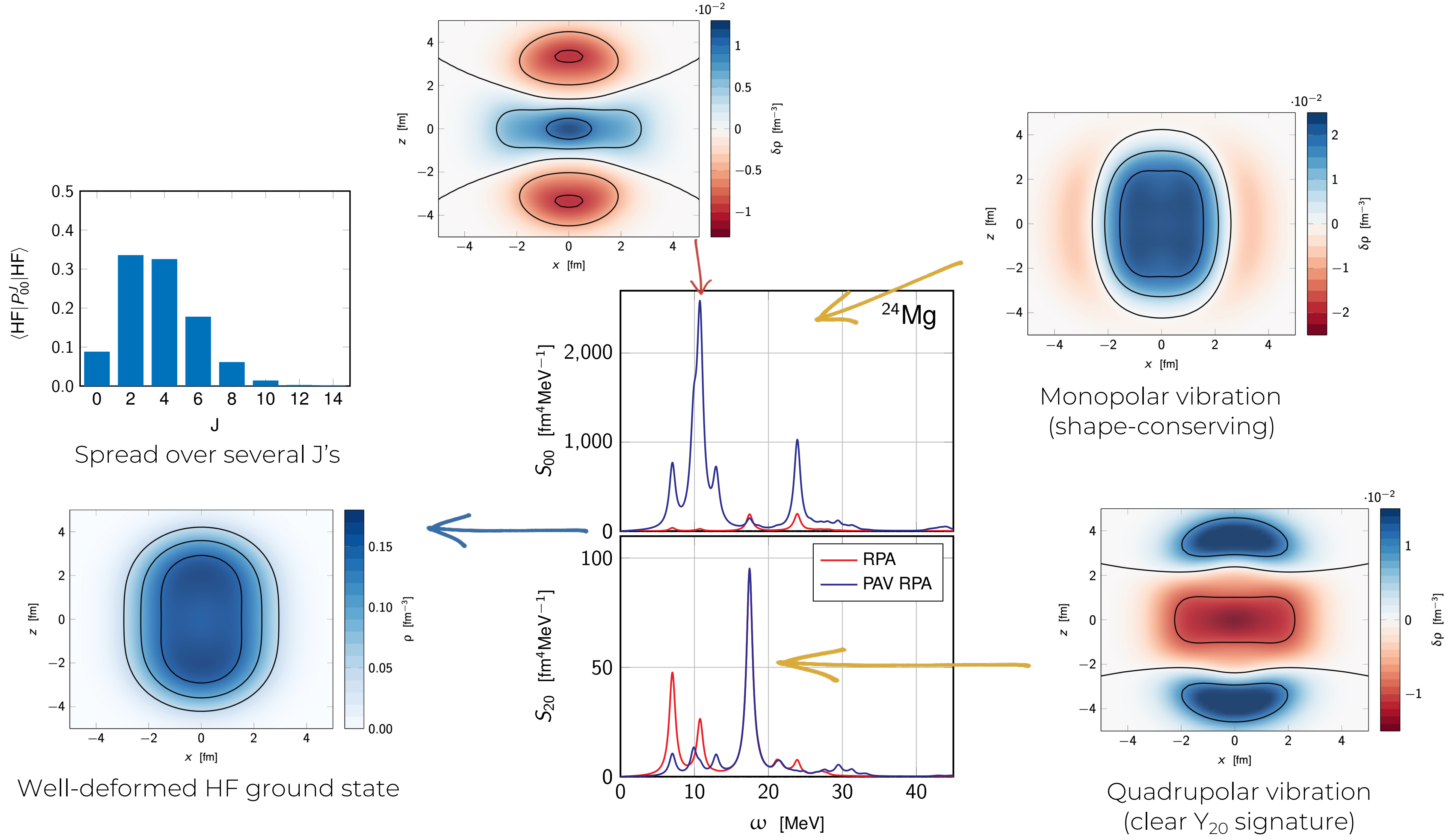
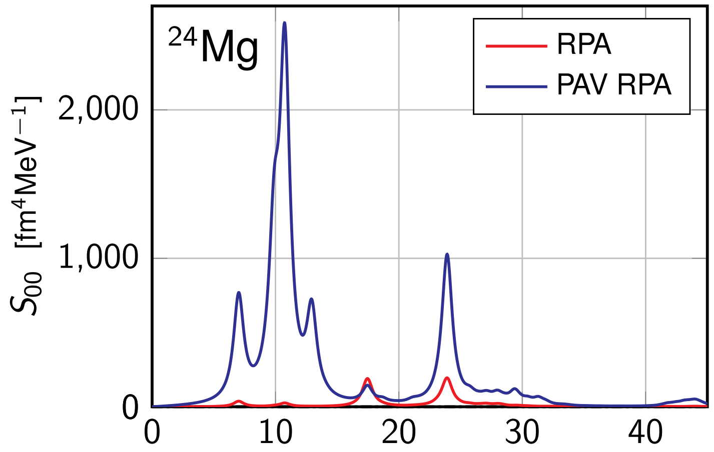


[PRC (2024) 109, 044315]

Rotation-vibration coupling

Where does the strength come from ?



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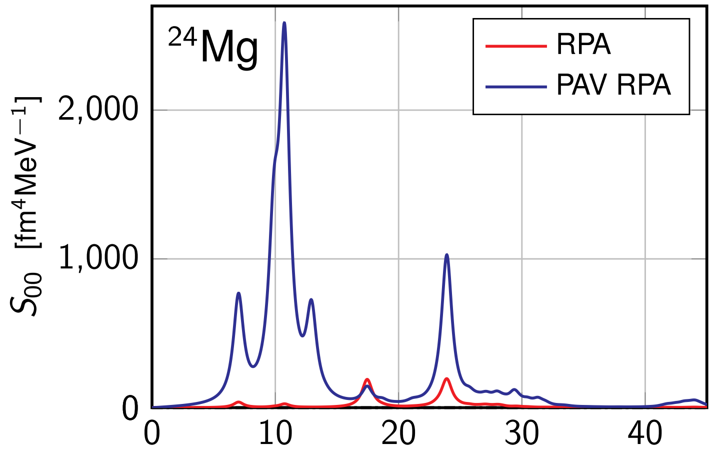

RPA : symmetry-breaking solutions $|n\rangle_{\mathrm{def}}$ (vibrational)

[PRC (2024) 109, 044315]

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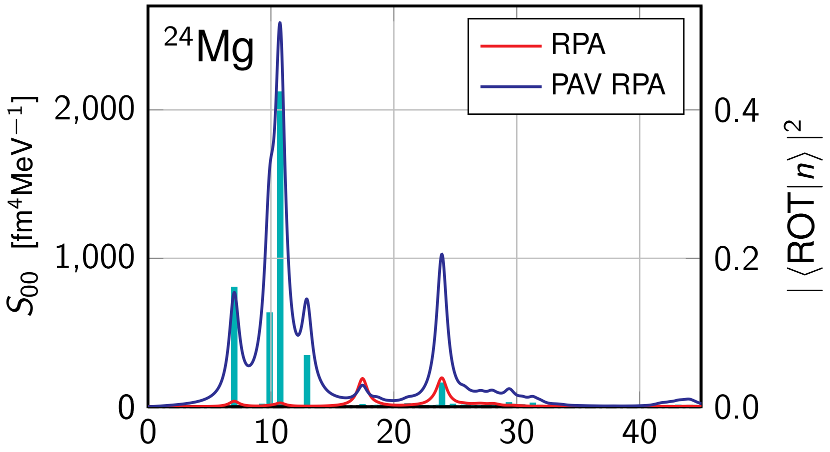

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Non-vanishing overlap with the rotational state !

$\langle \text{ROT}|n\rangle_{\text{def}}$ $|\text{ROT}\rangle \equiv N_{\text{ROT}} P^0_{00} |\text{HF}\rangle$

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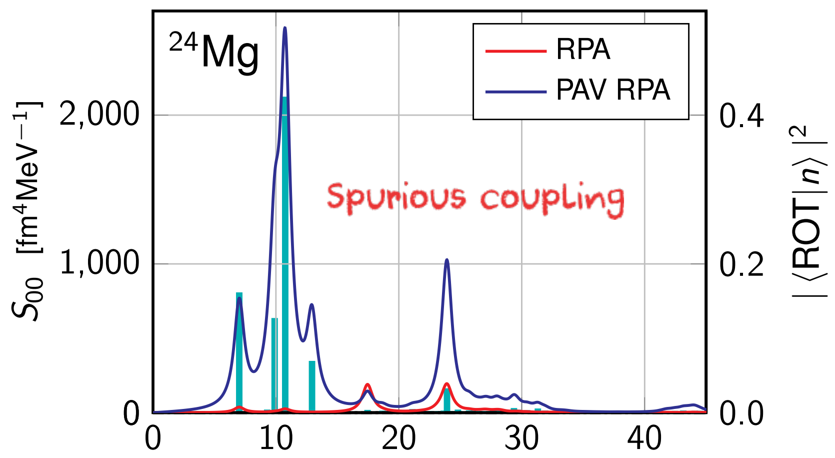

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RPA states have vibrational and rotational (spurious) content

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

[PRC (2024) 109, 044315]

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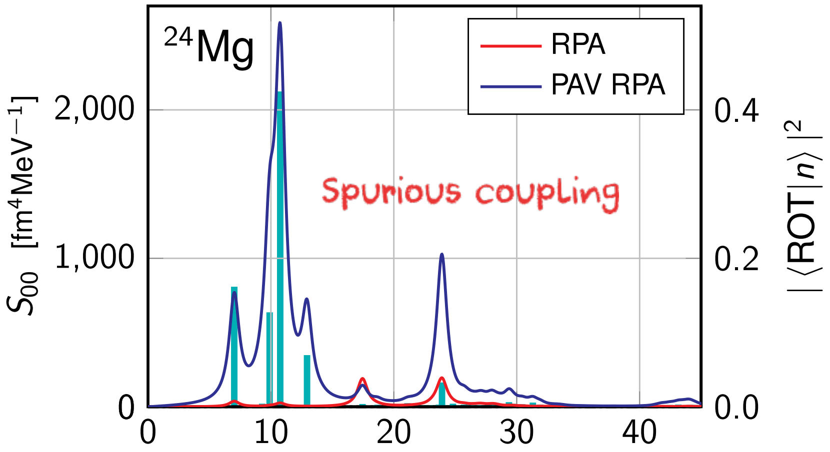

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[PRC (2024) 109, 044315]

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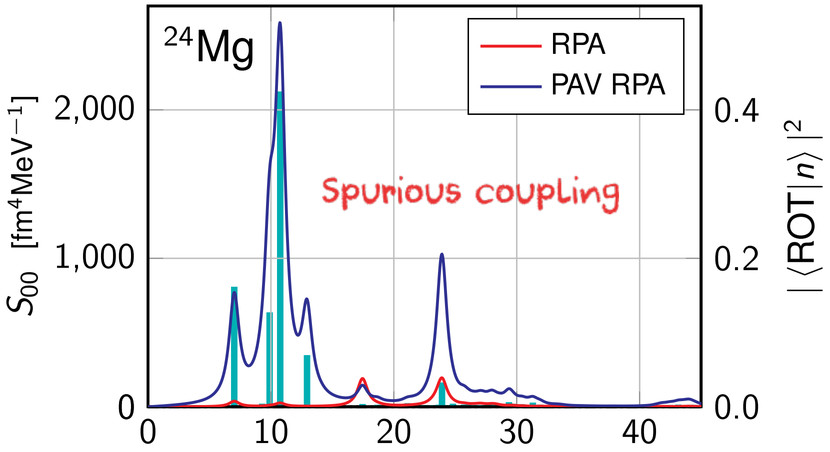

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[PRC (2024) 109, 044315]

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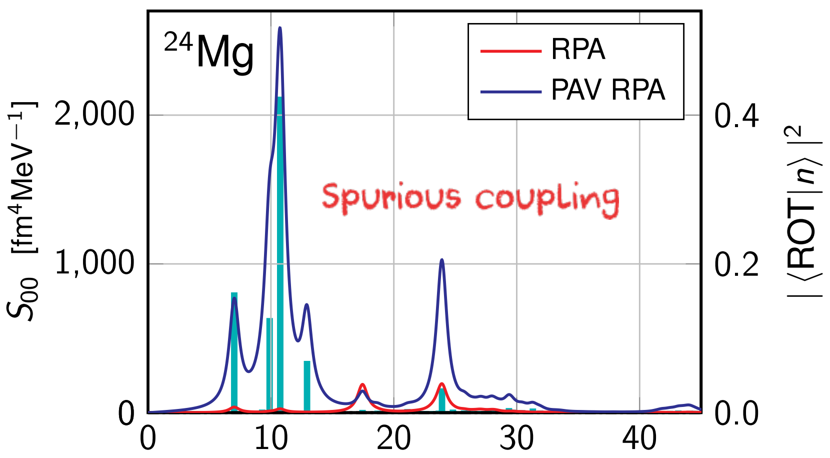

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$$\langle \mathrm{ROT}|\tilde{n}\rangle = 0 \quad \rightarrow \quad a_n = \langle \mathrm{ROT}|n\rangle$$

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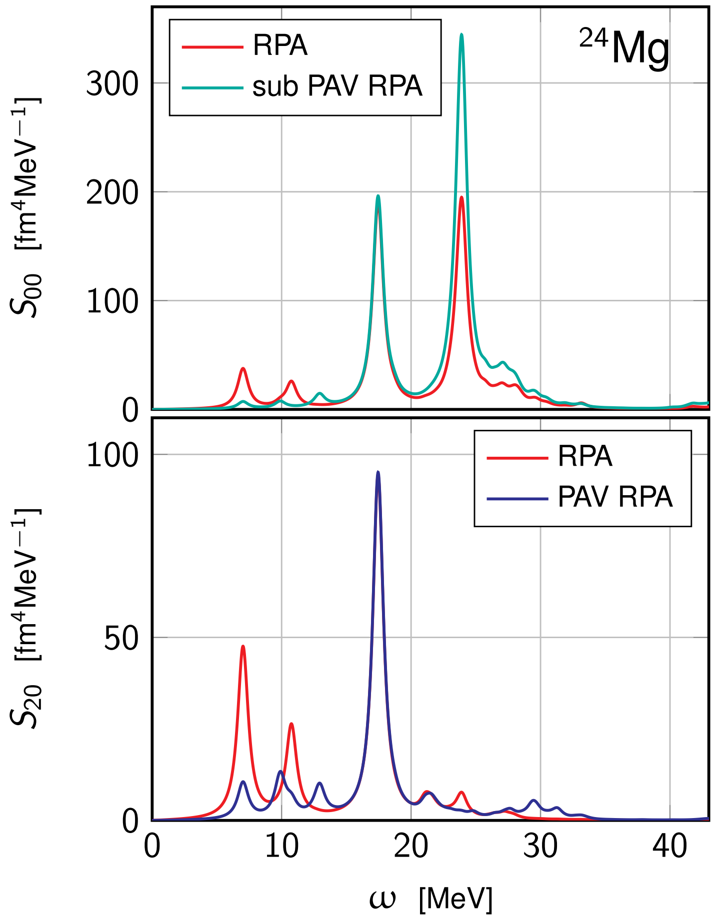

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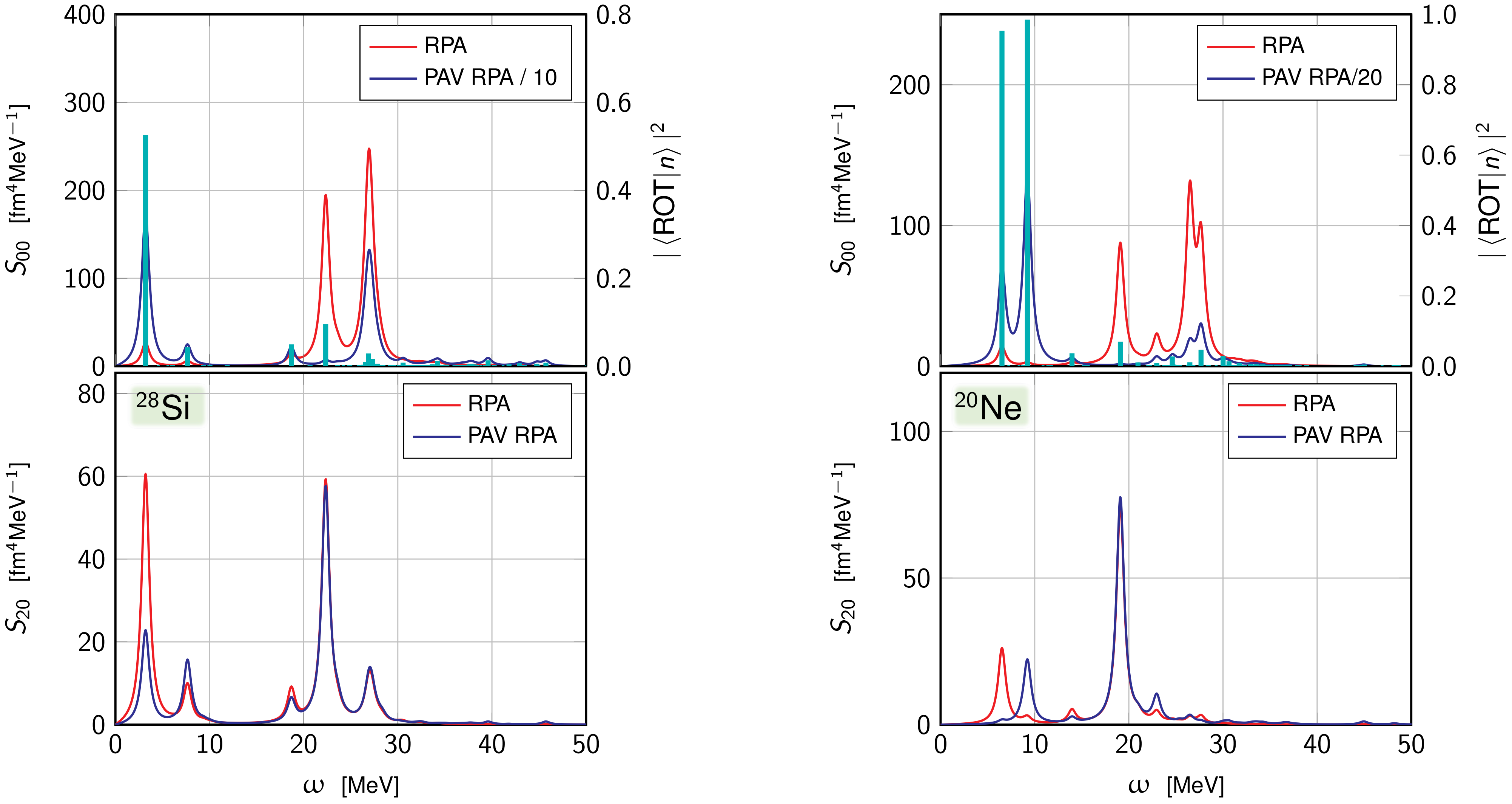
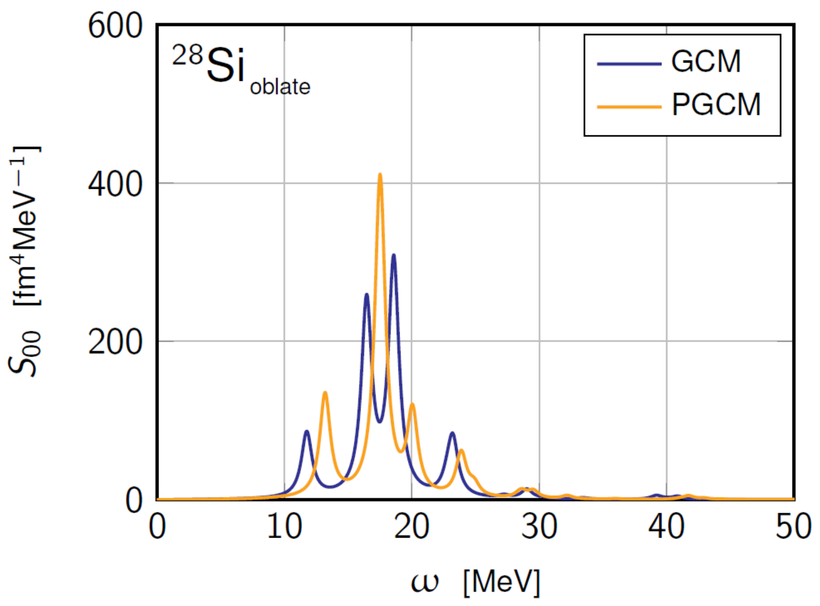
Subtraction + Projection

Observation in other systems



[arXiv:2407.01325]

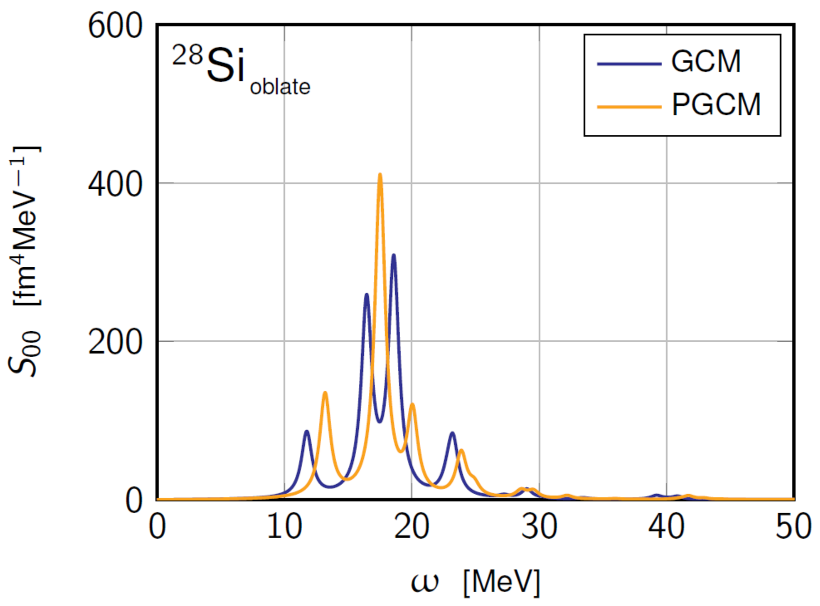
Comparison to ab initio PGCM



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

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

Comparison to ab initio PGCM



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Variational treatment of rotations in PGCM !

[arXiv:2407.01325]

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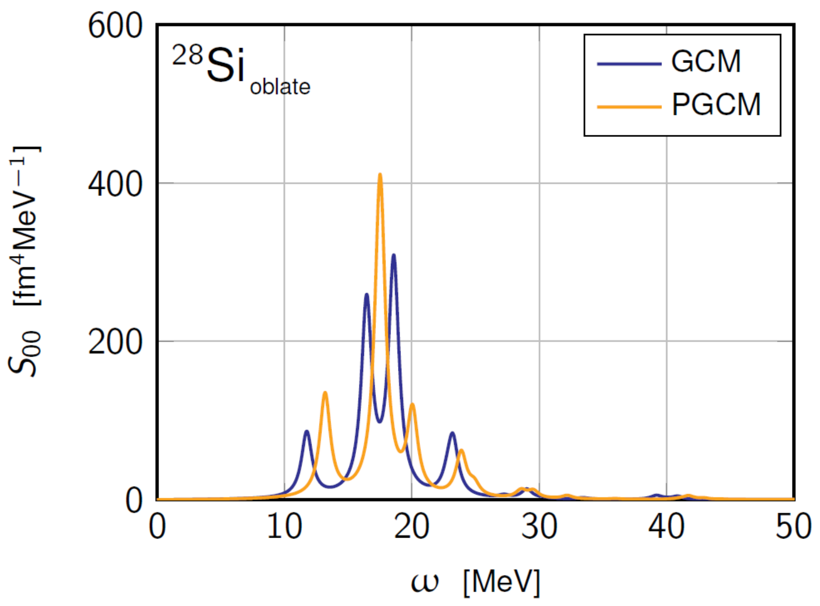

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Projection effects

- Not too dissimilar
- Increased **fragmentation** (e.g. ^{24}Mg)
- More quantitative agreement

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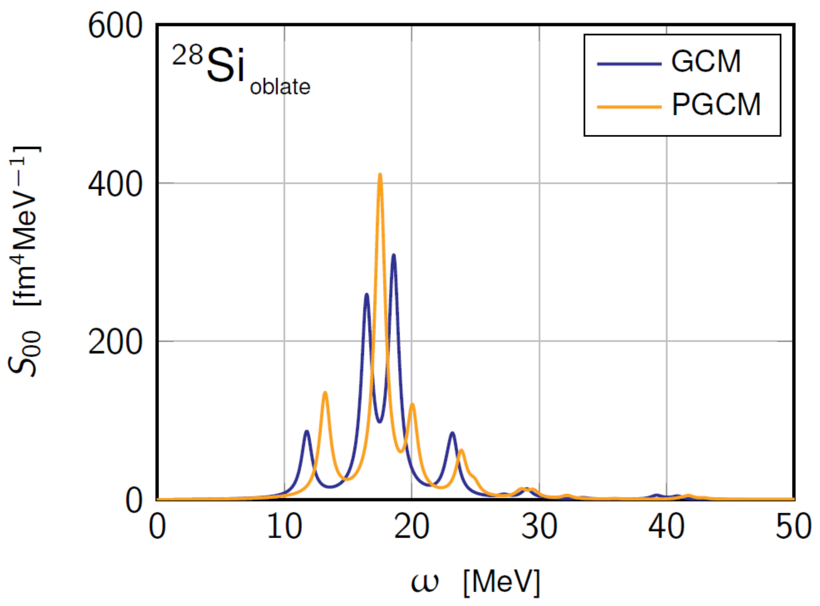

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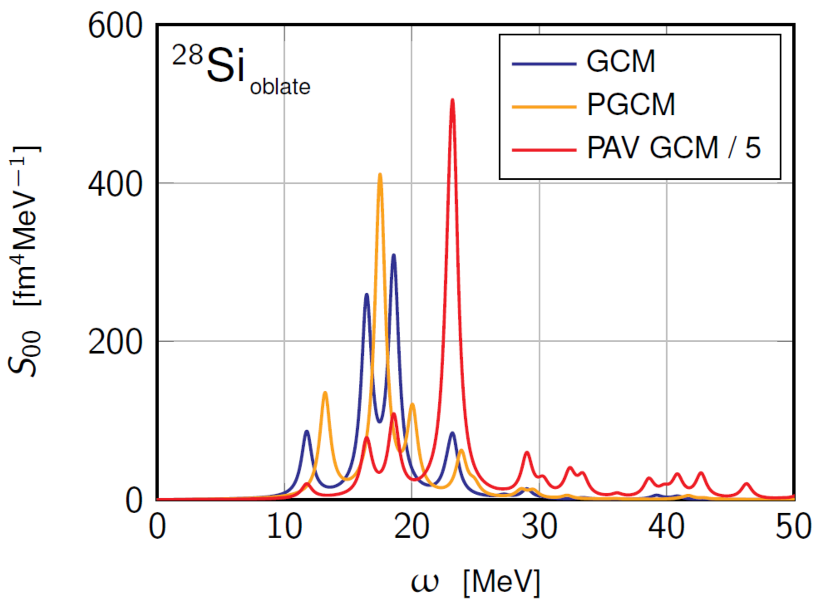
Can we treat projection a posteriori ?

Comparison to ab initio PGCM

[arXiv:2407.01325]



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PAV GCM: projection of symmetry-breaking solution

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

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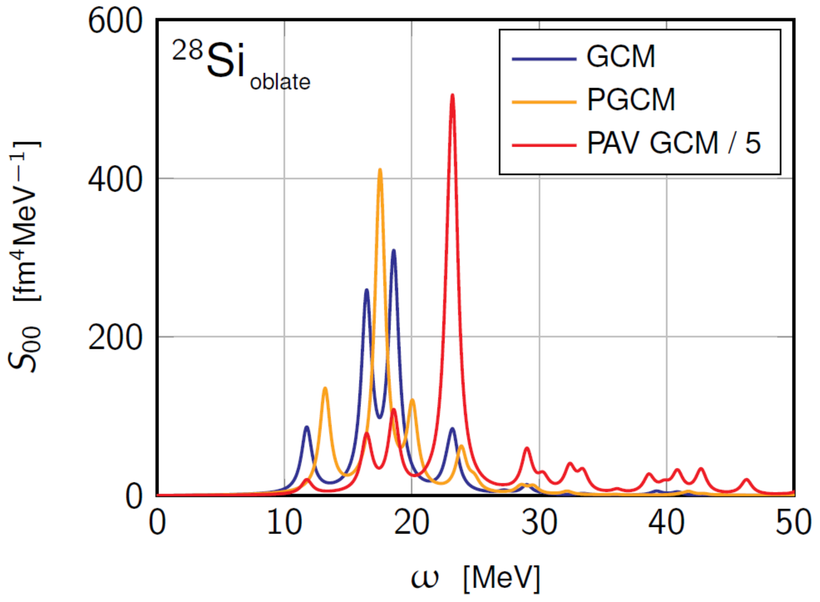

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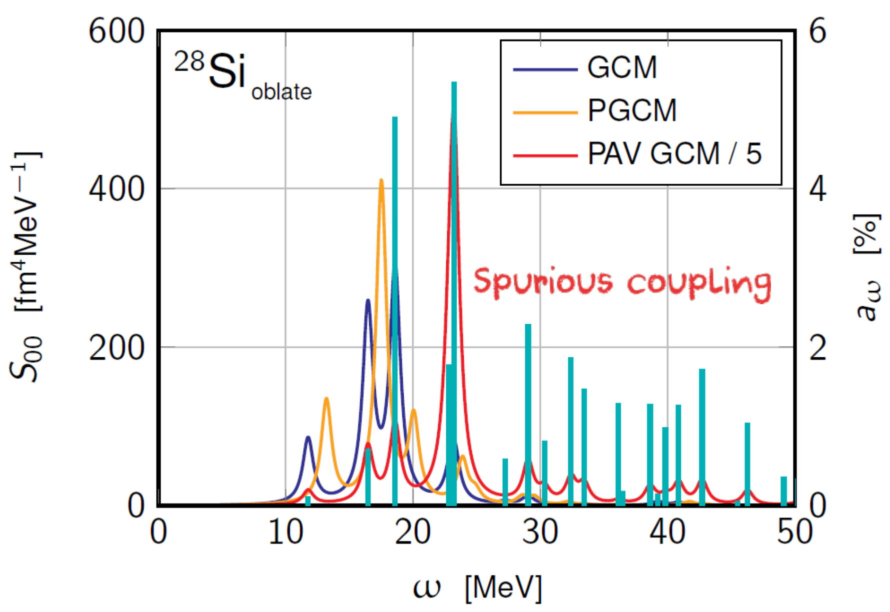

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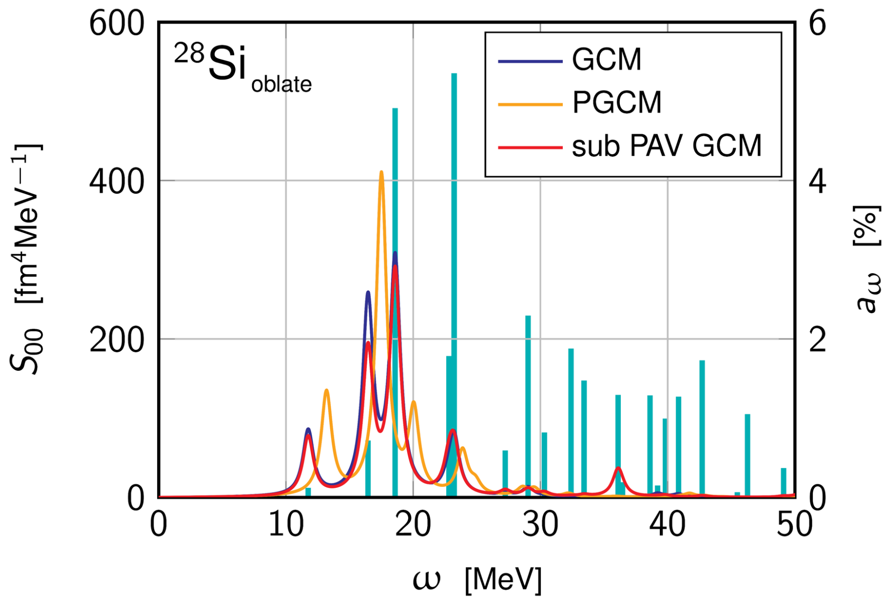

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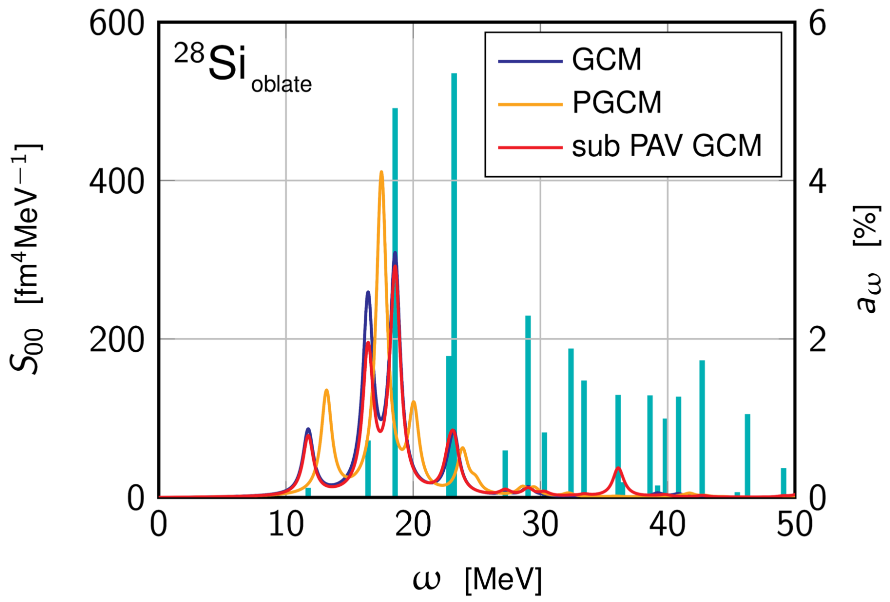

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Similar results in GCM and RPA

- Does not depend on the many-body method
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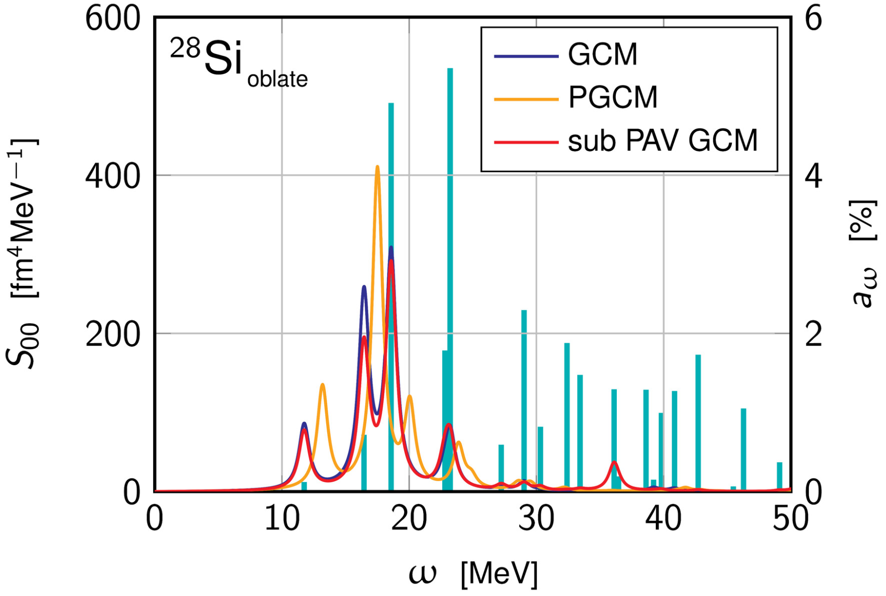

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Rotations must be treated variationally !

- PGCM already does
- Projected QRPA needed

Outline

Introduction

- Giant Resonances
- GCM and RPA

Random Phase Approximation

- Theoretical introduction
- Angular Momentum Projection

Results

- Rotation-Vibration coupling
- Comparison to ab initio PGCM

Conclusions

Summary

DIFFERENT FLAVOURS OF SYMMETRY BREAKING AND RESTORATION

(Q)RPA

Symmetry breaking

GCM

Symmetry conserving

Summary

DIFFERENT FLAVOURS OF SYMMETRY BREAKING AND RESTORATION

(Q)RPA	Symmetry breaking	**GCM**
Harmonic fluctuations around deformed HF(B)	✓ ✓	Large amplitudes superposition of def. HF(B) states

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PROJECTION AFTER DIAGONALIZATION PAV RPA [(1)]	✘ ✘	**PROJECTION AFTER DIAGONALIZATION** PAV GCM

Symmetry conserving

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

Summary

DIFFERENT FLAVOURS OF SYMMETRY BREAKING AND RESTORATION

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(Q)RPA			GCM
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PROJECTION AFTER DIAGONALIZATION PAV RPA [1]	✗	✗	**PROJECTION AFTER DIAGONALIZATION** PAV GCM
PROJECTION BEFORE DIAGONALIZATION P(Q)RPA [2]	✗	✓	**PROJECTION BEFORE DIAGONALIZATION** PGCM

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[PRC (2024) 109, 044315]		[arXiv:2407.01325]
PROJECTION AFTER DIAGONALIZATION ✓ PAV RPA [1] *New implementation*		✓ **PROJECTION AFTER DIAGONALIZATION** PAV GCM *New implementation*
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(Q)RPA

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[PRC (2024) 109, 044315]

PROJECTION AFTER DIAGONALIZATION ✓

⚠ Spurious coupling

PAV RPA (1)

New implementation

PROJECTION BEFORE DIAGONALIZATION ✗

P(Q)RPA (2)

GCM

✓ Large amplitudes superposition of def. HF(B) states

[arXiv:2407.01325]

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[PRC (2024) 109, 044315]

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PROJECTION BEFORE DIAGONALIZATION ✗

P(Q)RPA (2)

Needed for proper comparison with experiments !

GCM

✓ Large amplitudes superposition of def. HF(B) states

[arXiv:2407.01325]

✓ **PROJECTION AFTER DIAGONALIZATION**

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Thank you for the attention

Thomas Duguet
Jean-Paul Ebran
Mikael Frosini
Vittorio Somà

Gianluca Colò
Danilo Gambacurta

TECHNISCHE UNIVERSITÄT DARMSTADT

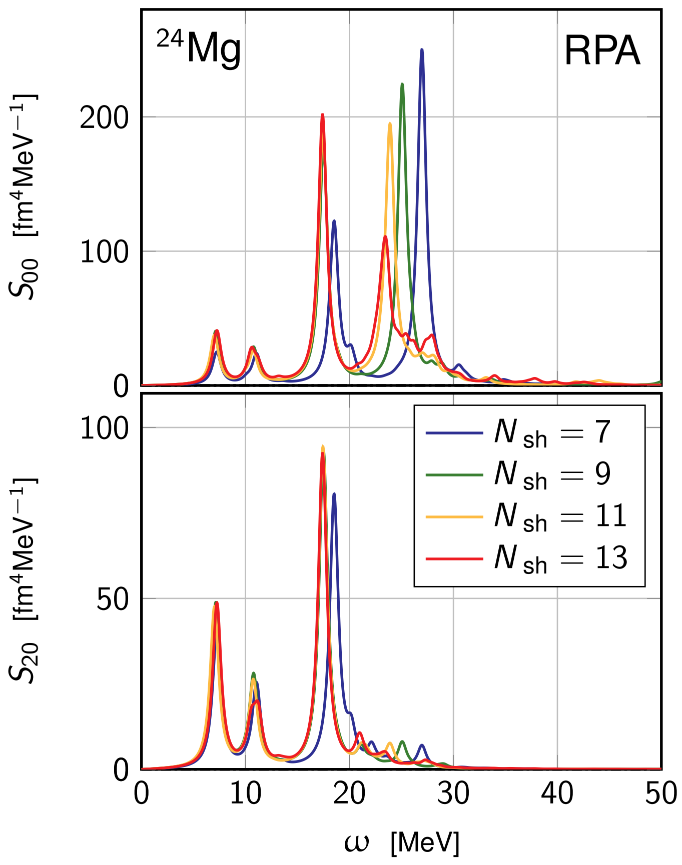
Robert Roth
Achim Schwenk
Alexander Tichai

Backup slides

Setting

RPA response stability wrt basis variations

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

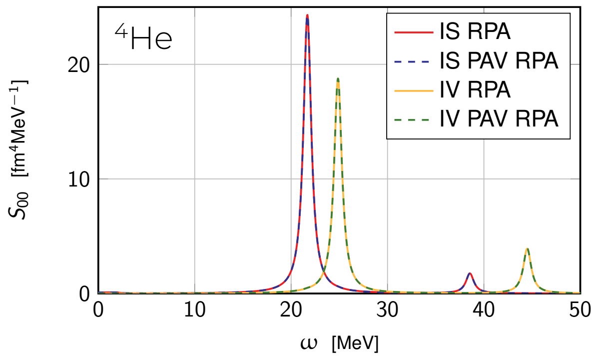


$N_{\rm sh}$	$E_{\rm HF}$ [MeV]	r [fm]	β
7	-195.65	2.991	0.378
9	-196.21	3.009	0.392
11	-196.93	3.011	0.383
13	-197.15	3.016	0.390

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

AMP Benchmarks

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



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

Extended derivation

Standard RPA derivation

$$\begin{aligned}\langle n|T|\mathrm{RPA}\rangle &= \langle \mathrm{RPA}|TQ_n^\dagger|\mathrm{RPA}\rangle \\ &= \langle \mathrm{RPA}|\left[T, Q_n^\dagger\right]|\mathrm{RPA}\rangle \\ &\approx \langle \mathrm{HF}|\left[T, Q_n^\dagger\right]|\mathrm{HF}\rangle \\ &= \sum_{ph}\left\{X_{ph}^n\,\langle h|T_{\lambda\mu}|p\rangle + Y_{ph}^n\,\langle p|T_{\lambda\mu}|h\rangle\right\}\end{aligned}$$

Projected RPA derivation

$$\begin{aligned}\langle \mathrm{RPA}|T_{\lambda\mu}P^J_{K_0-\mu,K}|n\rangle &= \langle \mathrm{RPA}|T_{\lambda\mu}P^J_{K_0-\mu,K}Q_n^\dagger|\mathrm{RPA}\rangle \\ &= \langle \mathrm{RPA}|T_{\lambda\mu}P^J_{K_0-\mu,K}Q_n^\dagger - Q_n^\dagger P^J_{K_0-\mu,K}T_{\lambda\mu}|\mathrm{RPA}\rangle \\ &\approx \langle \mathrm{HF}|T_{\lambda\mu}P^J_{K_0-\mu,K}Q_n^\dagger - Q_n^\dagger P^J_{K_0-\mu,K}T_{\lambda\mu}|\mathrm{HF}\rangle \\ &= \sum_{\mathrm{ph}} X^{\mathrm{ph}}\langle \mathrm{HF}|T_{\lambda\mu}P^J_{K_0-\mu,K}a_p^\dagger a_h|\mathrm{HF}\rangle + Y^{\mathrm{ph}}\langle \mathrm{HF}|a_h^\dagger a_p P^J_{K_0-\mu,K}T_{\lambda\mu}|\mathrm{HF}\rangle\end{aligned}$$

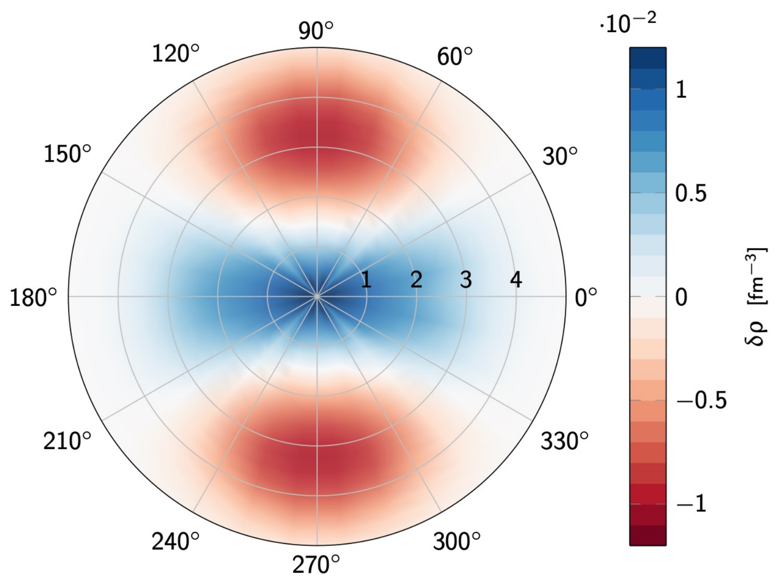
Reduced transition amplitudes

$$\langle \mathrm{RPA}||T_\lambda||n\rangle = (2J_0+1)N_0N_n(-1)^{J_0-K_0}\sum_{\mathrm{ph}}\sum_{\mu}\left[X_n^{\mathrm{ph}} + (-1)^\mu Y_n^{\mathrm{ph}}\right]\begin{pmatrix} J_0 & \lambda & J \\ -K_0 & \mu & K_0-\mu\end{pmatrix}\int_{-1}^{1} d(cos\beta)\; d^J_{K_0-\mu,K}(\beta)\langle \mathrm{HF}|T_{\lambda\mu}e^{i\beta J_y}a_p^\dagger a_h|\mathrm{HF}\rangle$$

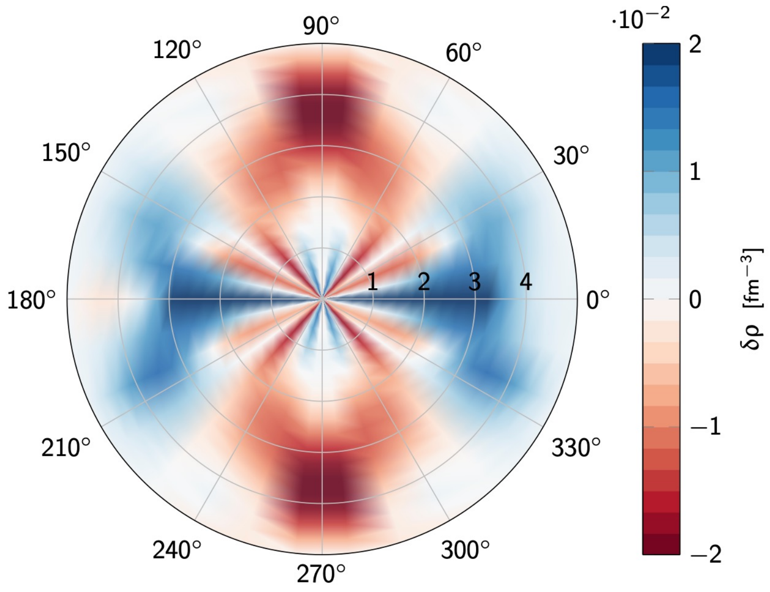
$$N_0 = \left[\int_{-1}^{1} d(cos\beta)\; d^{J_0}_{K_0,K_0}(\beta)\langle \mathrm{HF}|e^{i\beta J_y}|\mathrm{HF}\rangle\right]^{-1/2} \qquad N_n = \left[\sum_{\mathrm{p,h;p',h'}}\left(X^n_{ph}X^n_{p'h'} - Y^n_{ph}Y^n_{p'h'}\right)\int_{-1}^{1} d(cos\beta)\; d^J_{K,K}(\beta)\langle \mathrm{HF}|a_{h'}^\dagger a_{p'}e^{i\beta J_y}a_p^\dagger a_h|\mathrm{HF}\rangle\right]^{-1/2}$$

Comparison to rotational transition density

Anomalous phonon



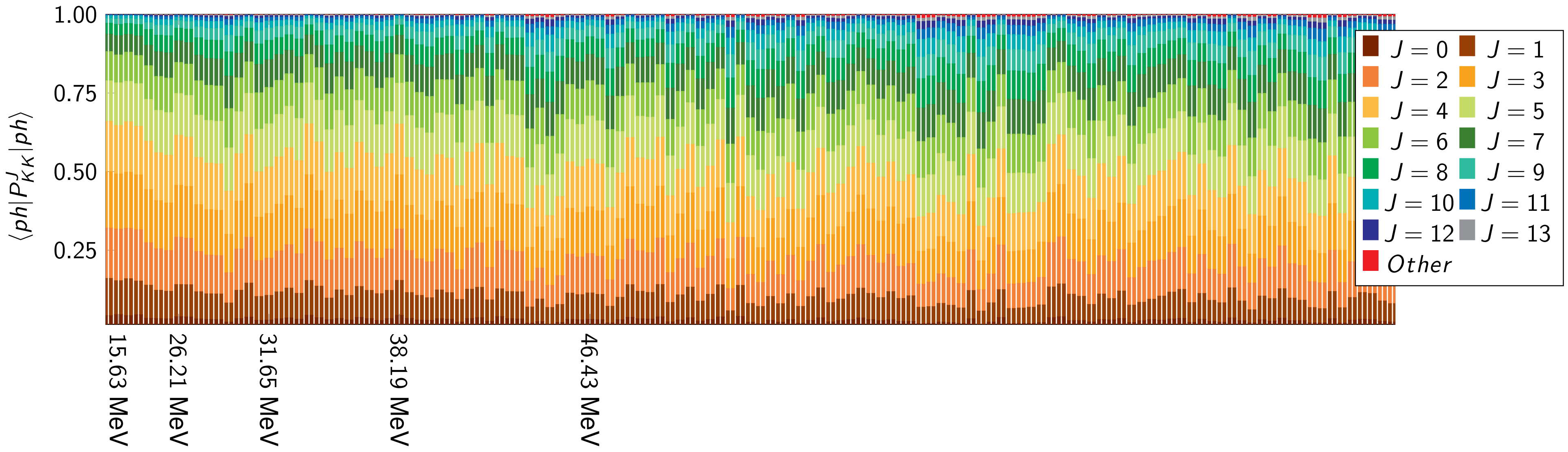
Rotational state

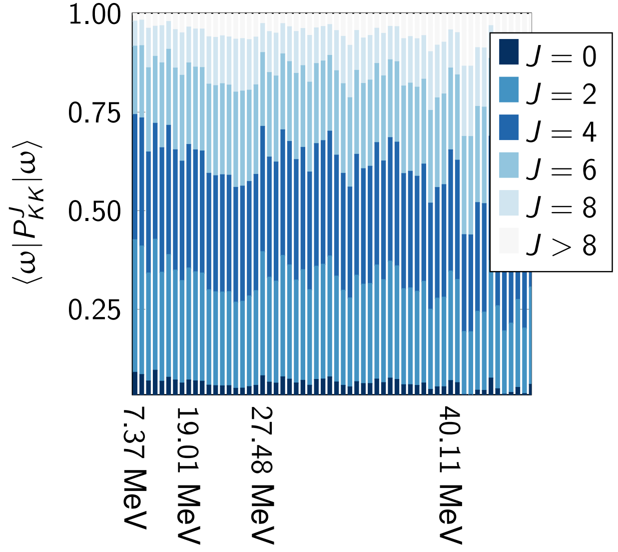


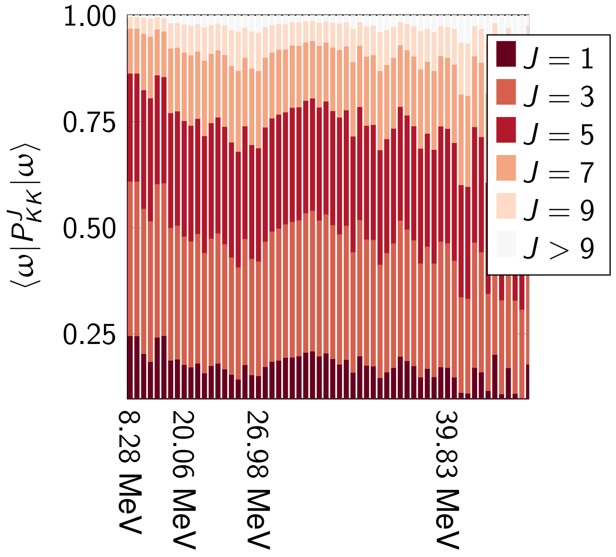
Overlap maximised at $\alpha \sim 24^\circ$

$$\rho_\alpha = \left(\frac{\hat{R}_y(\alpha) + \hat{R}_y(-\alpha)}{2} \right) \rho_0$$

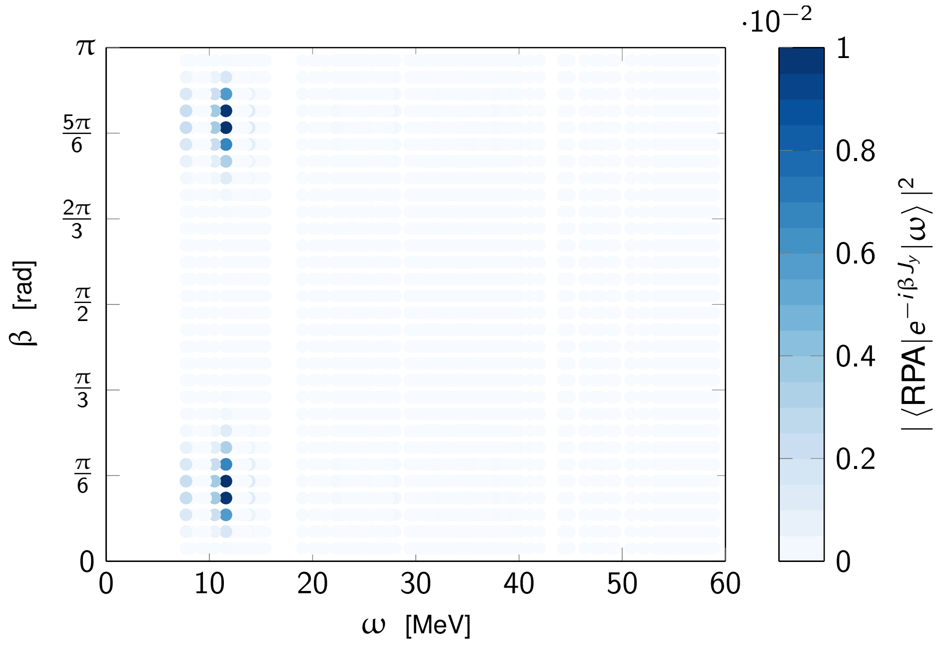
AMP identity resolutions



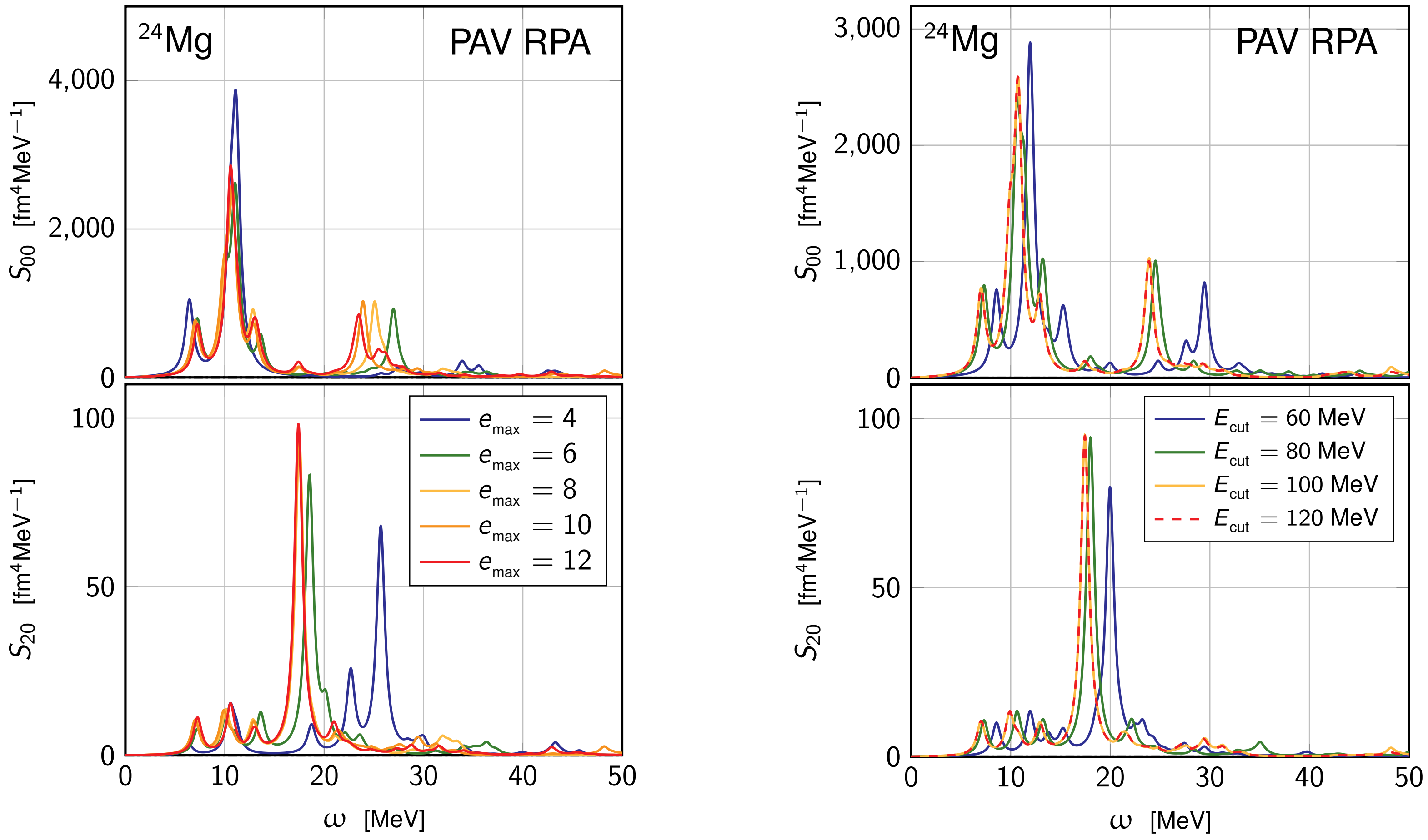




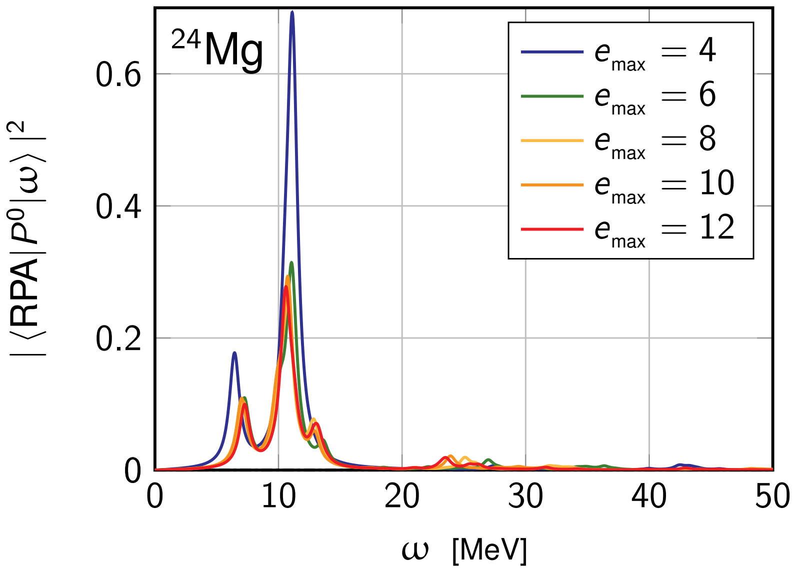
Rotational overlap

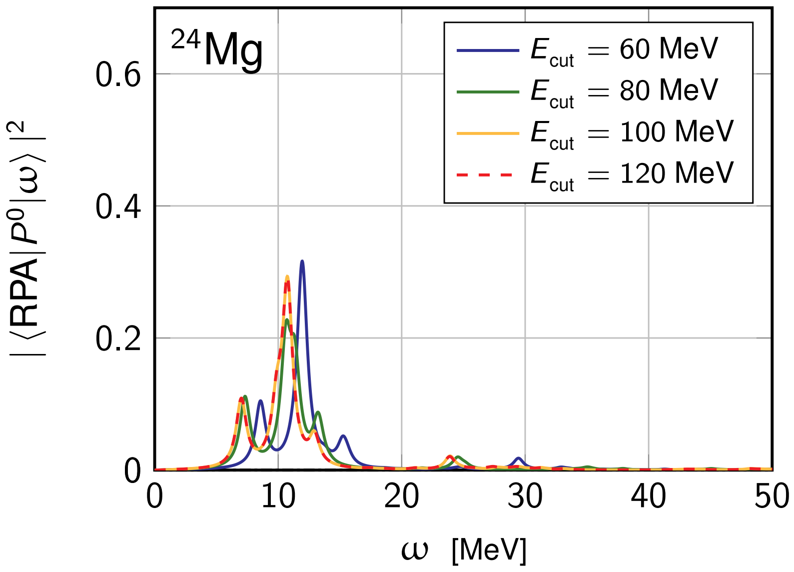


PAV RPA convergence



PAV RPA convergence





PAV RPA convergence