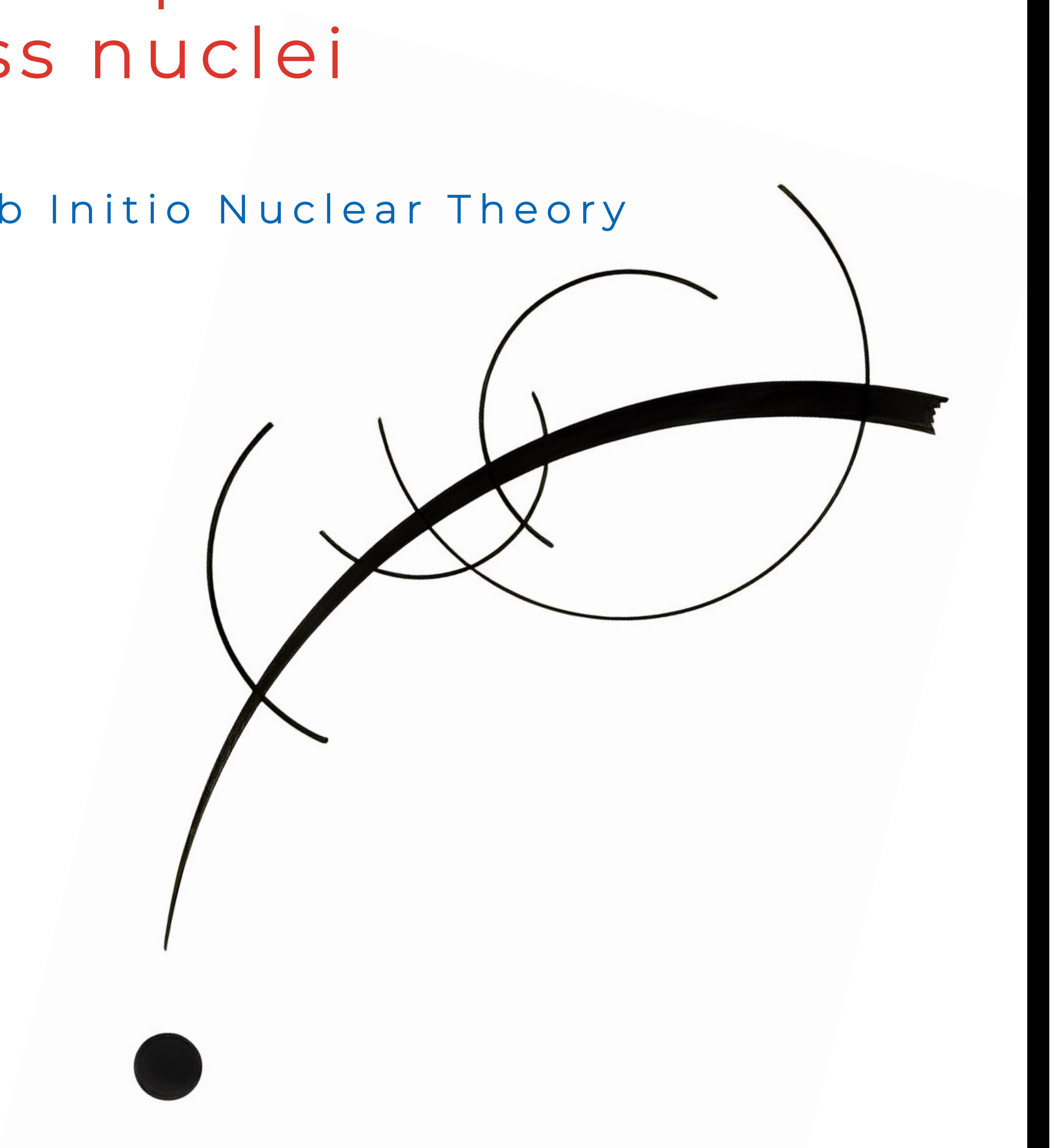
Ab initio description of monopole resonances in light- and medium-mass nuclei

PAINT2024 – Workshop on Progress in Ab Initio Nuclear Theory

TRIUMF, Vancouver

February 27th, 2024



Andrea Porro

Technische Universität Darmstadt

SFB 1245

TECHNISCHE UNIVERSITÄT DARMSTADT

Outline

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1 Giant Resonances

- Physical introduction
- Existing ab initio theoretical tools

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- Formalisms
- Uncertainty quantification

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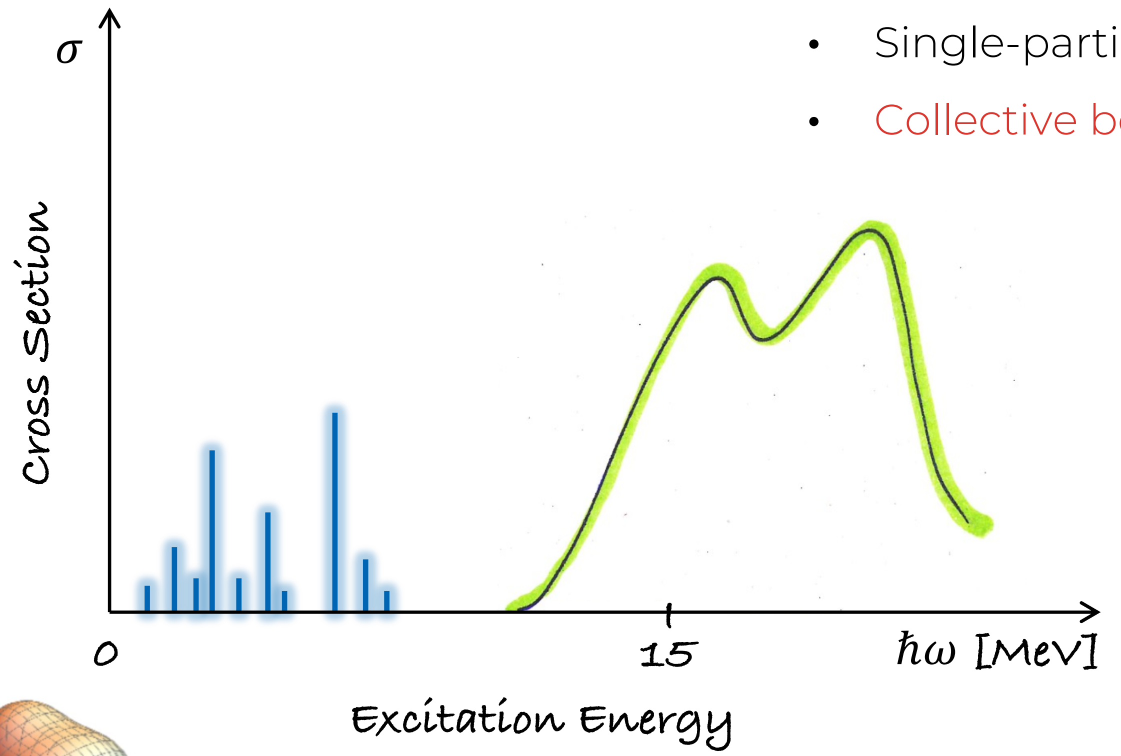

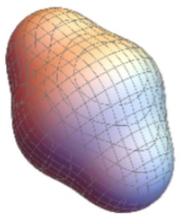

Dual nature of nucleus

- Single-particle features
- Collective behaviour

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

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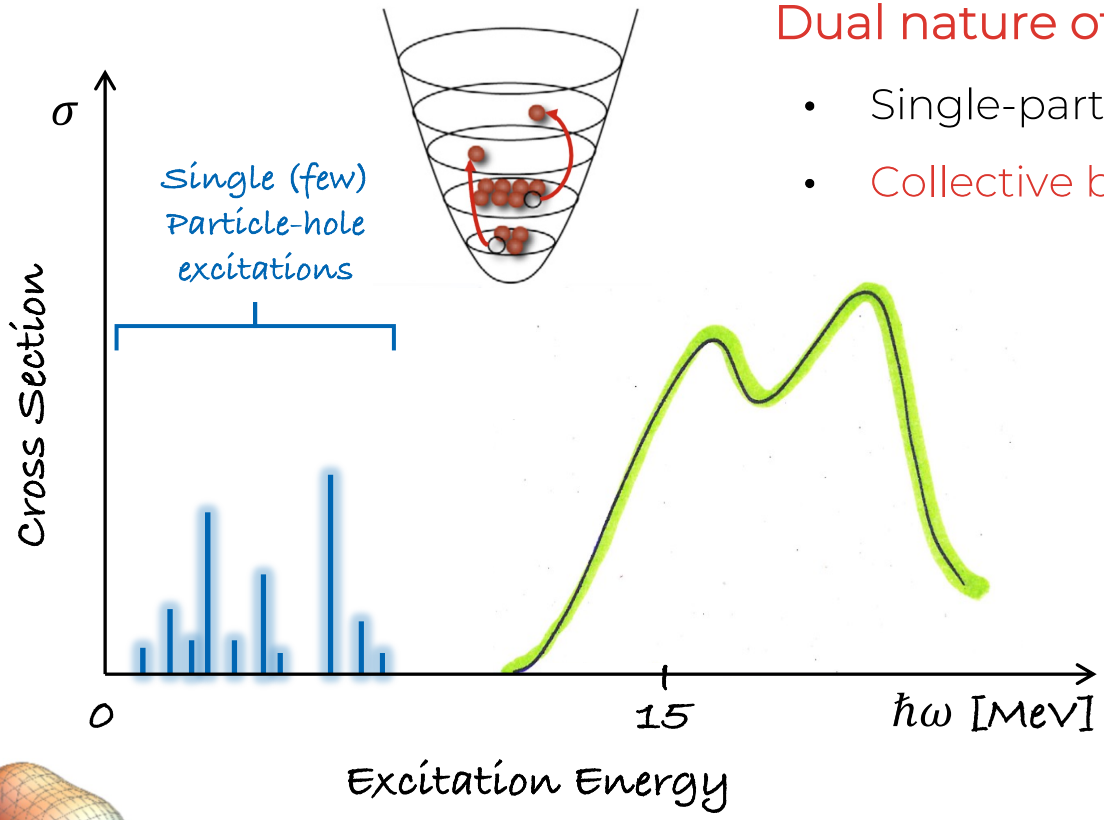

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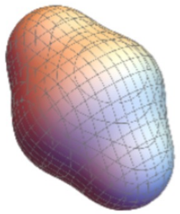

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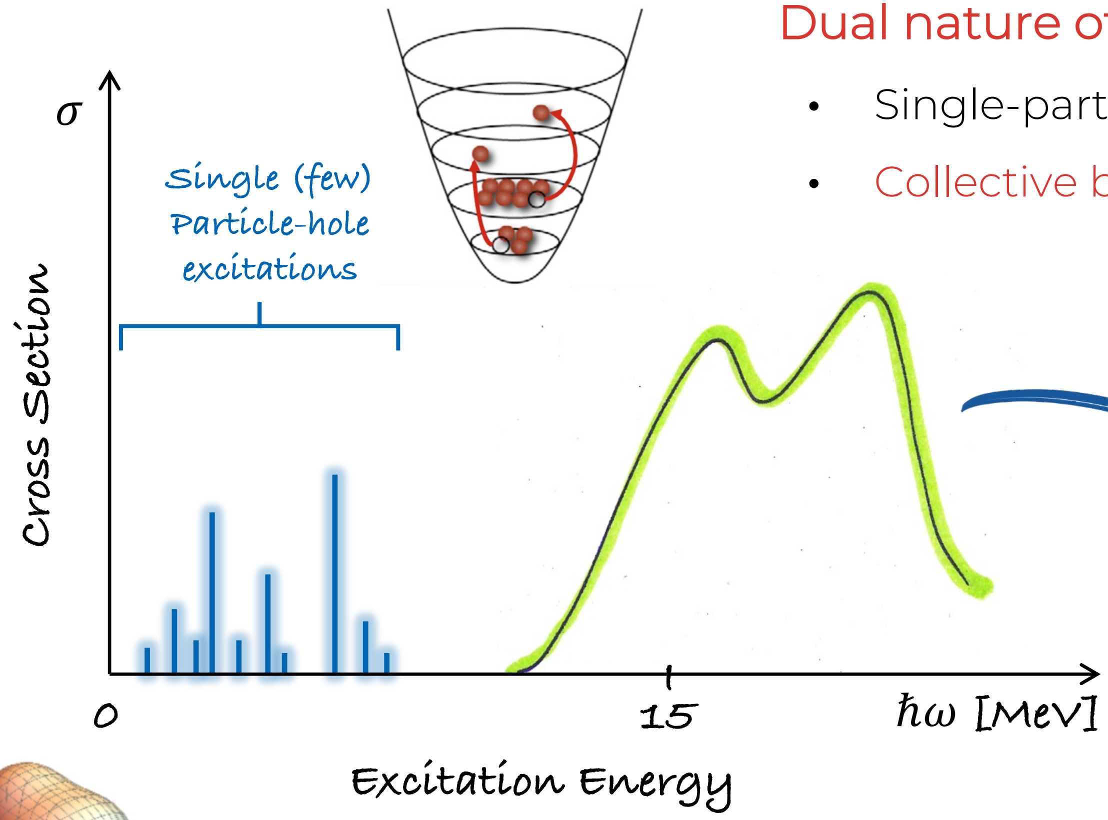

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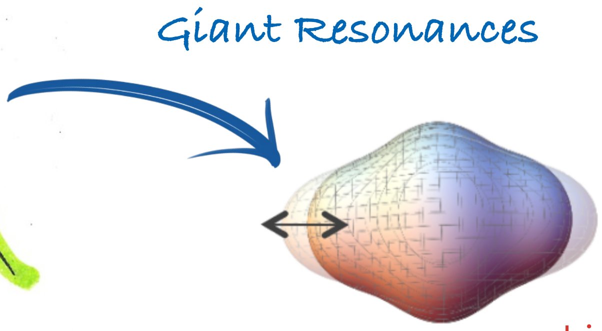
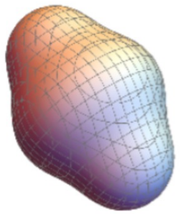


Liquid drop picture

vibrations, oscillations



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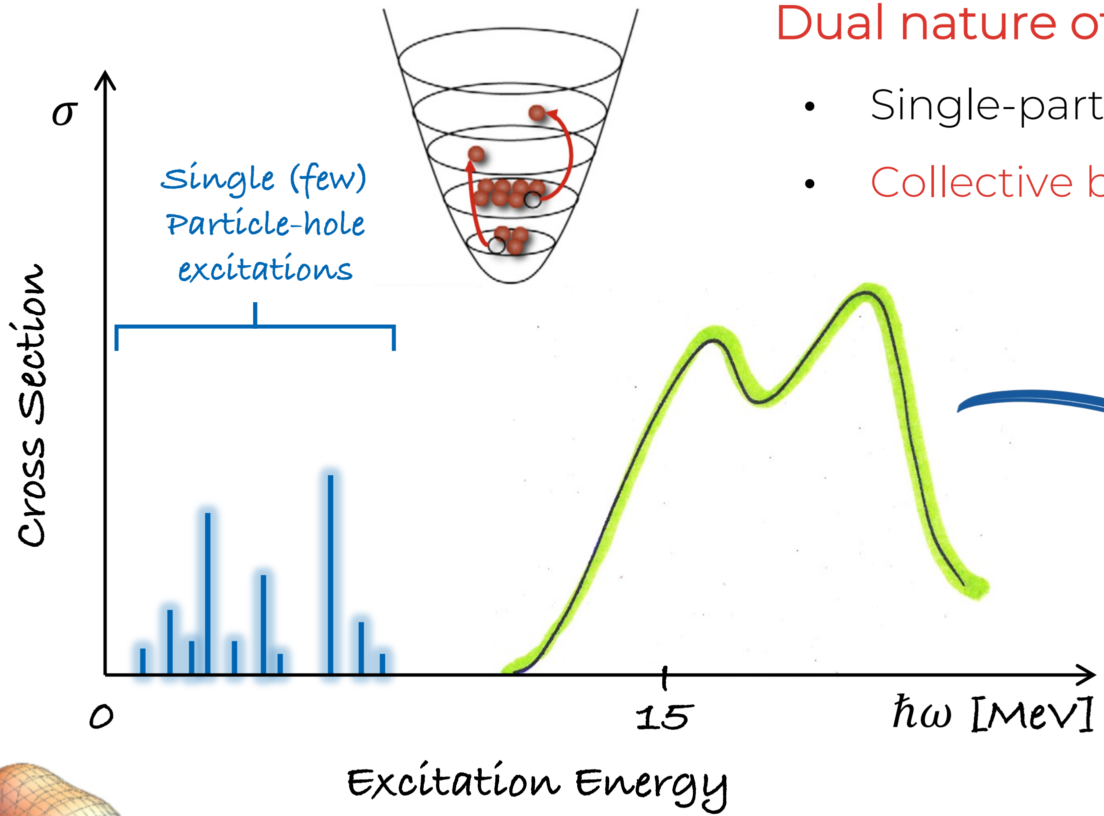

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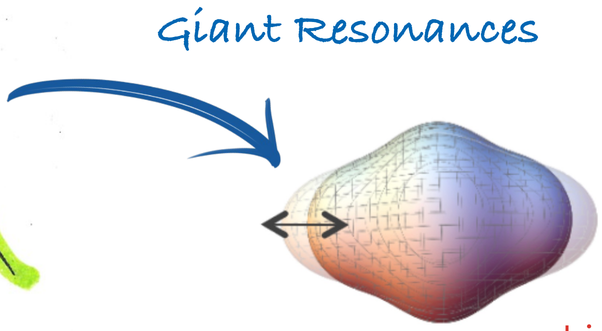

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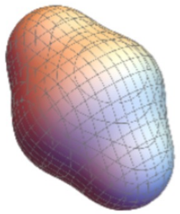

Giant Resonances (GRs)

clearest manifestation of collective motion

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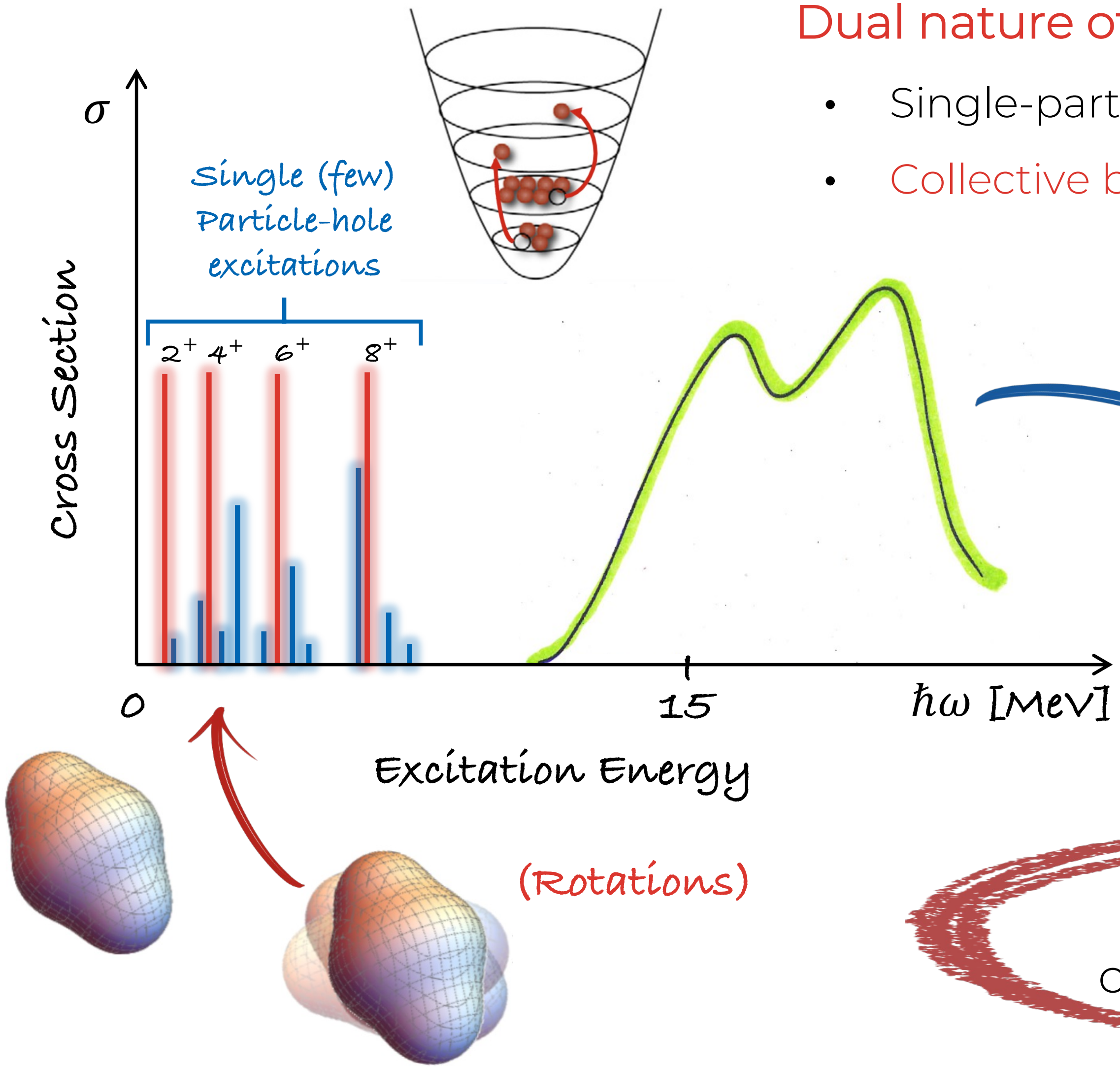

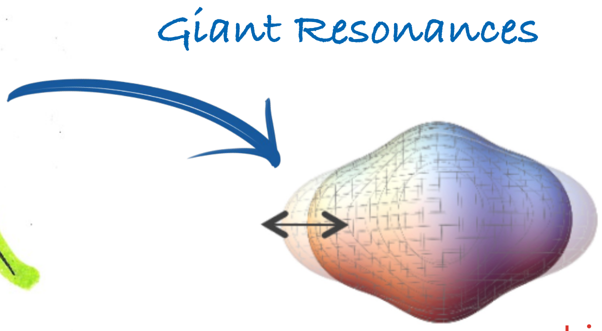

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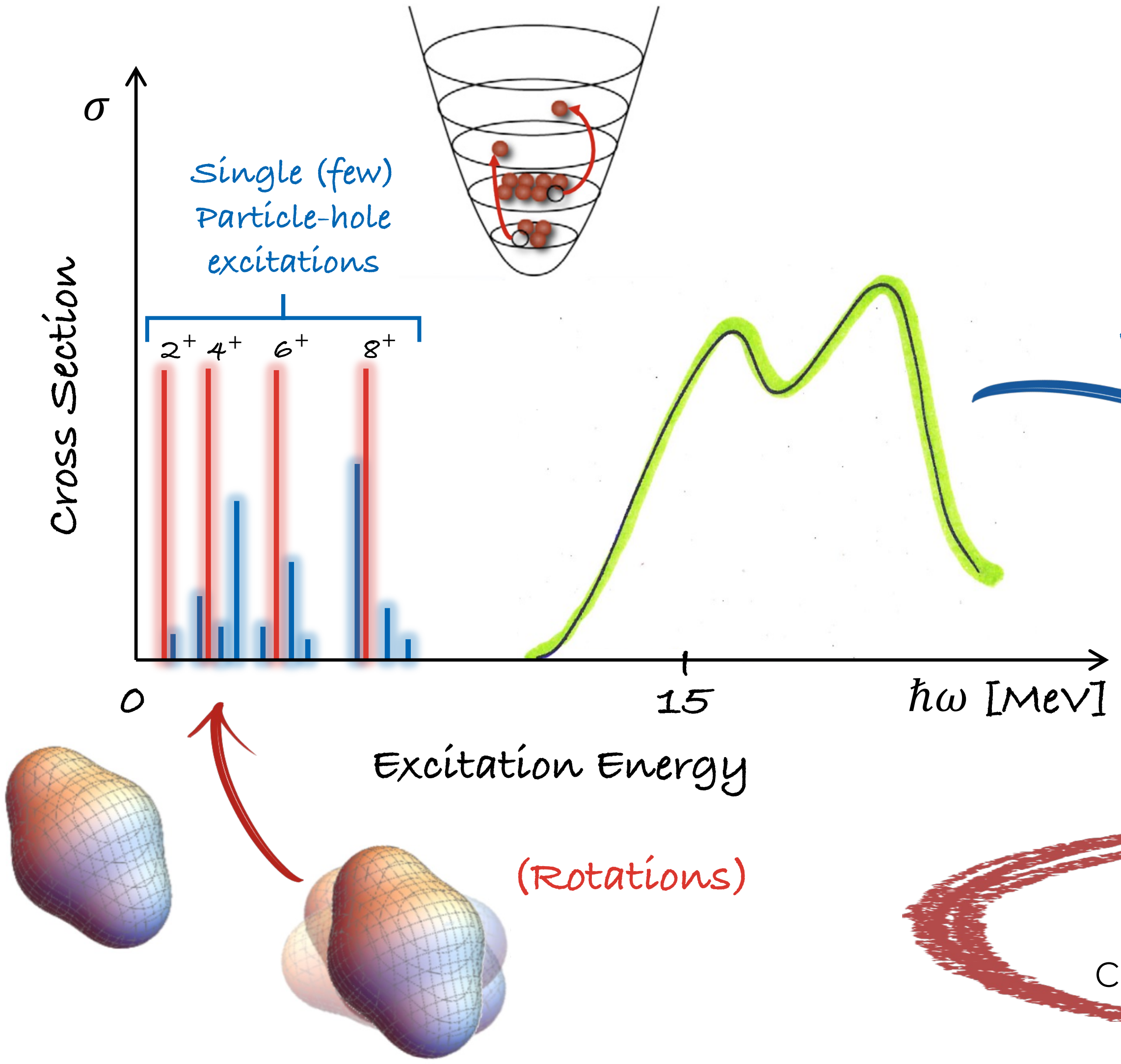

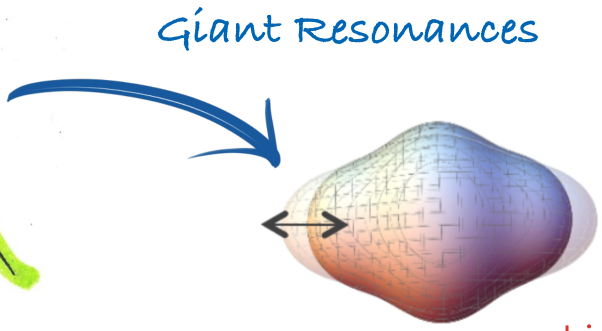

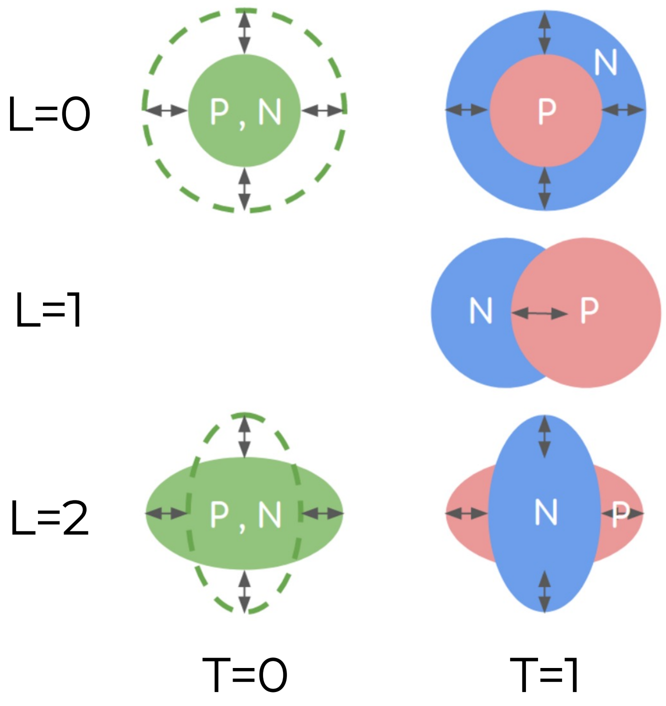

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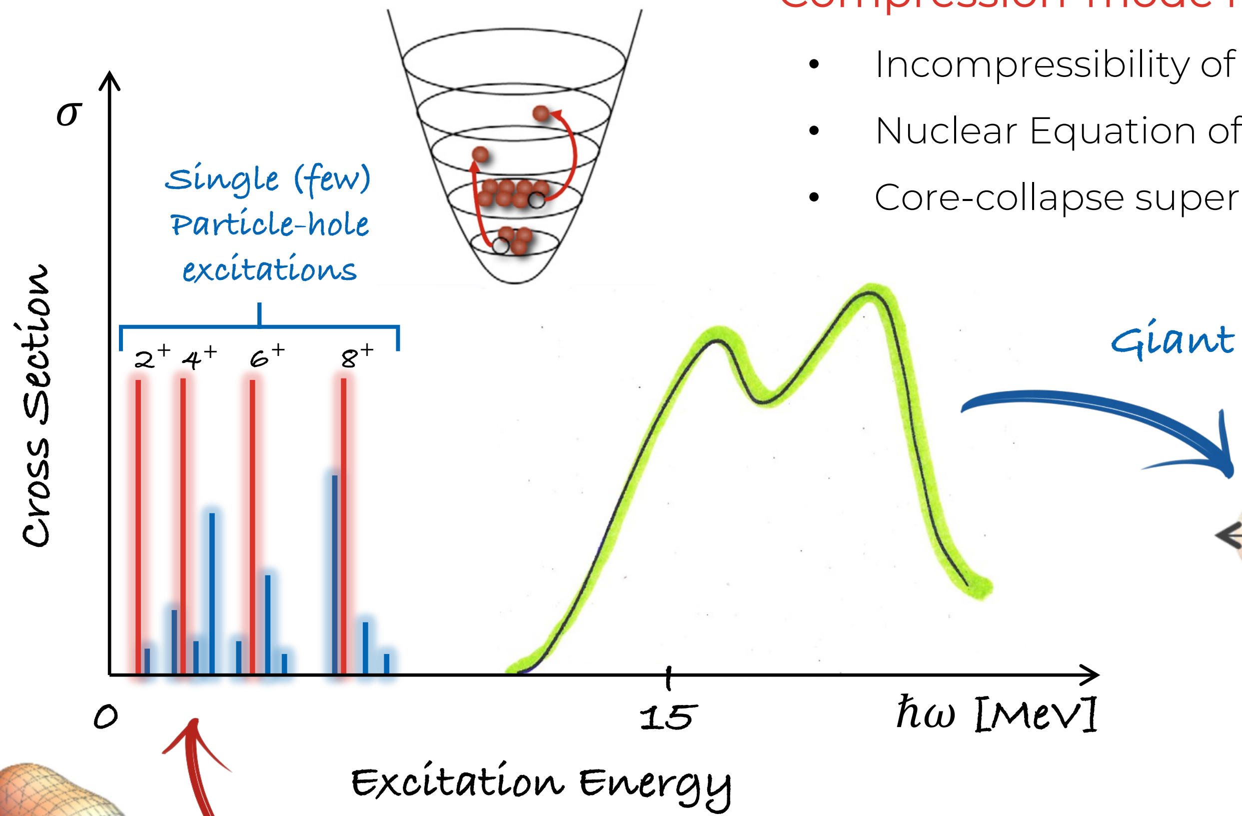
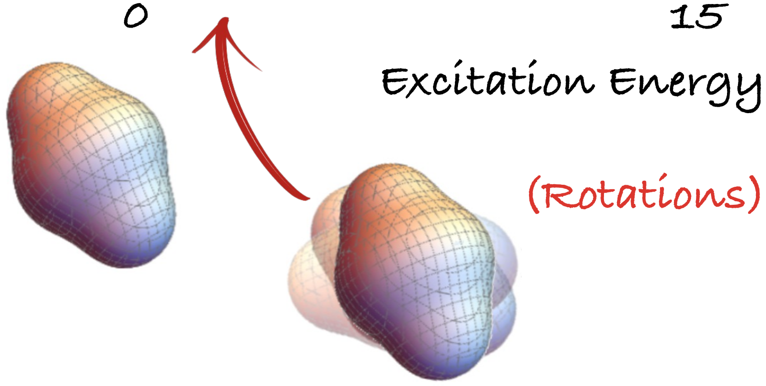
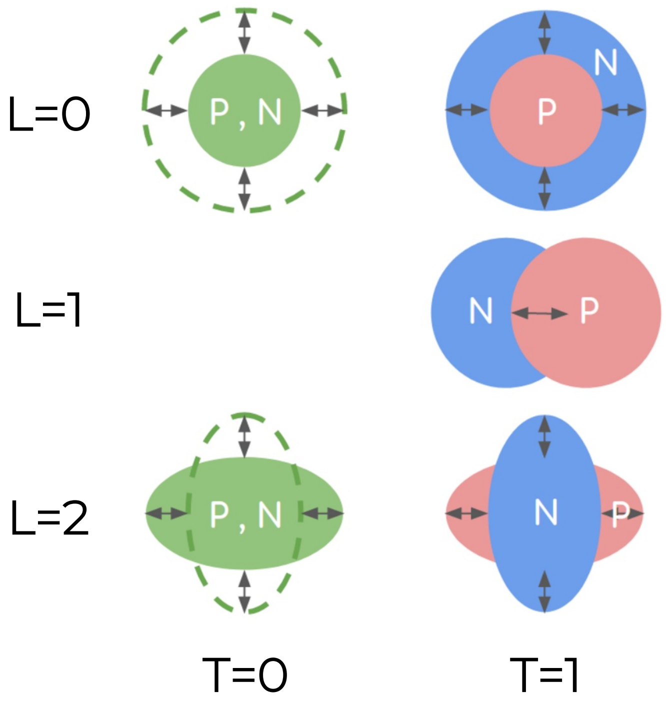
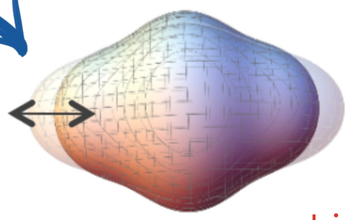




Compression-mode resonances

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





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EOM and VS extensions

- **IMSRG** and **CC**
- Suited for **weakly-collective** excitations only

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CC-LIT Lorenz integral transform (sperical)

SA-NCSM Application to deformed systems (^{20}Ne)

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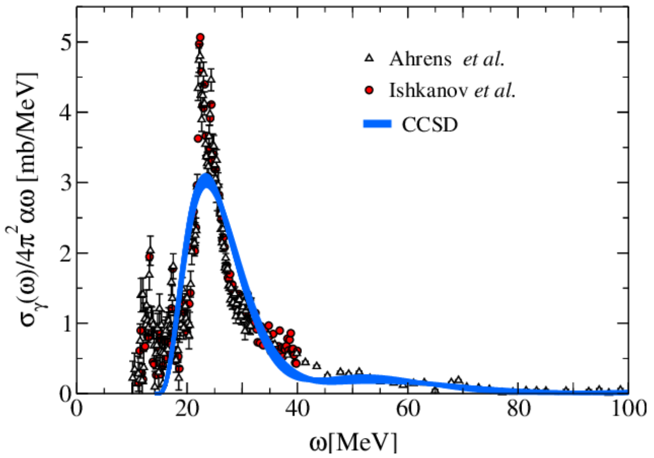

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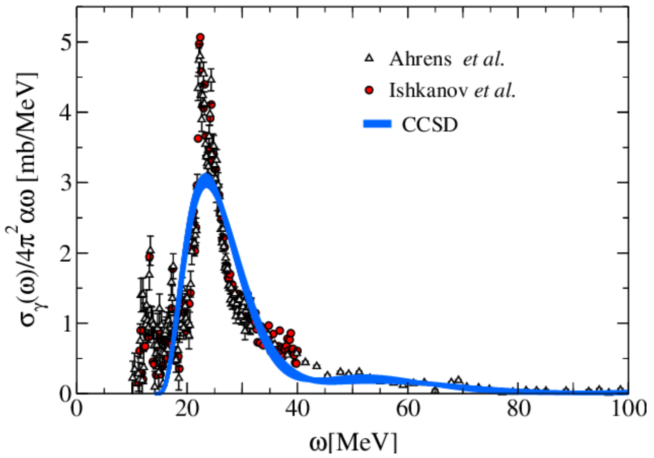

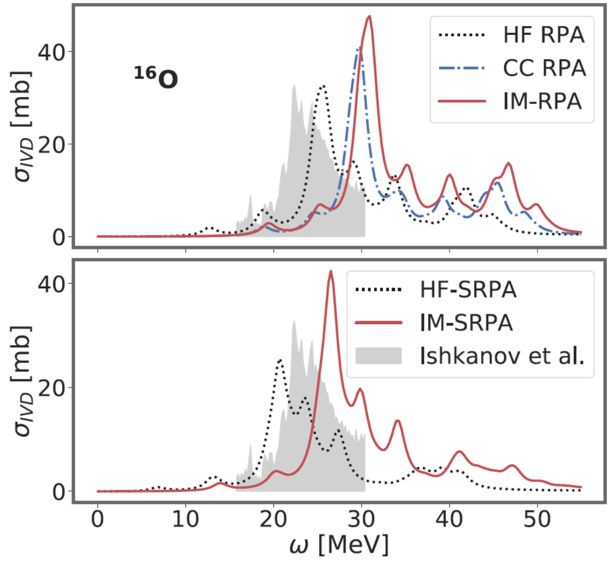

(Q)RPA

- Spherical (Q)RPA, 2nd RPA, CC-RPA, IMSRG-RPA, IMSRG-2nd RPA

[R. Trippel, PhD Thesis, 2016]

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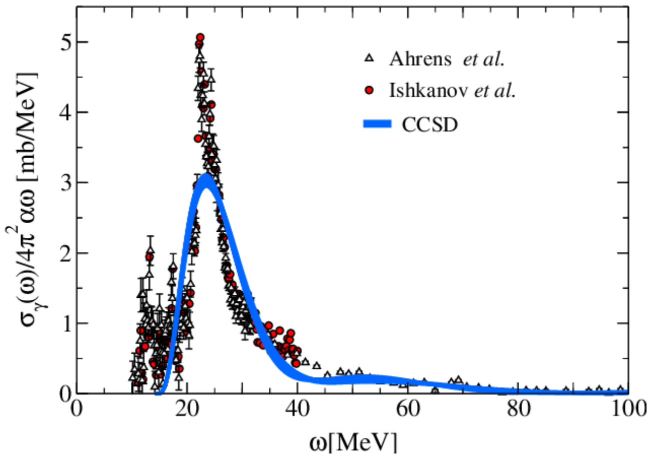

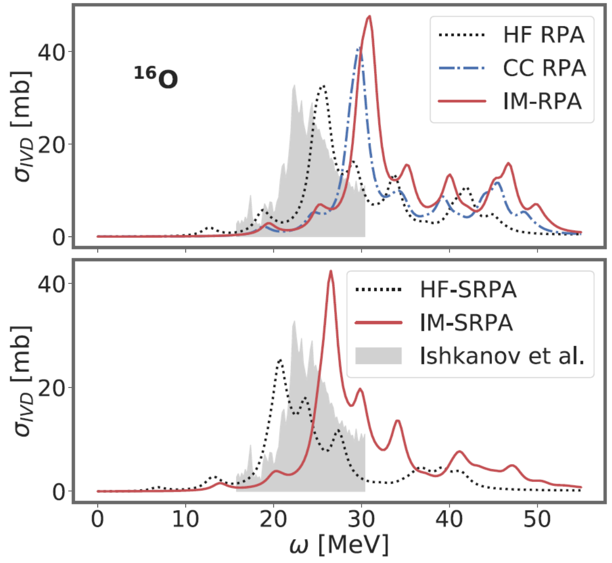

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- Spherical (Q)RPA, 2nd RPA, CC-RPA, IMSRG-RPA, IMSRG-2nd RPA
- SCGF, RPA with dressed propagators

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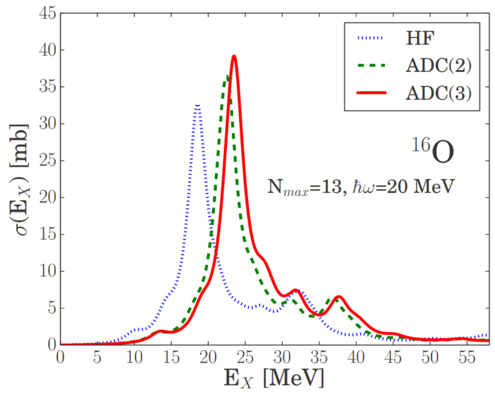

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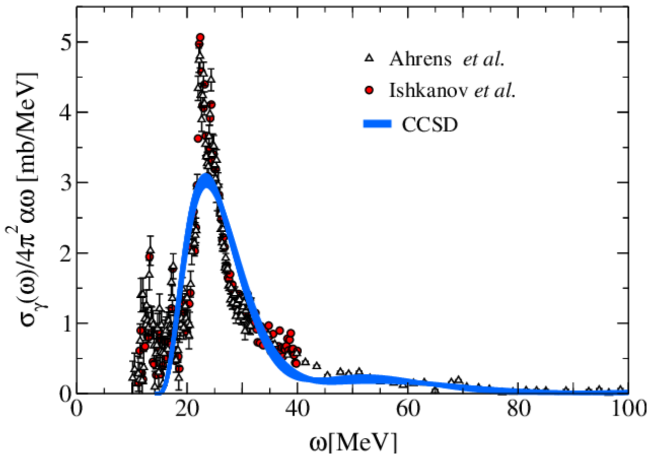
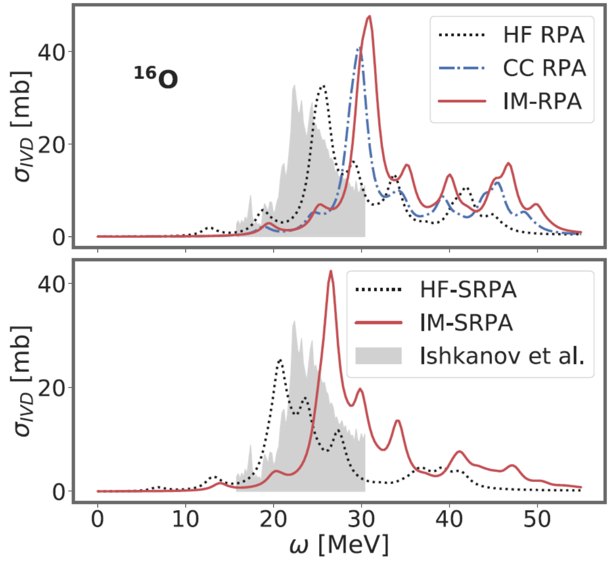




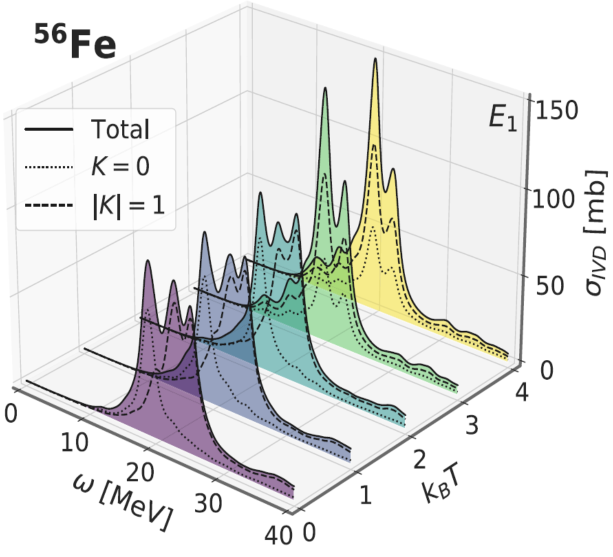
(Q)RPA

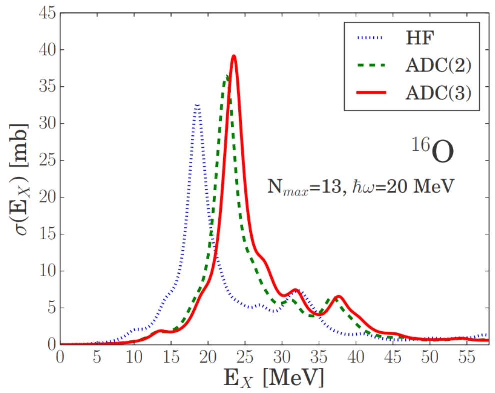
- Spherical (Q)RPA, 2nd RPA, CC-RPA, IMSRG-RPA, IMSRG-2nd RPA
- SCGF, RPA with dressed propagators
- (Q)RPA for axially- and triaxally-deformed systems

[R. Trippel, PhD Thesis, 2016]

[Barbieri, Raimondi, PRC, 2019]

[Beaujeault-Taudière, Frosini, Ebran, Duguet, Roth, Somà, PRC, 2023]





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Projected Generator Coordinate Method

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

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Open-shell systems

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→ Strong static correlations

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Symmetry-breaking reference states

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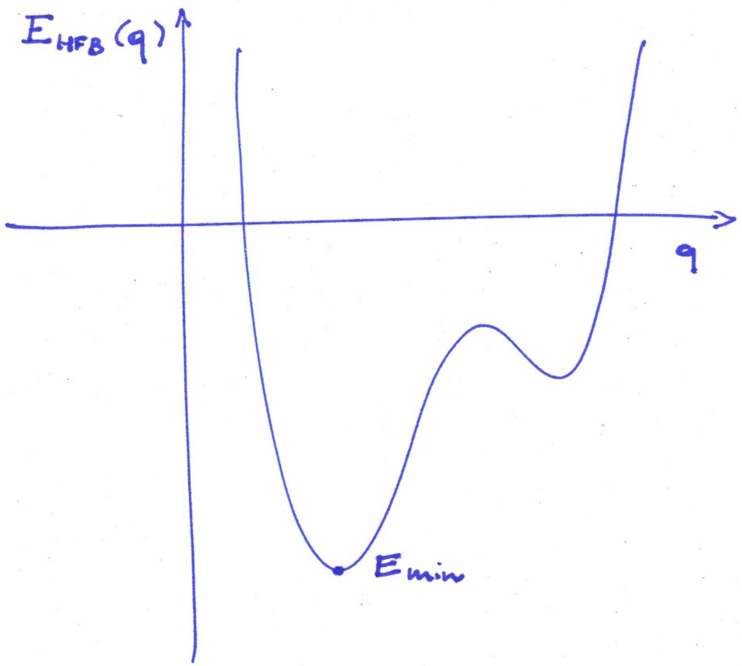
Open-shell systems → Strong static correlations → Symmetry-breaking reference states

1 *Constrained HFB solutions*

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



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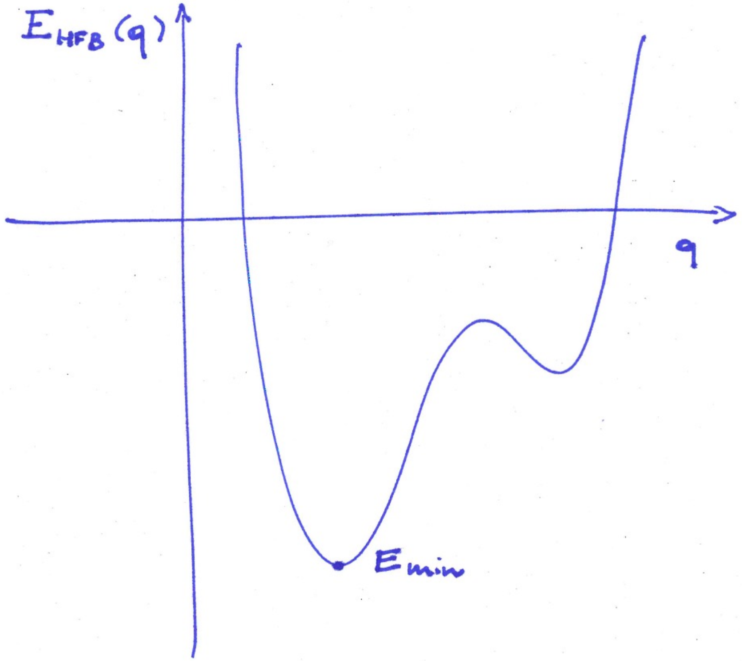
Generator coordinates

(q can be any coordinate)



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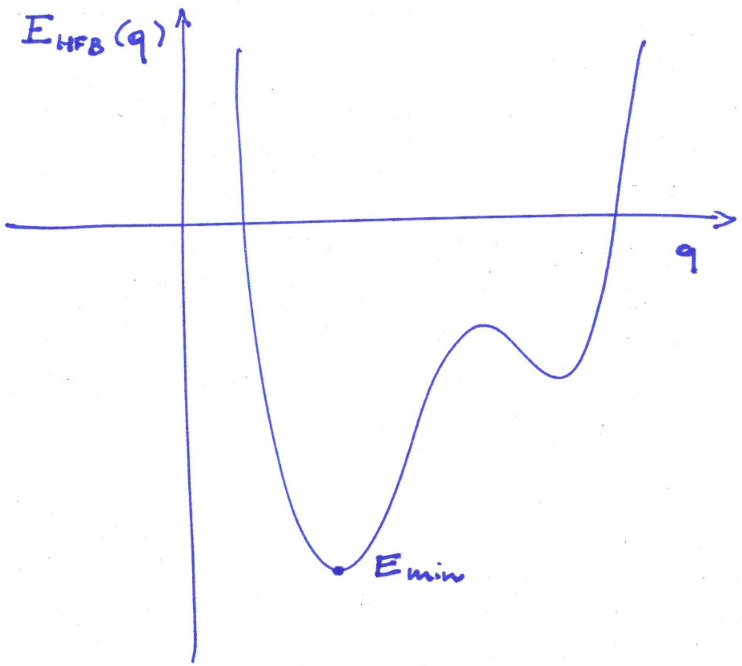

2 PGCM ansatz

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

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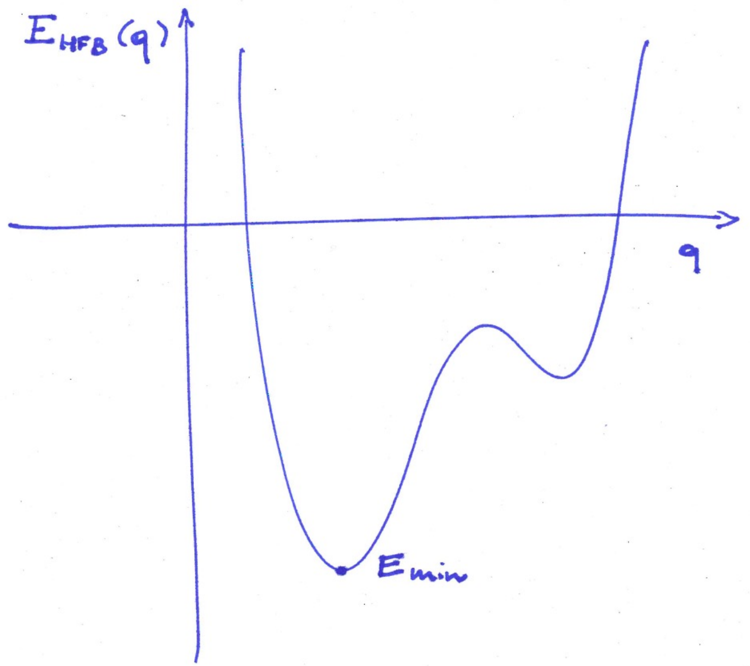

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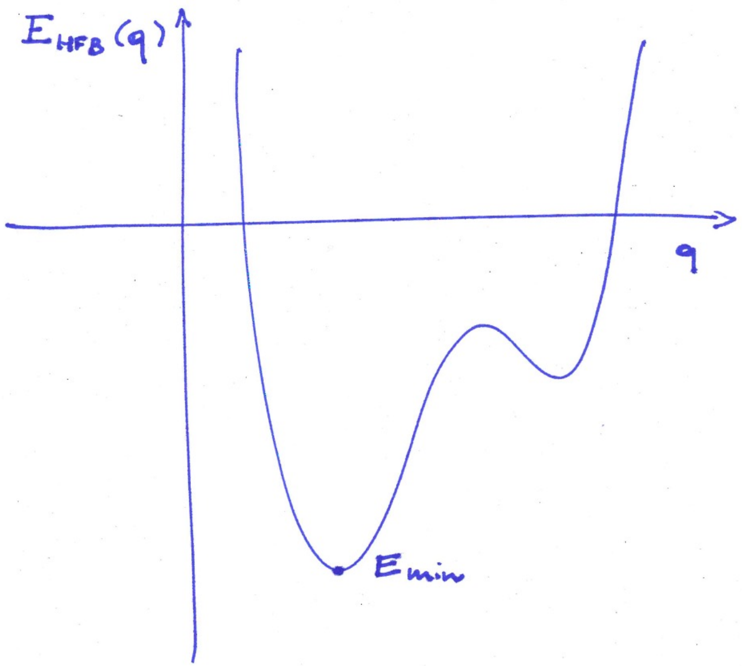

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Variational method

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

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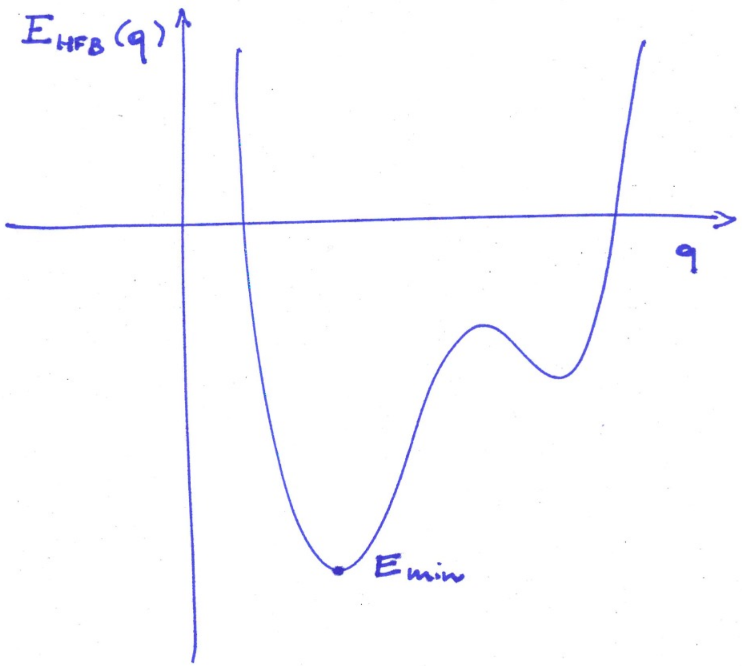

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Schrödinger-like equation

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

Kernels evaluation

$$\mathcal{H}(p,q) \equiv \langle \Phi(p) | H | \Phi(q) \rangle$$
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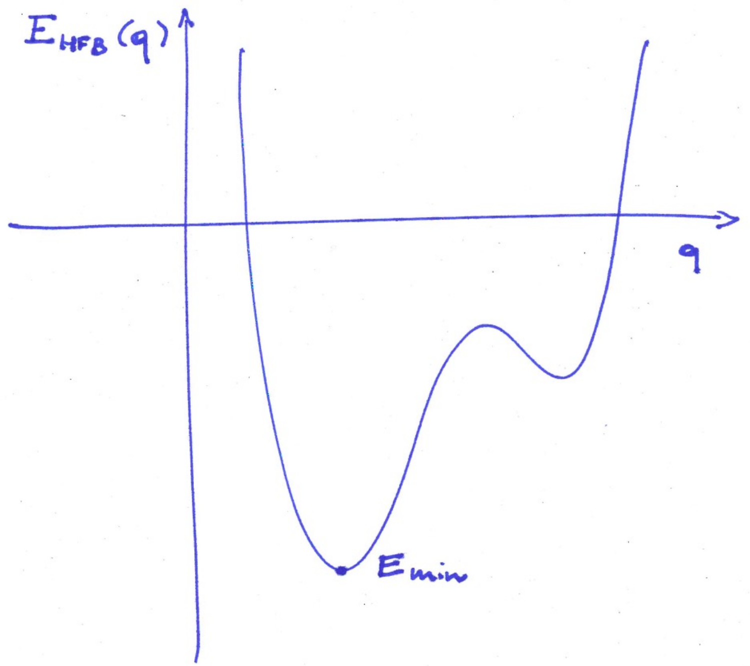
Projected Generator Coordinate Method

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

Diagonalization in a physically-informed reduced Hilbert space



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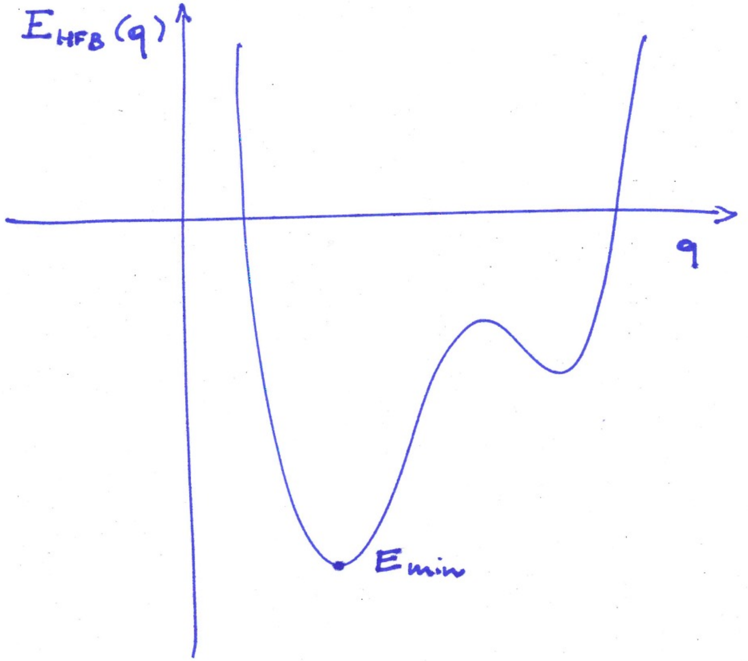

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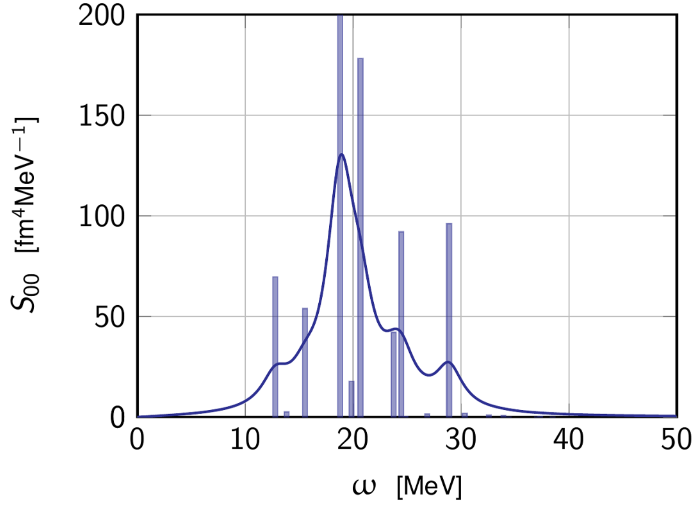
Setting

Studied quantity: monopole strength

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

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



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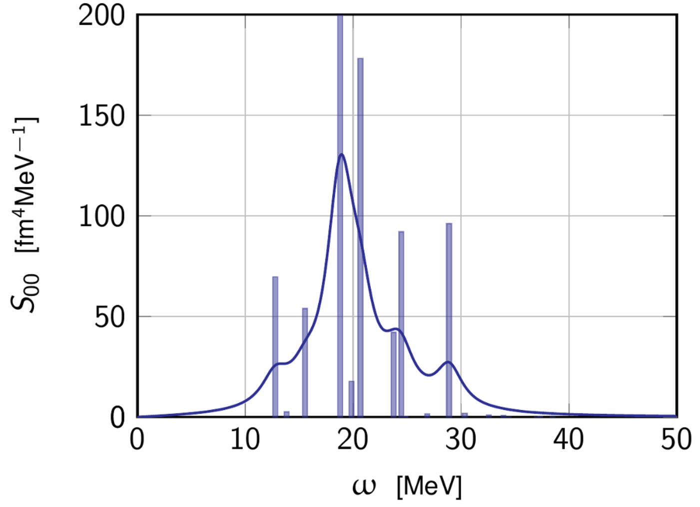
JM=00



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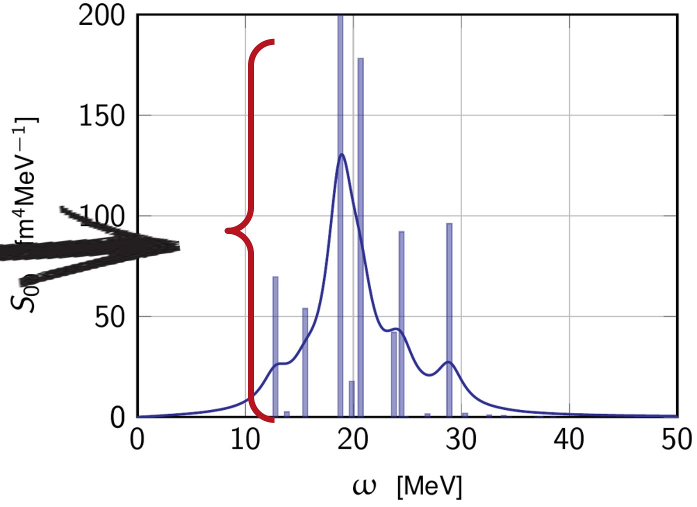

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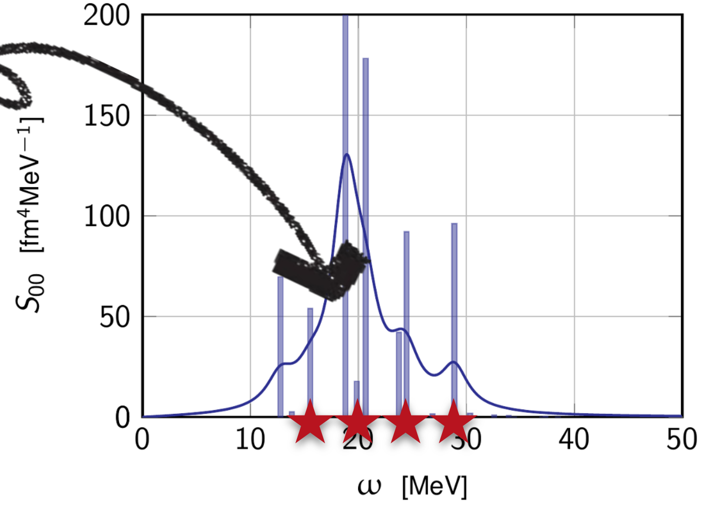
Studied quantity: monopole strength

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

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



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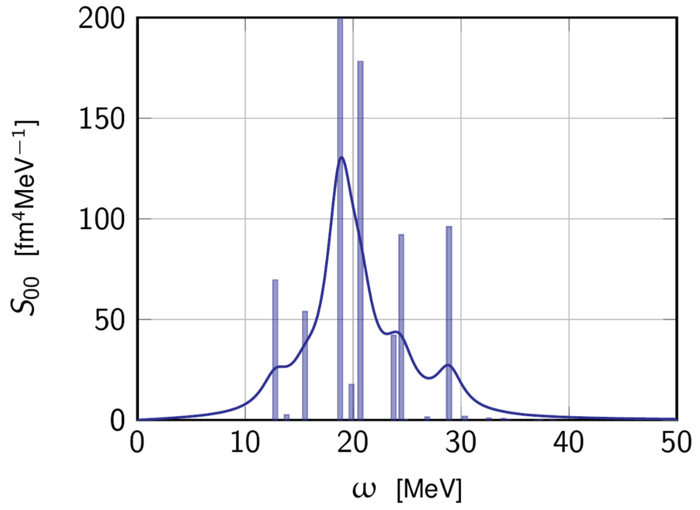

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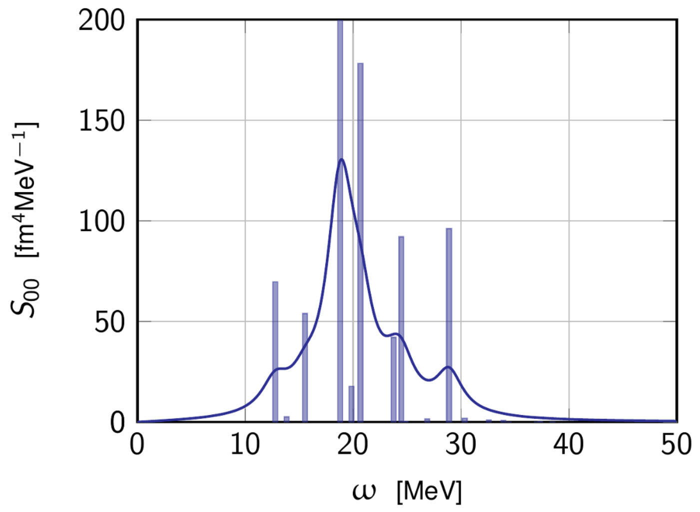

Related moments

$$m_k \equiv \int_0^\infty S_{00}(\omega)\, \omega^k \, d\omega$$
$$= \sum_\nu (E_\nu - E_0)^k |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2$$

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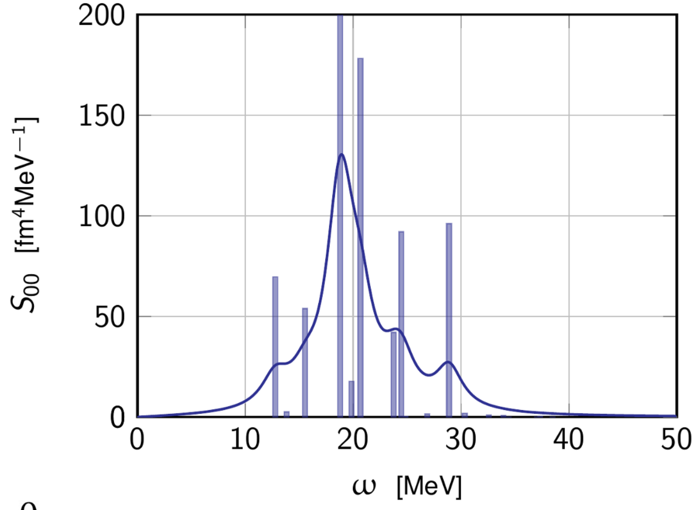

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Quantify the most relevant features of the strength $\bar{E}_1 = \frac{m_1}{m_0}$ $\sigma^2 = \frac{m_2}{m_0} - \left(\frac{m_1}{m_0}\right)^2 \geq 0$

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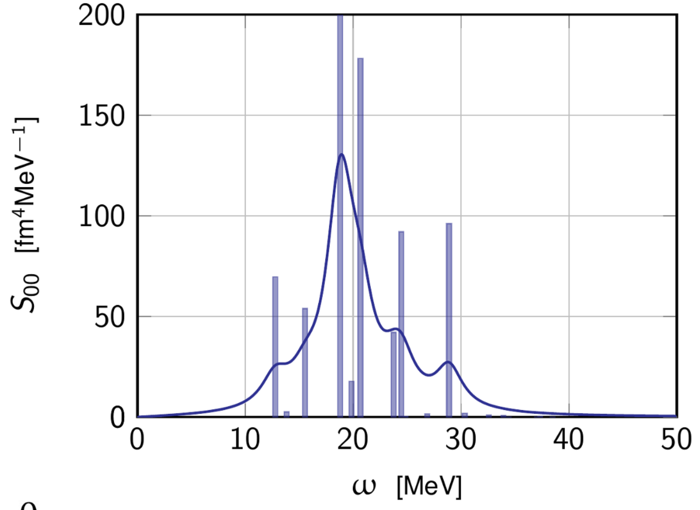

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Ab-initio PGCM and QRPA consistent numerical settings (systematic study in ^{46}Ti)

- Quantities expanded on harmonic oscillator basis (characterised by **ħω,** e_{max}, e_{3max})

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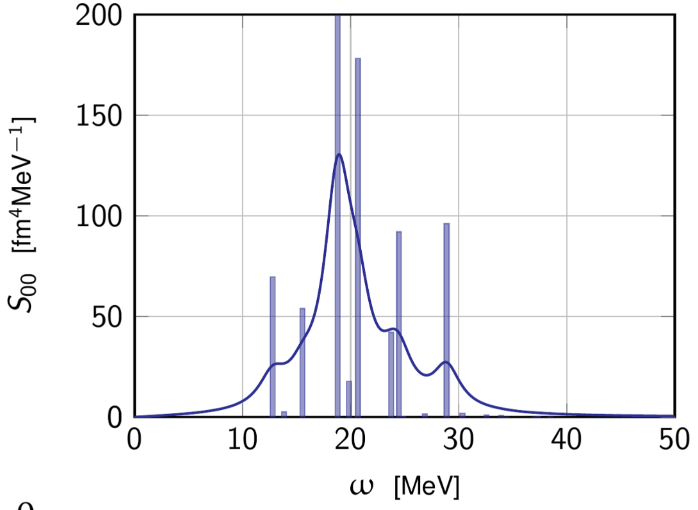

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Ab-initio PGCM and QRPA consistent numerical settings (systematic study in ^{46}Ti)

- Quantities expanded on harmonic oscillator basis (characterised by **ħω,** e_{max}, e_{3max})
- Family of chiral NN + in-medium 3N interactions (NLO, N2LO and N3LO)
  - T. Hüther, K. Vobig, K. Hebeler, R. Machleidt and R. Roth, "Family of chiral two-plus three-nucleon interactions for accurate nuclear structure studies", *Phys. Lett. B,* 808, 2020
  - In-vacuum SRG evolution (**α**=0.04 fm^4, **α**=0.08 fm^4)
  - M. Frosini, T. Duguet, B. Bally, Y. Beaujeault-Taudière, J.-P. Ebran and V. Somà, "In-medium k-body reduction of n-body operators", *The European Physical Journal A*, *57*(4), 2021

Uncertainty budget

Many-body truncation

- Comparison to **PGCM-PT**
- Only tested for **low-lying exc**
- **Correlated** to **SRG** and **generator coords**

SRG dependence

- **Strong** centroid **dependence** ~ 10 %
- Dispersion relative error ~ 20 %
- **Truncates** both **H** and **many-body**

Chiral Order

- Good **overall convergence**
- Centroid relative error ~ 1,6 %
- Dispersion relative error ~ 9,8 %

Generator coordinates choice

- **Empirical knowledge**, two coords **r** and β_2
- More **systematic** choice **needed**

Harmonic Oscillator width

- Good **overall convergence**
- Centroid relative error ~ 1,6 %
- Dispersion relative error ~ 6 %

Three-body treatment

- NO2B approximation
- 1-2 % uncertainty in low-lying exc
- Not tested for giant resonances

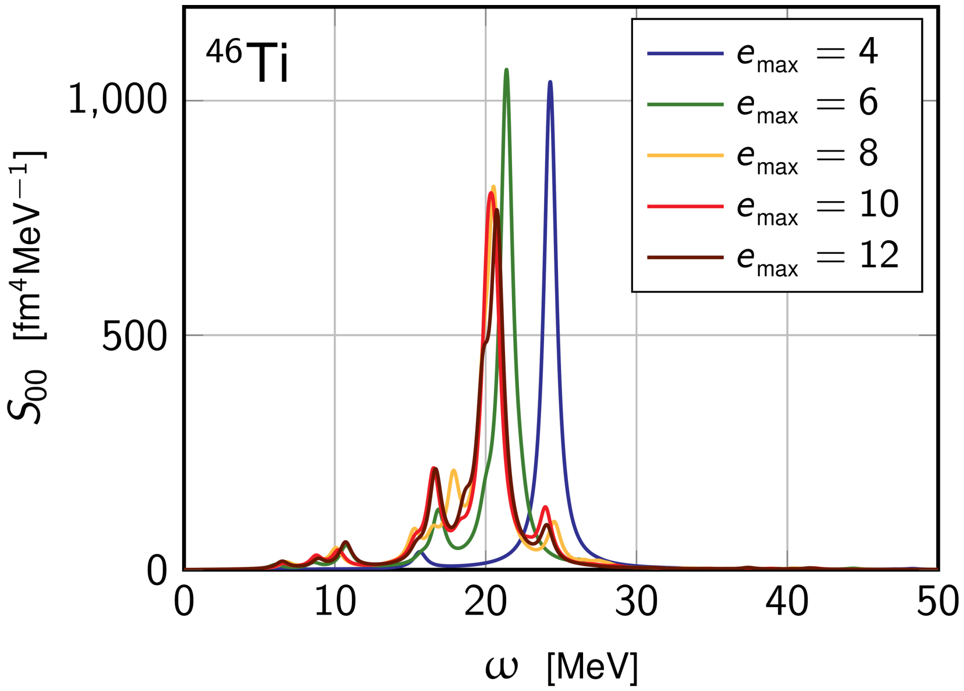
Finite Basis Size

- Good **overall convergence**
- Centroid relative error ~ 0,6 %
- Dispersion relative error ~ 1,7 %
- $\mathbf{e_{3max}}$ not studied (14 safe for GS)

Hamiltonian parameters

- **LEC** dependence of χ forces
- **Few interactions** compared
- **Correlated** to SRG
- Need for **emulators** (EC)

Finite Basis Size



- Good overall convergence

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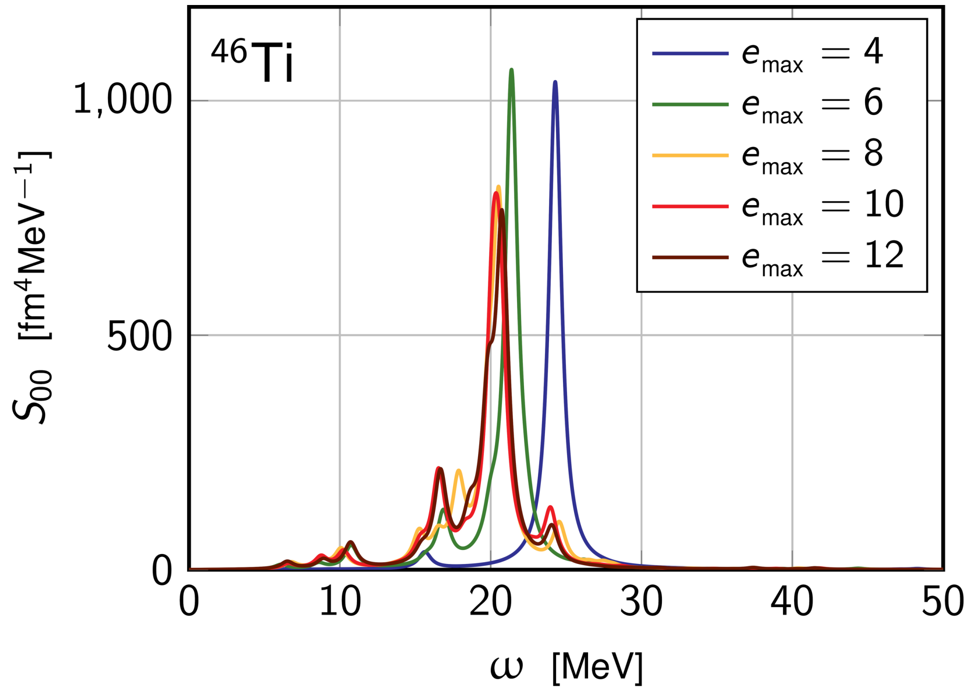

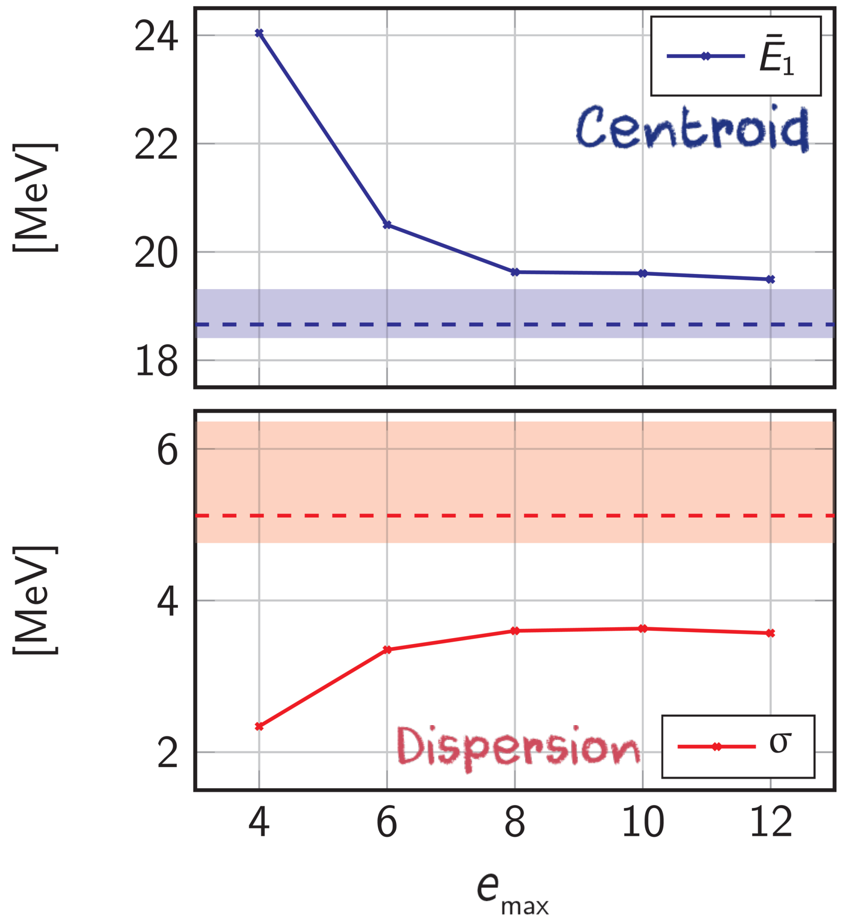

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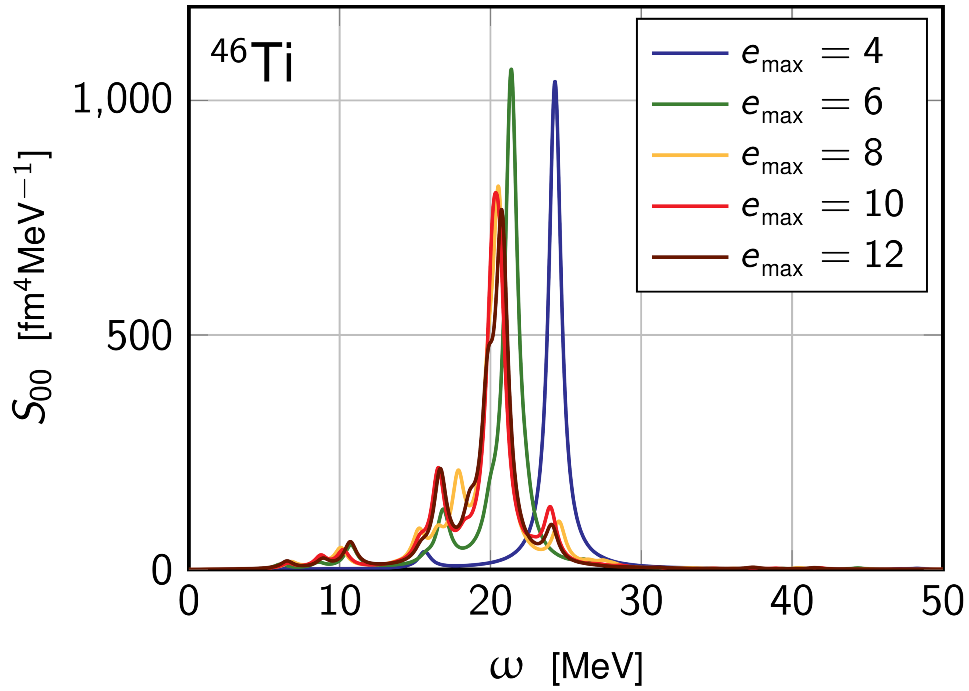

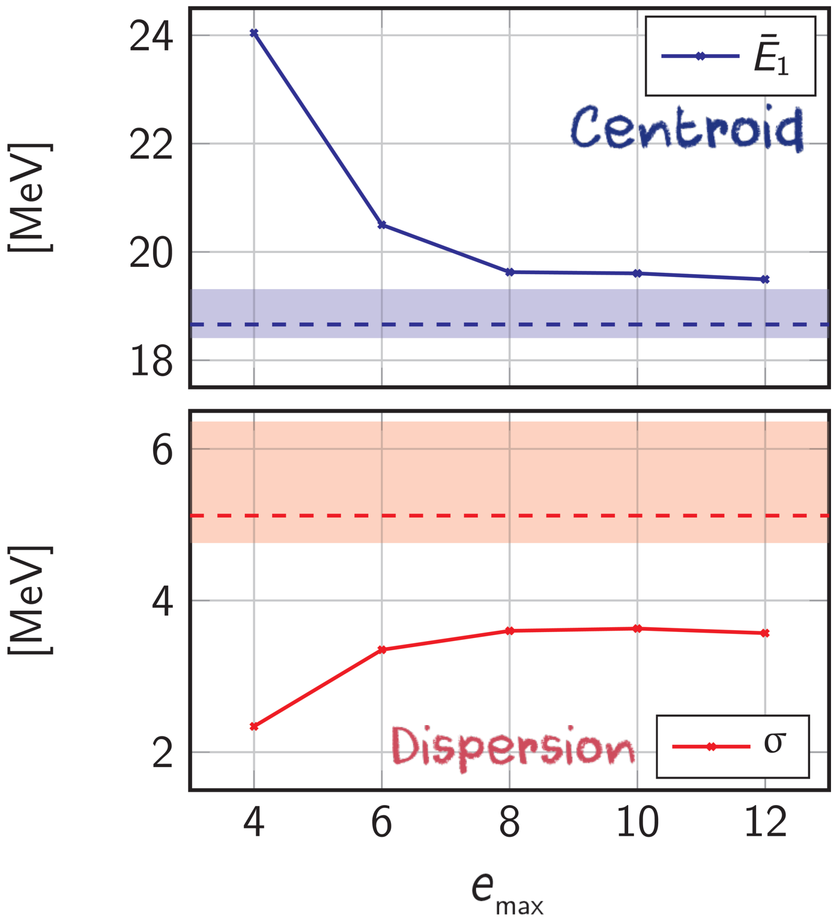

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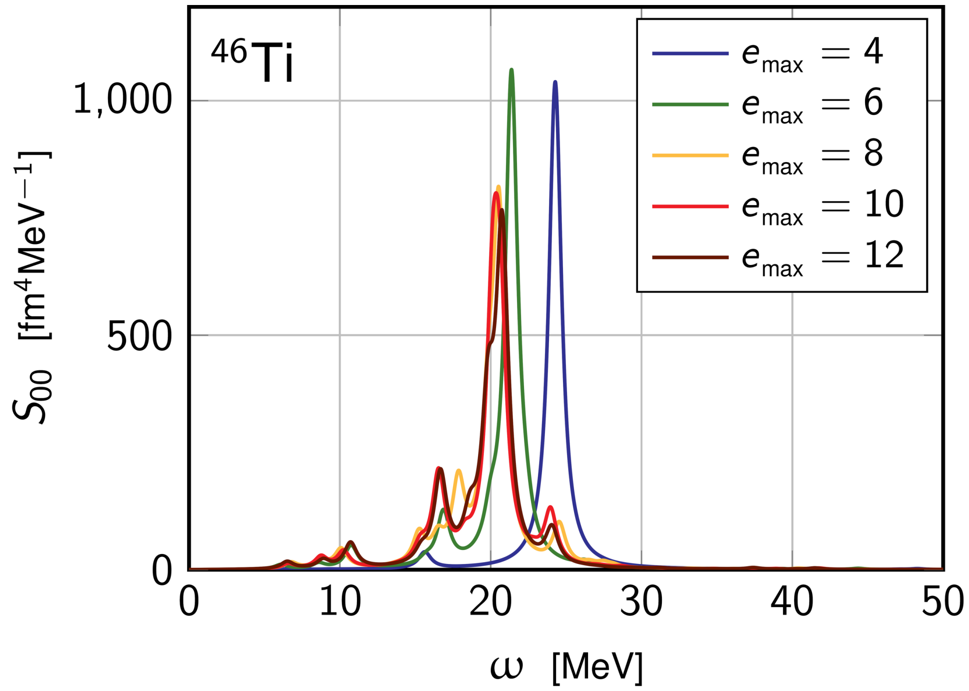

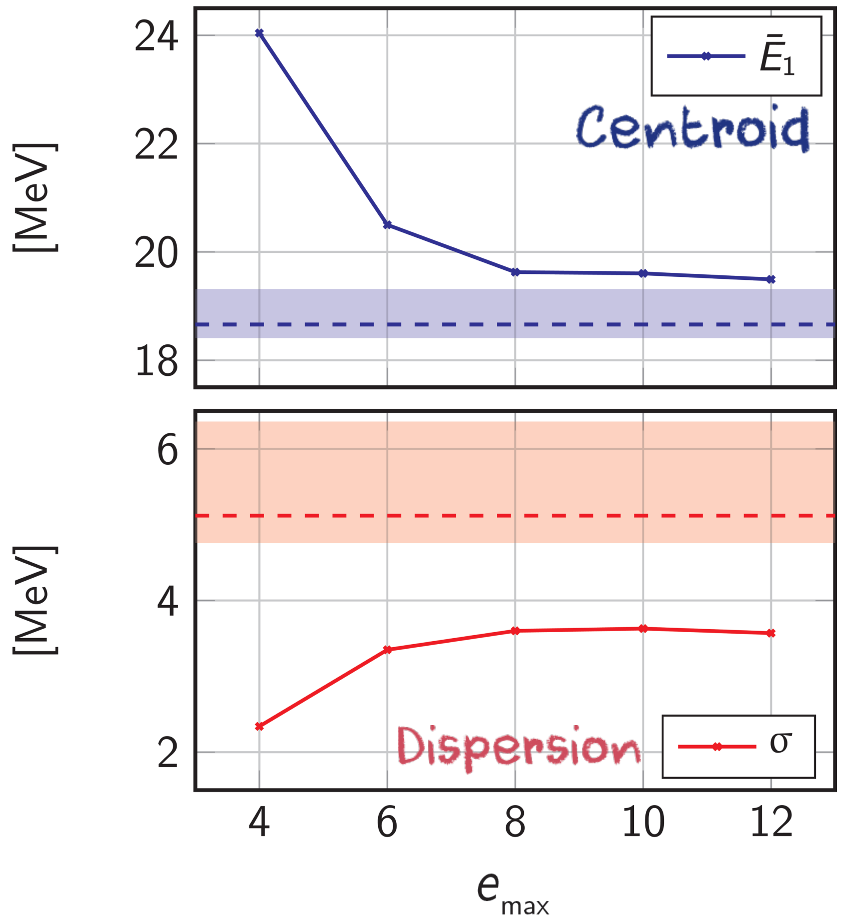

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[Myiagi et al., PRC, 2022]

Outline

1 Giant Resonances

- Physical introduction
- Existing ab initio theoretical tools

2 Ab initio PGCM

- Formalisms
- Uncertainty quantification

3 Chosen results

Conclusions and perspectives

Selected applications

- Shape coexistence
- Deformation

Projection effects

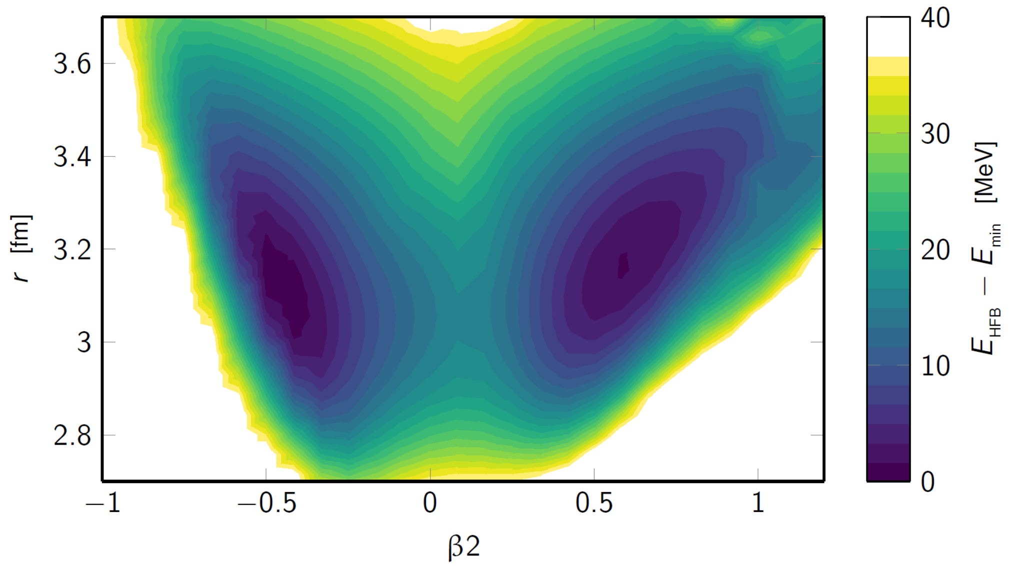
- PAV and VAP strategies
- Rotation-vibration coupling

From finite nuclei to Astrophysics

- Preliminary incompressibility results

Shape coexistence effects in ^{28}Si

Total Energy Surface $E_{HFB}(\beta_2,r)$



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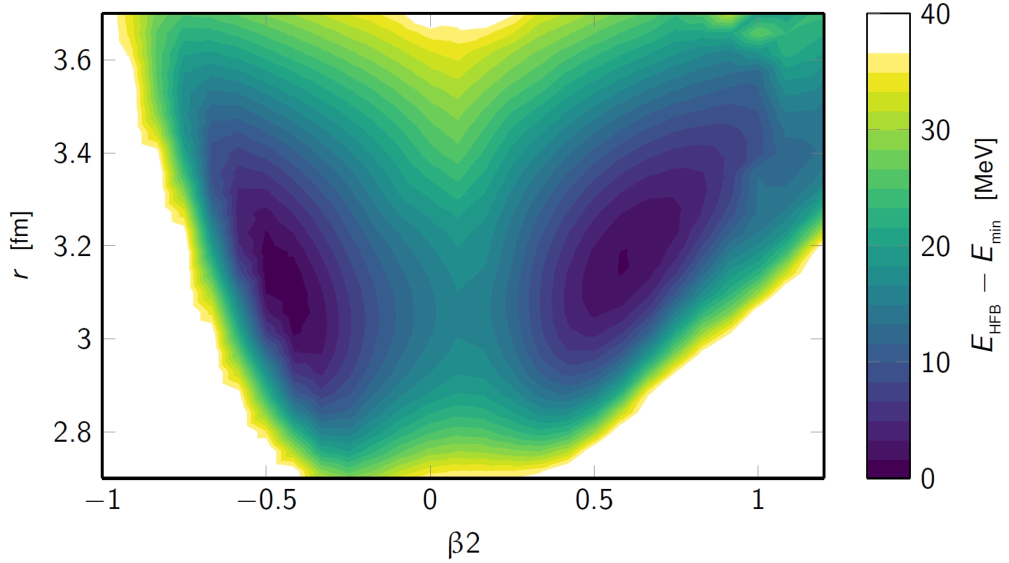
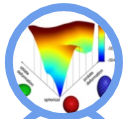
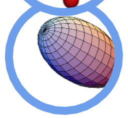



Shape coexistence [Jenkins et al., 2012]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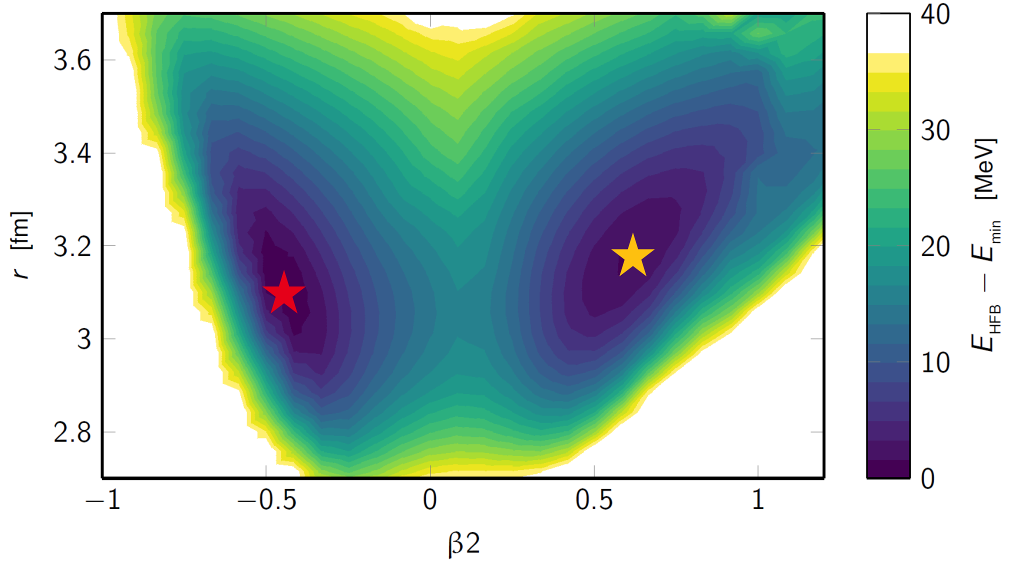

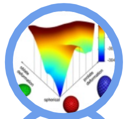

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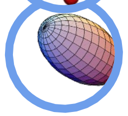

Deformation

- Oblate GS and prolate-shape isomer

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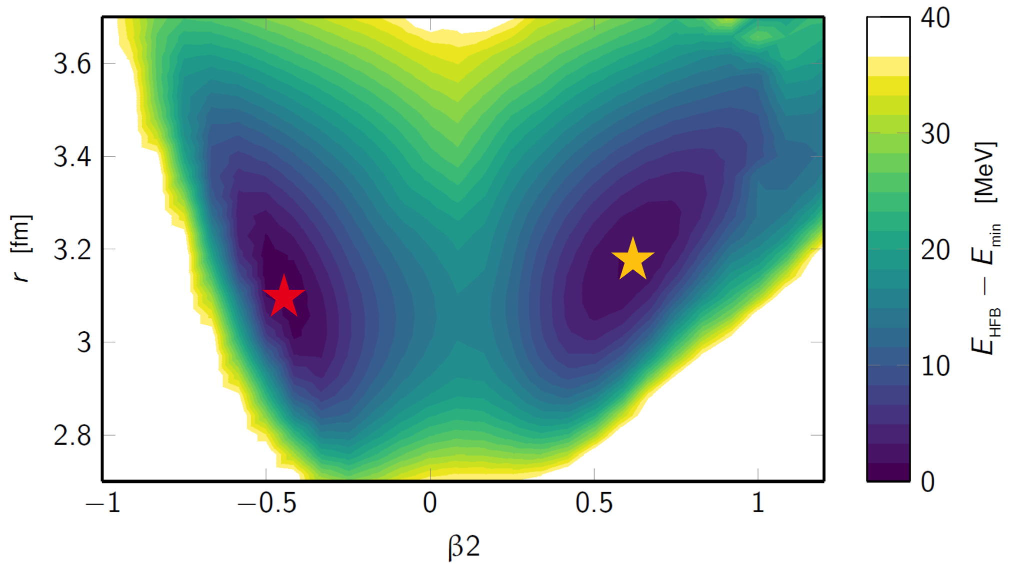

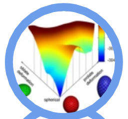

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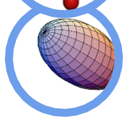

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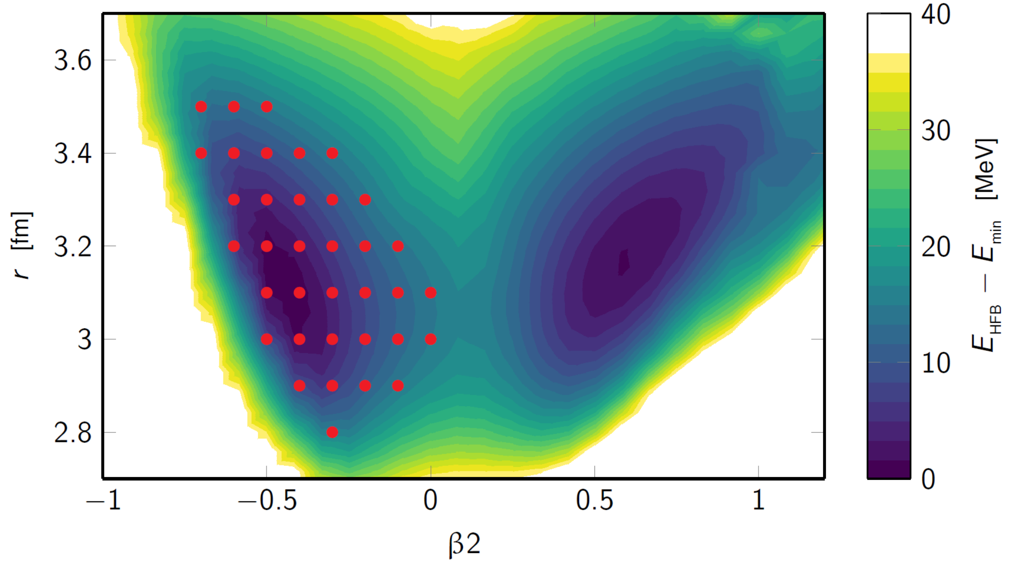

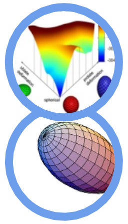

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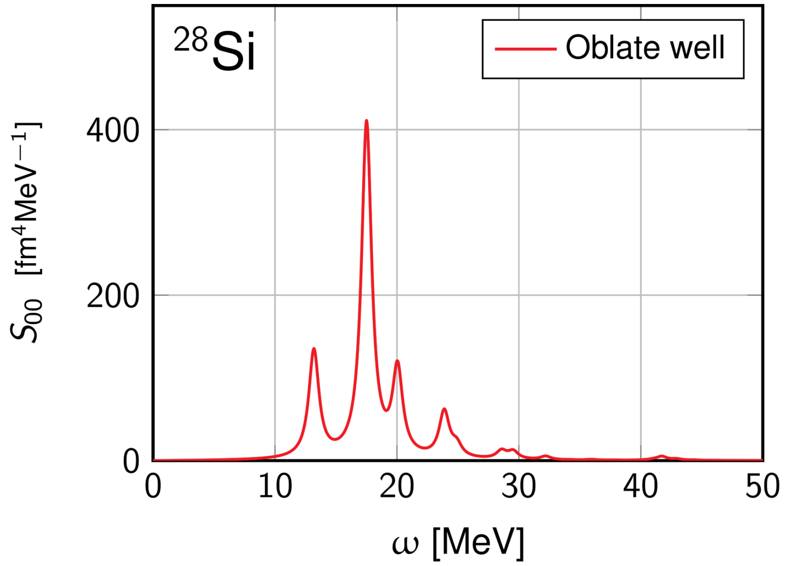

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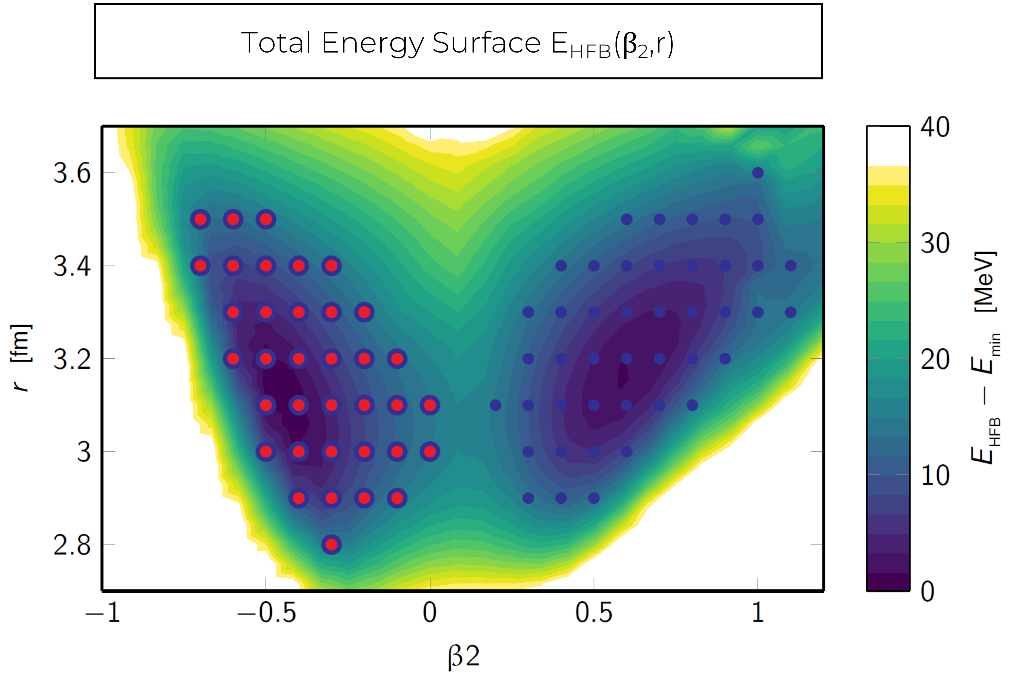

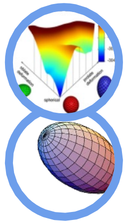

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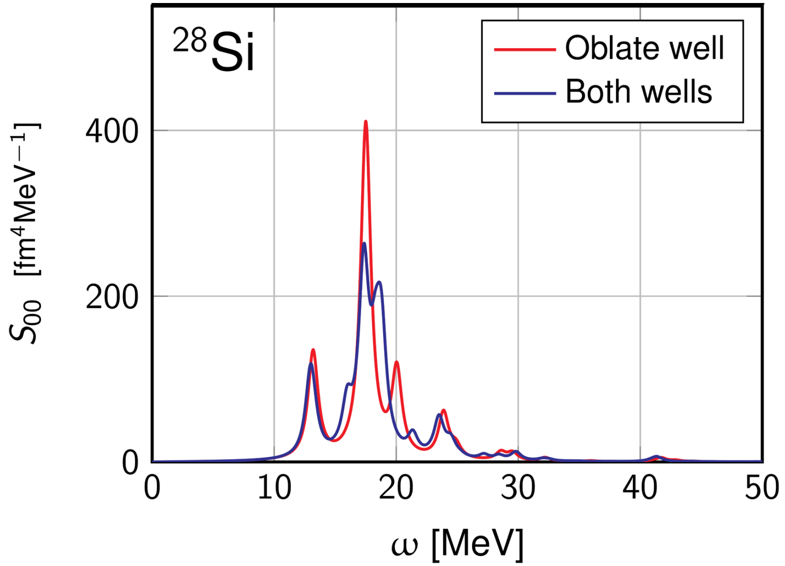

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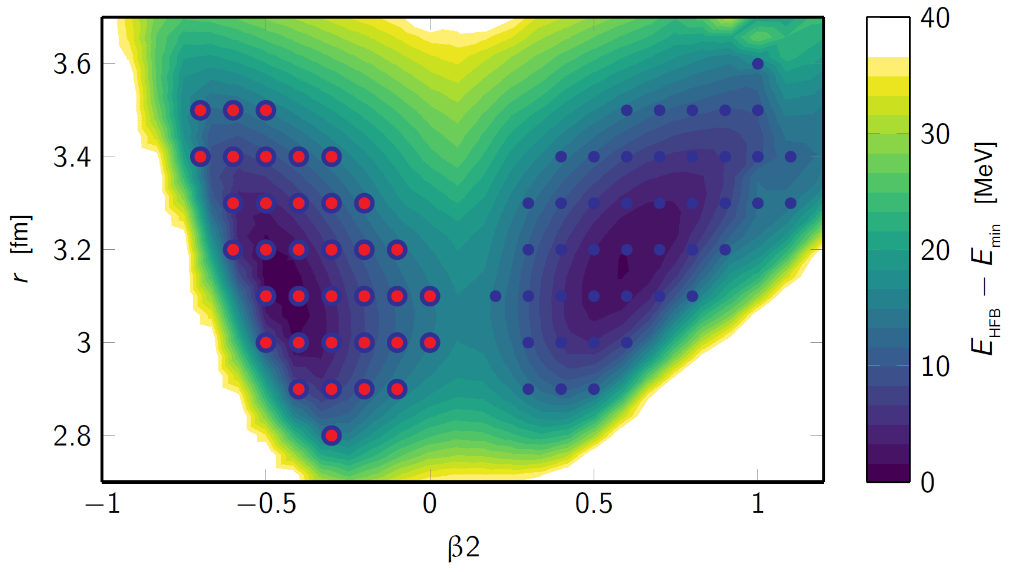

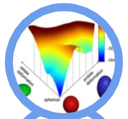

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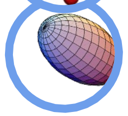

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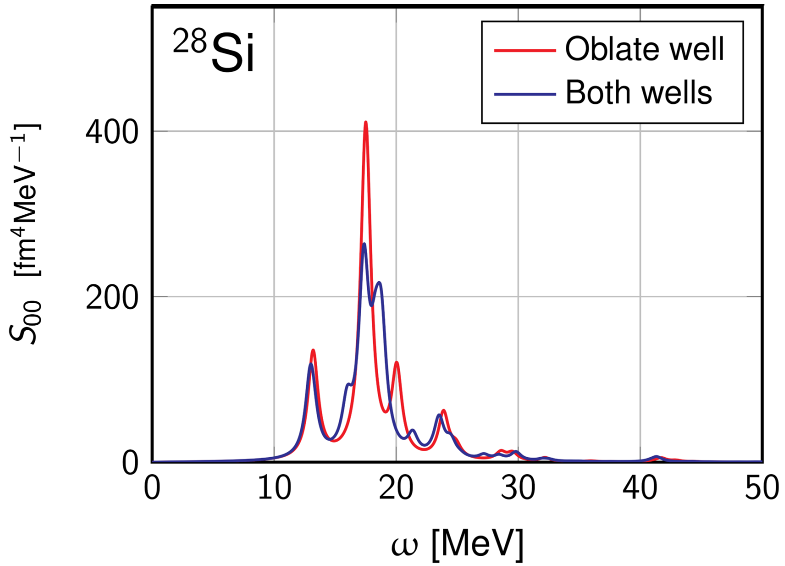

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Nuclei with stronger signature ?

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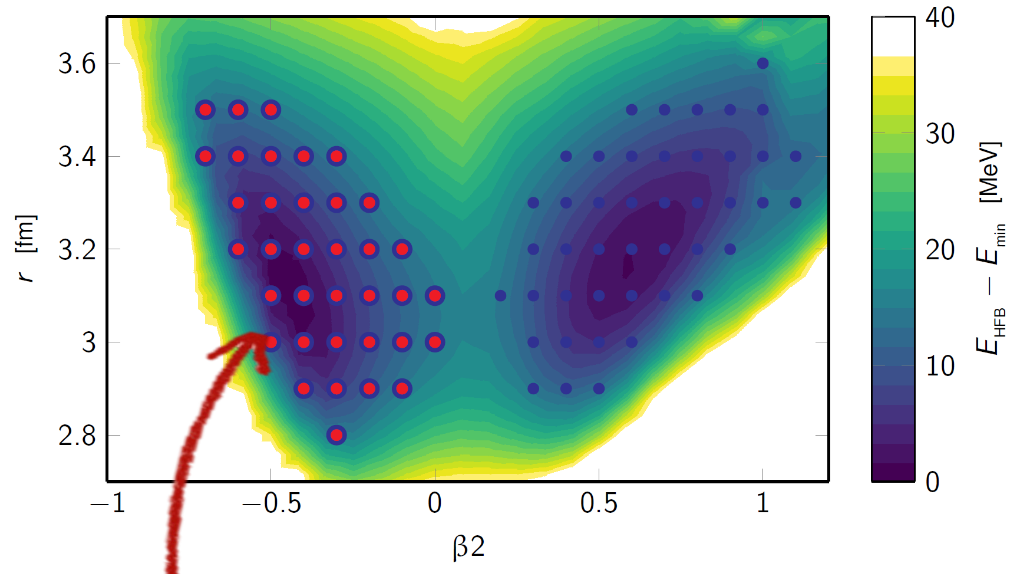

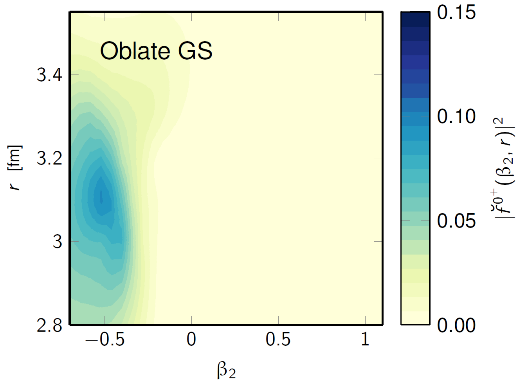

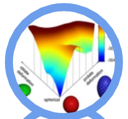

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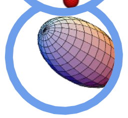

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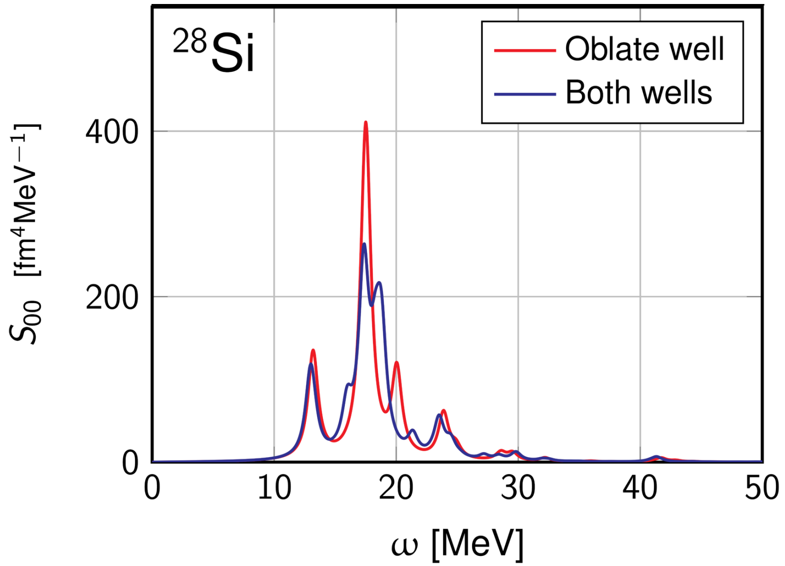

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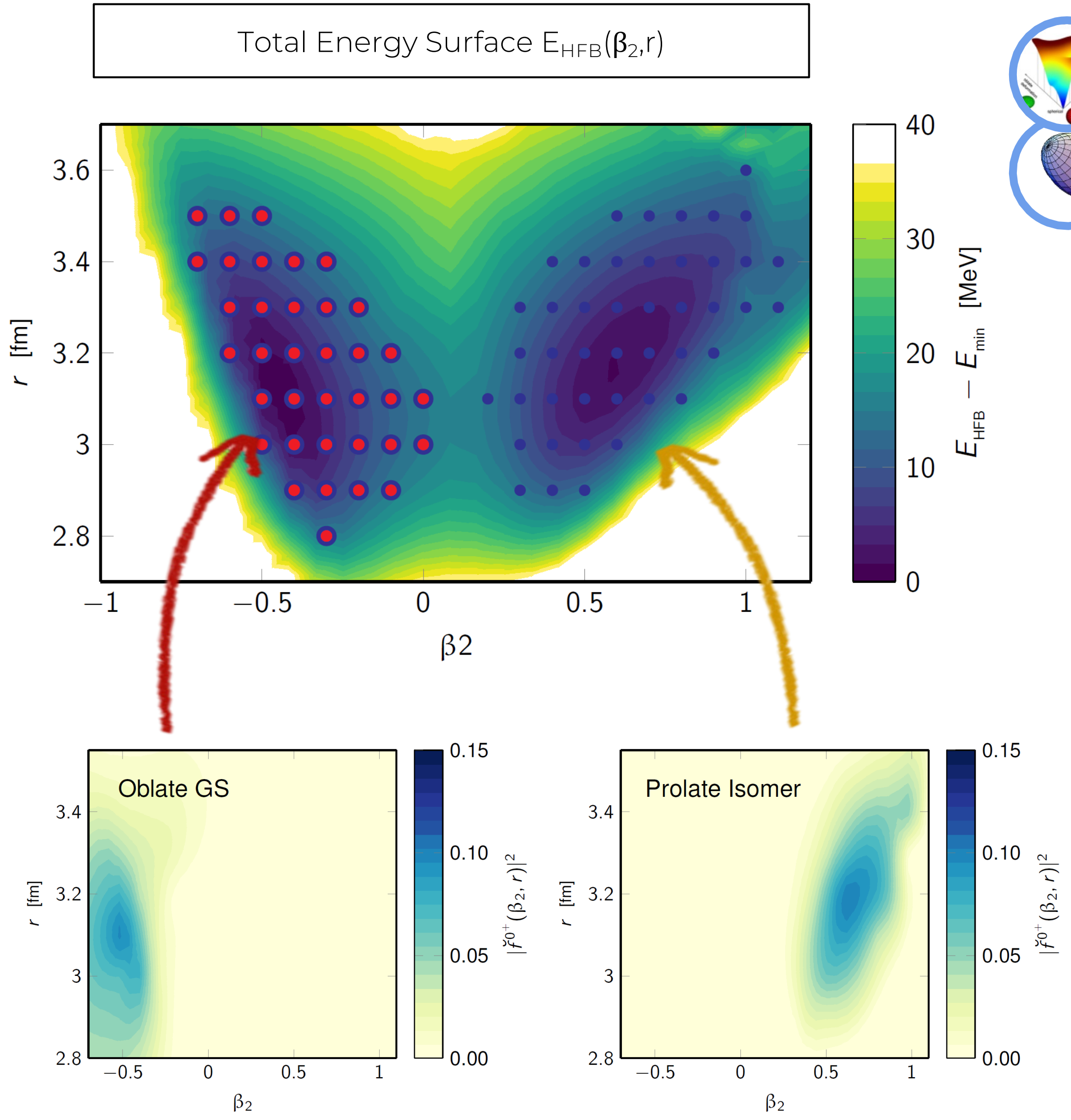

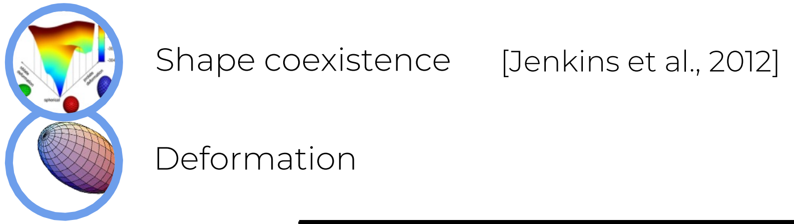

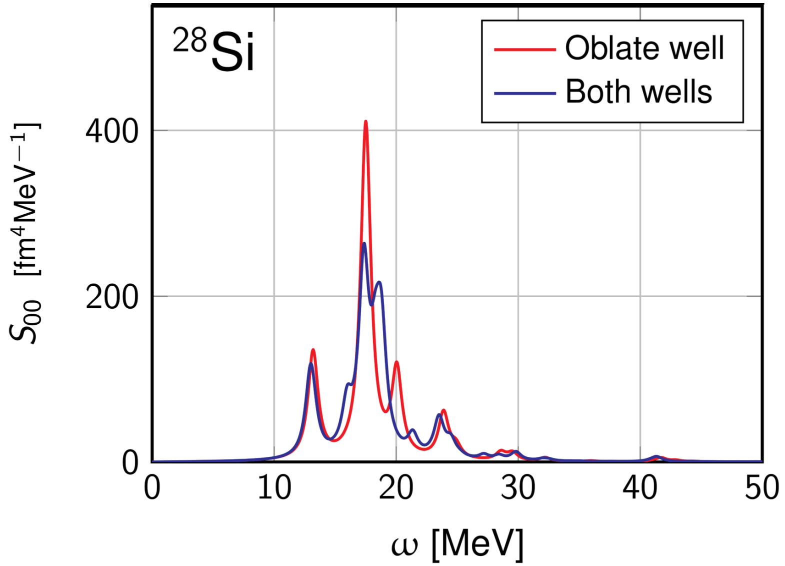

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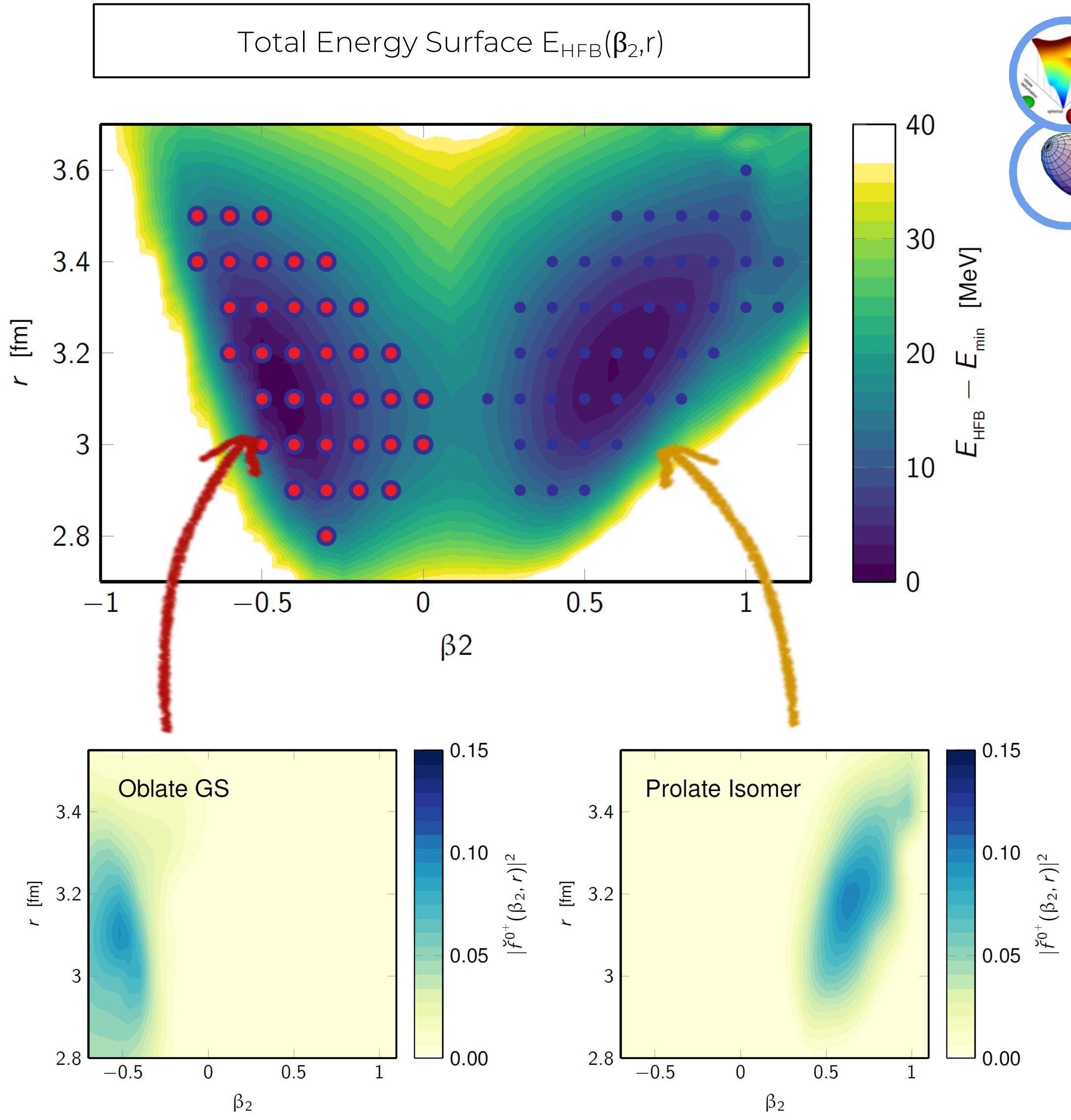

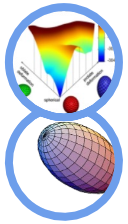

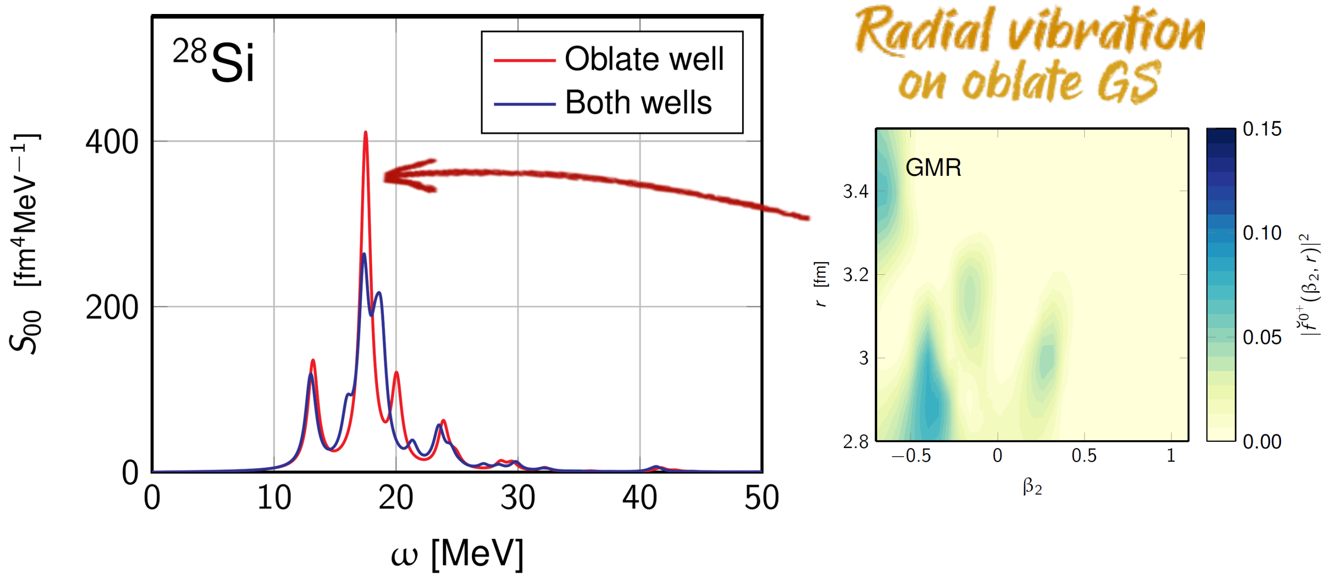

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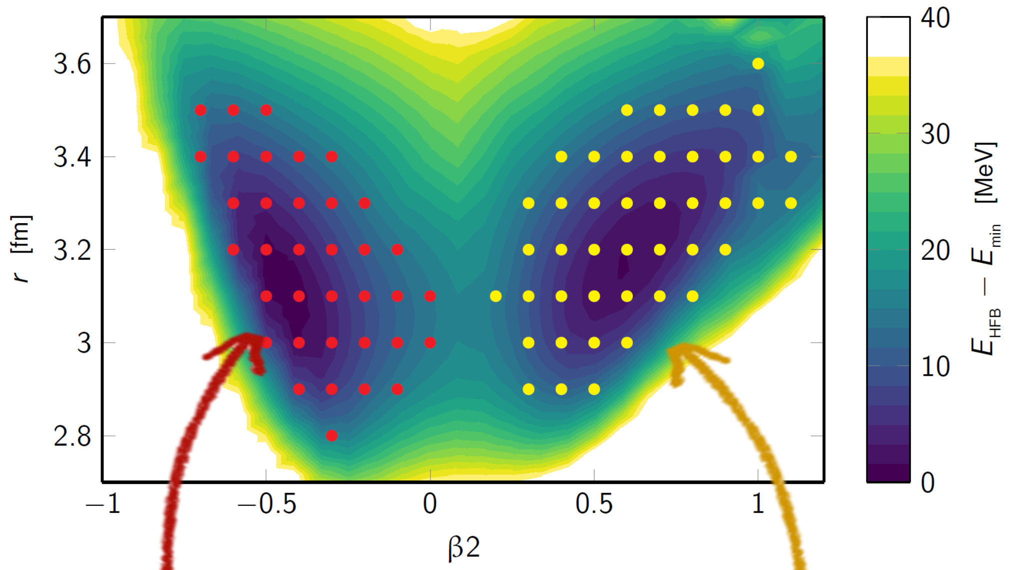

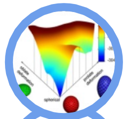

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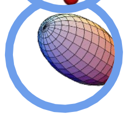

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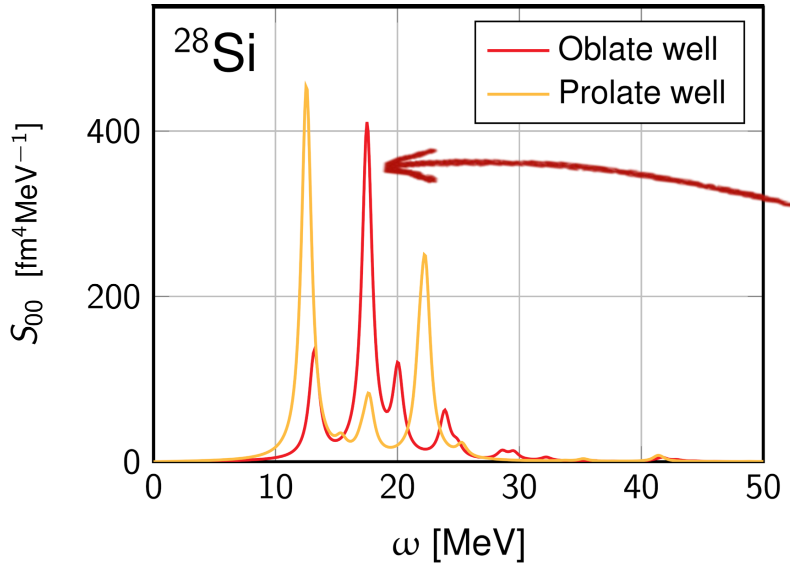
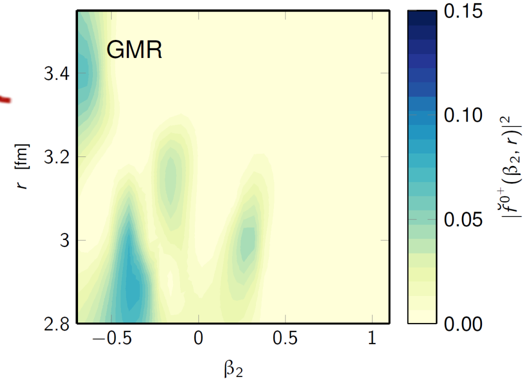
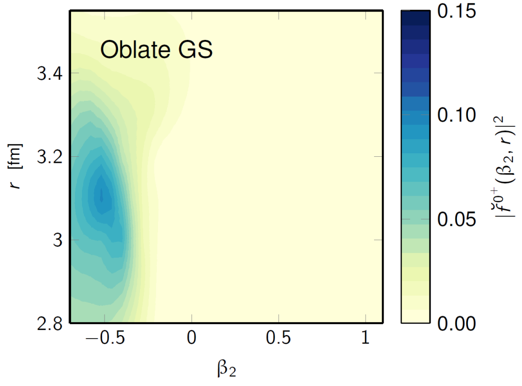
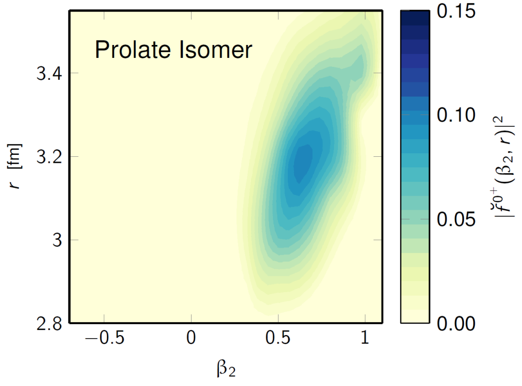


Radial vibration on oblate GS







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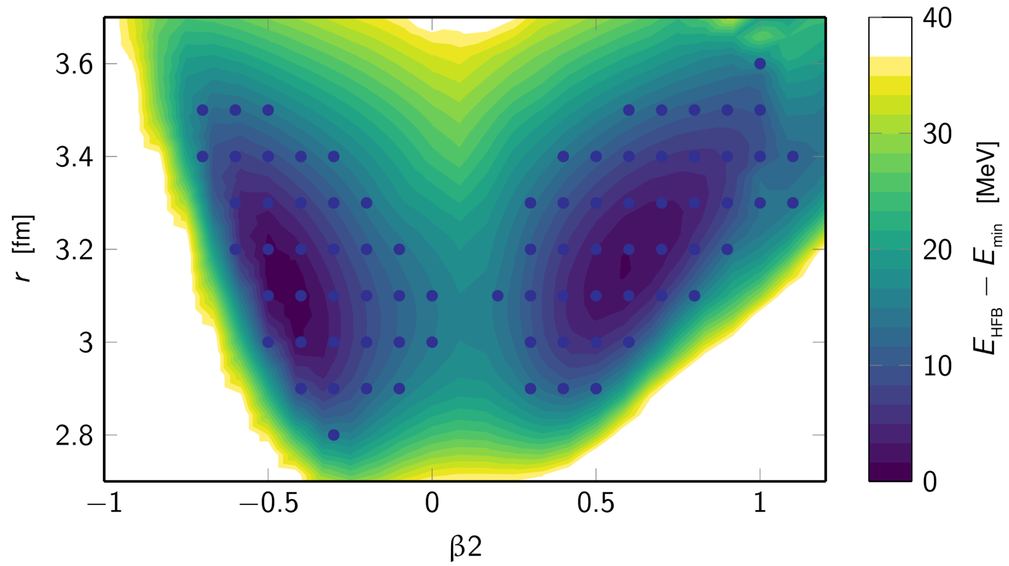

Deformation effects in prolate ^{28}Si

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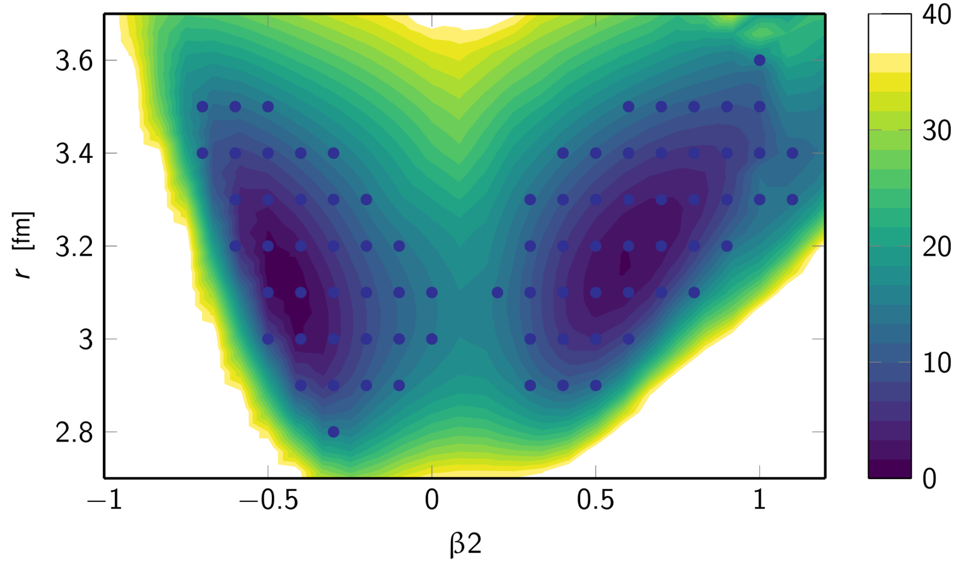
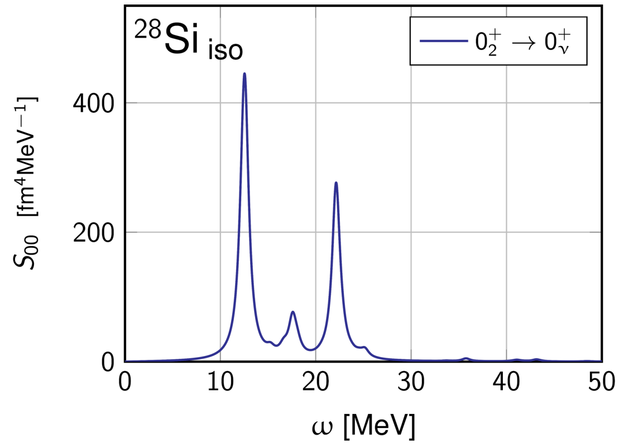
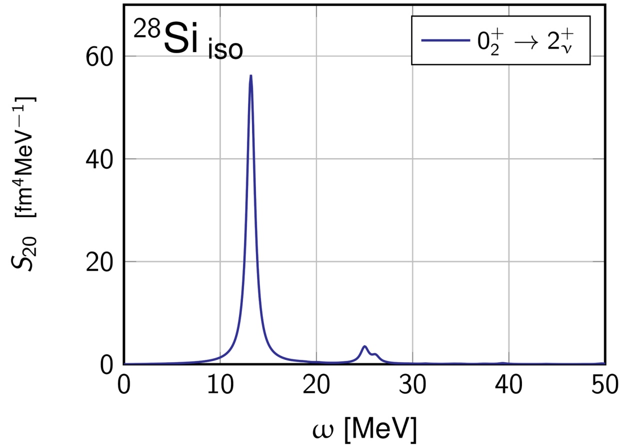


Monopole Strength



K=0 Quadrupole Strength



- Focus on the prolate-shape isomer
- Coupling to GQR generates splitting
  - x High peak = shifted "spherical" breathing mode
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- Two-peak GMR on the prolate shape isomer

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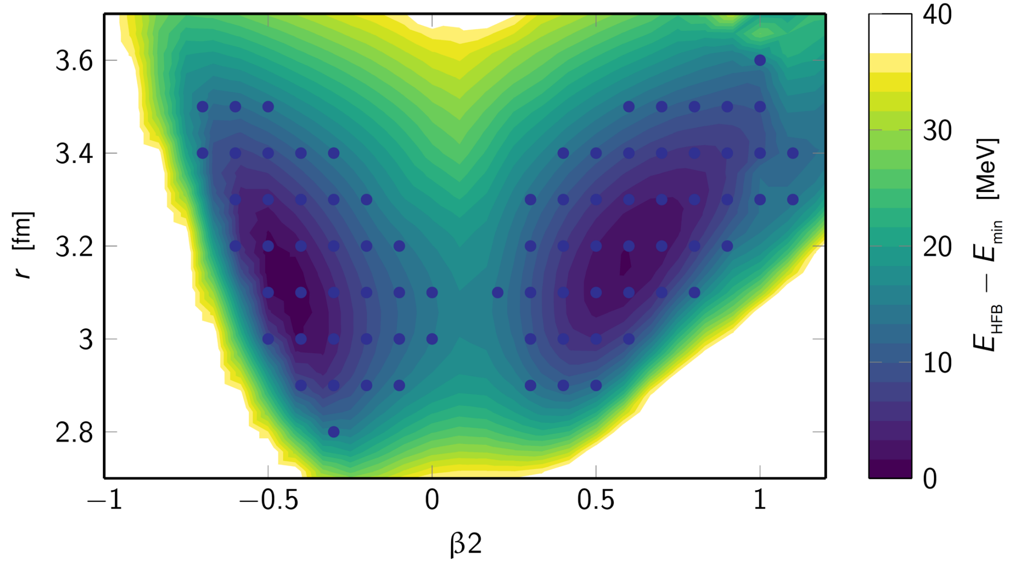

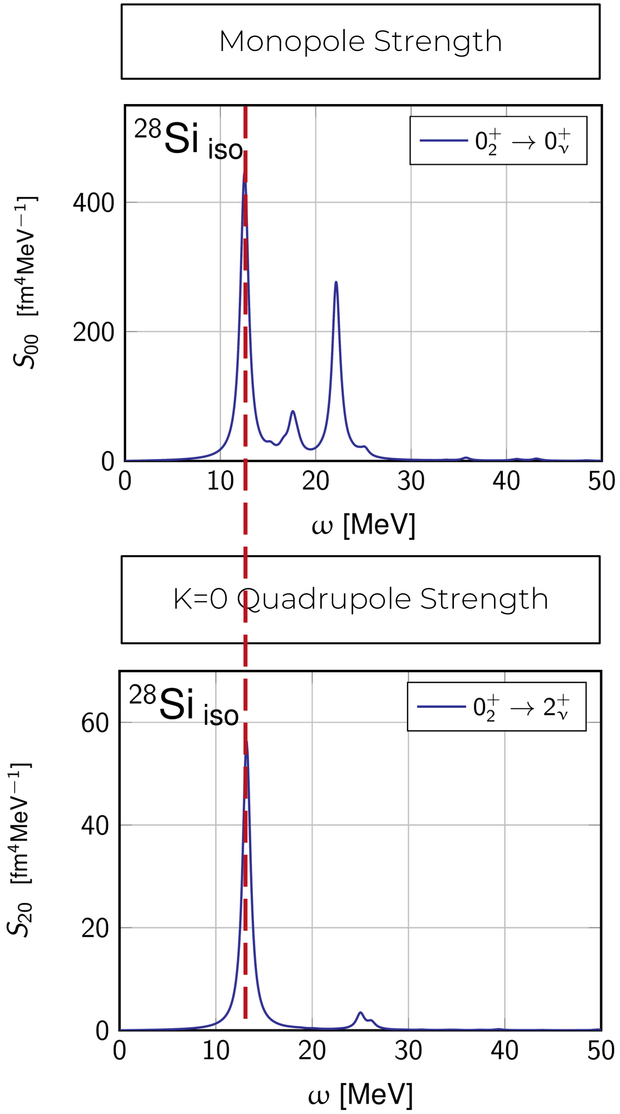

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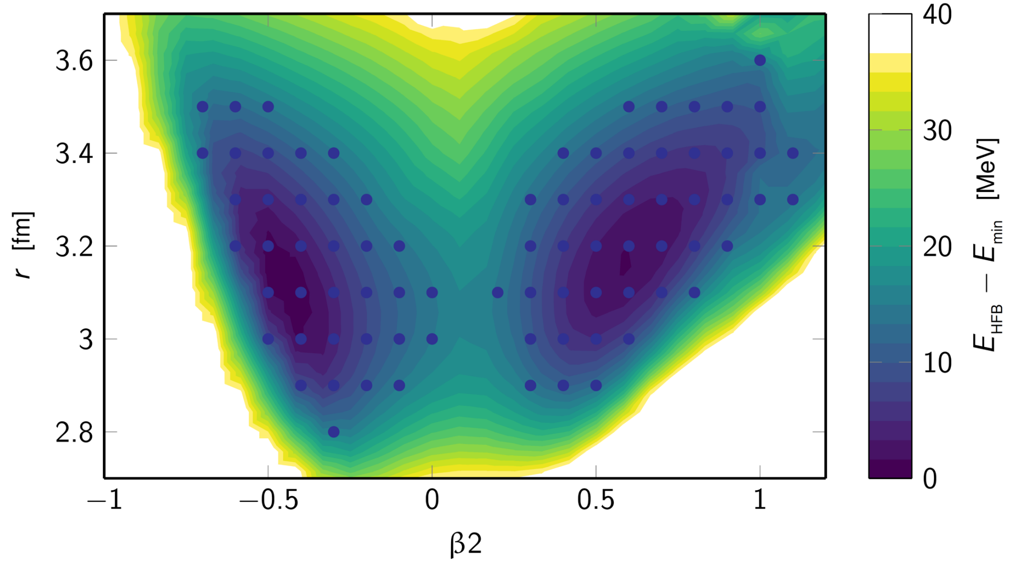

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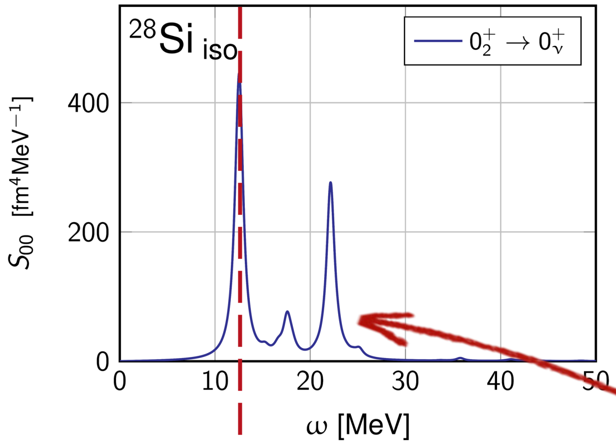

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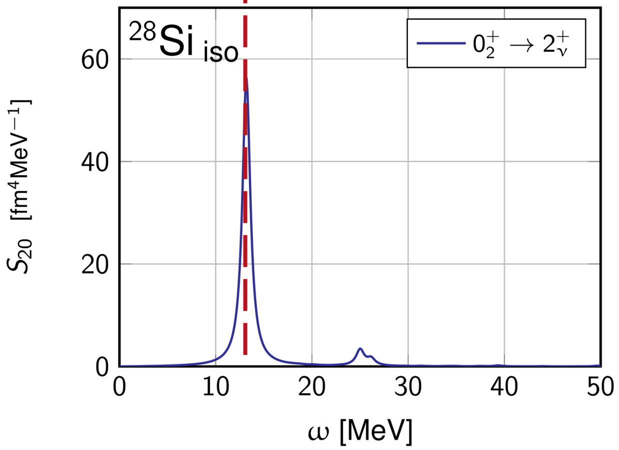

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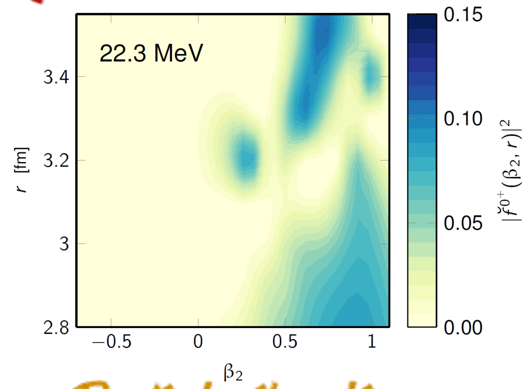

Radial vibration

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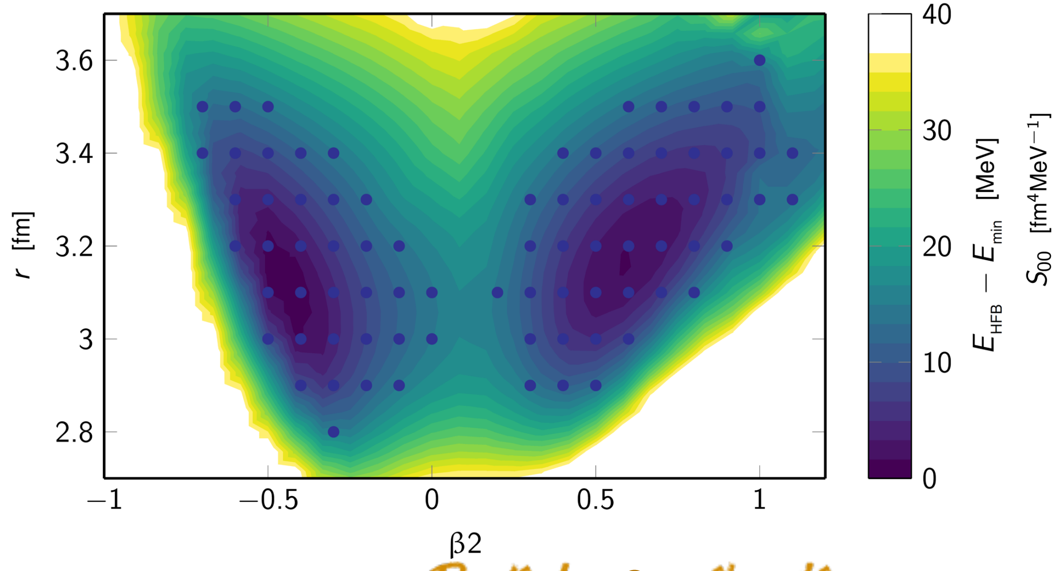
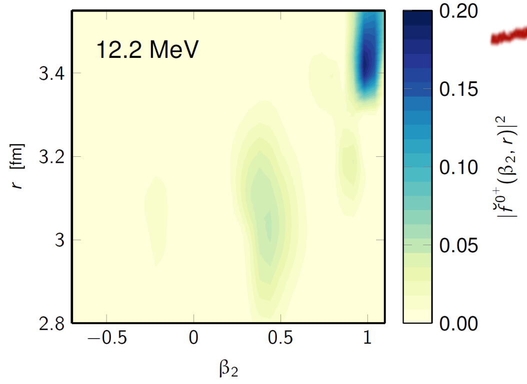


Radial + β_2 vibration



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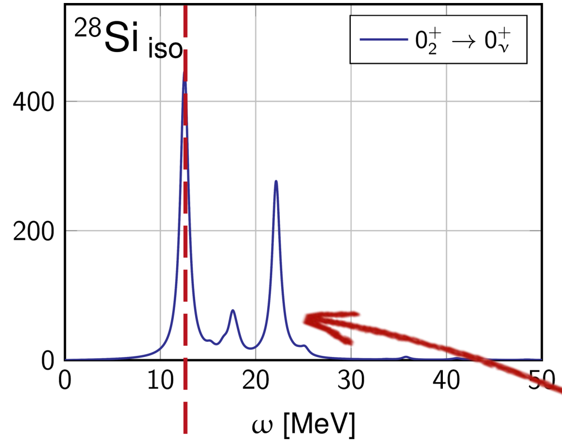

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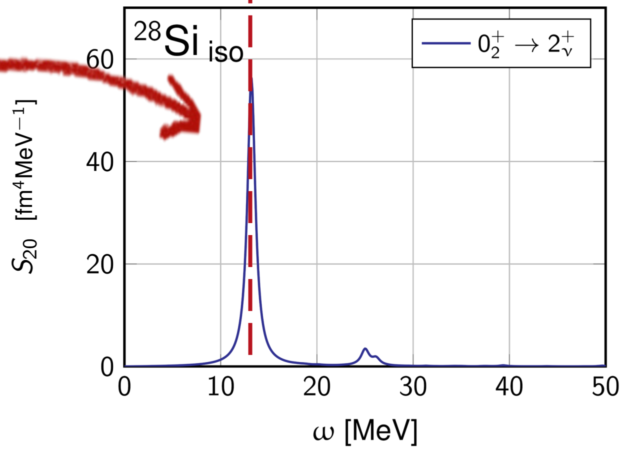

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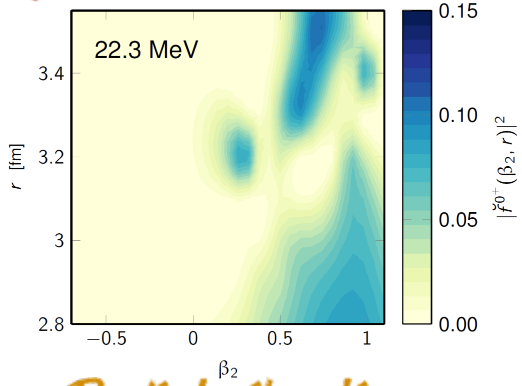
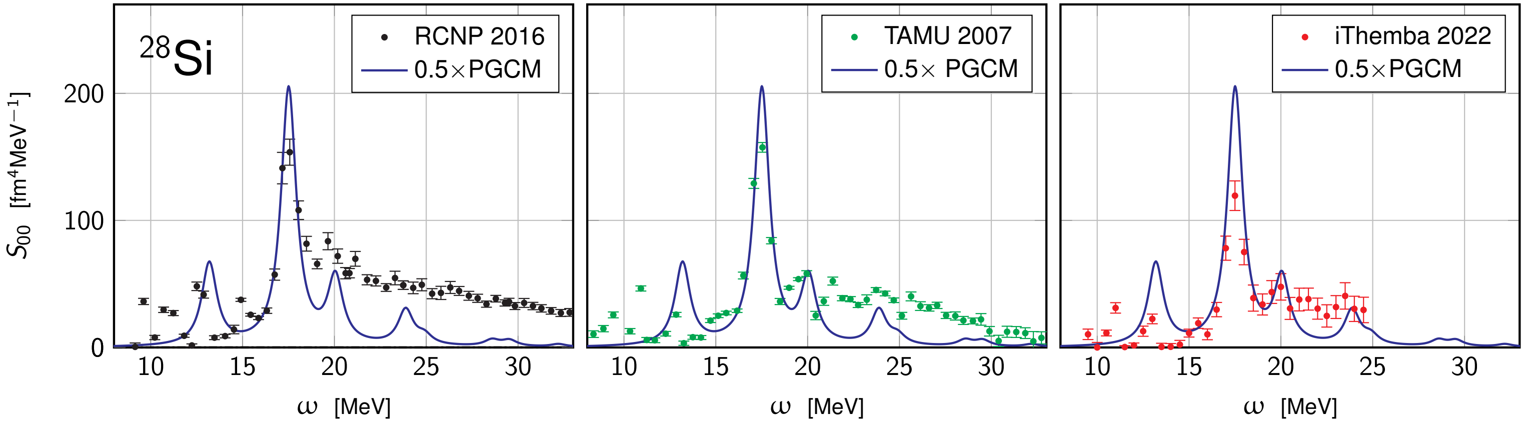


Radial vibration

Comparison to experimental data



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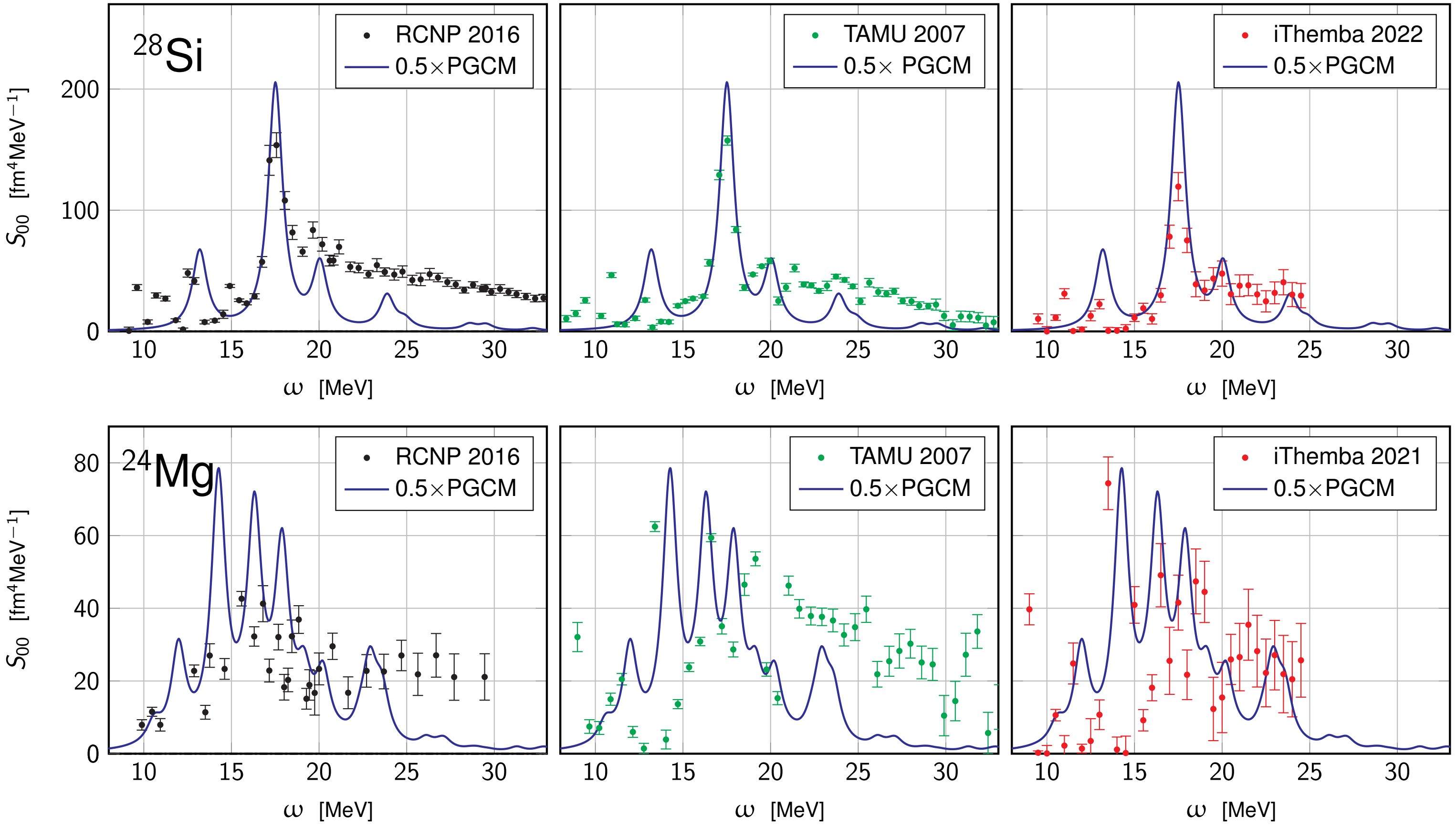

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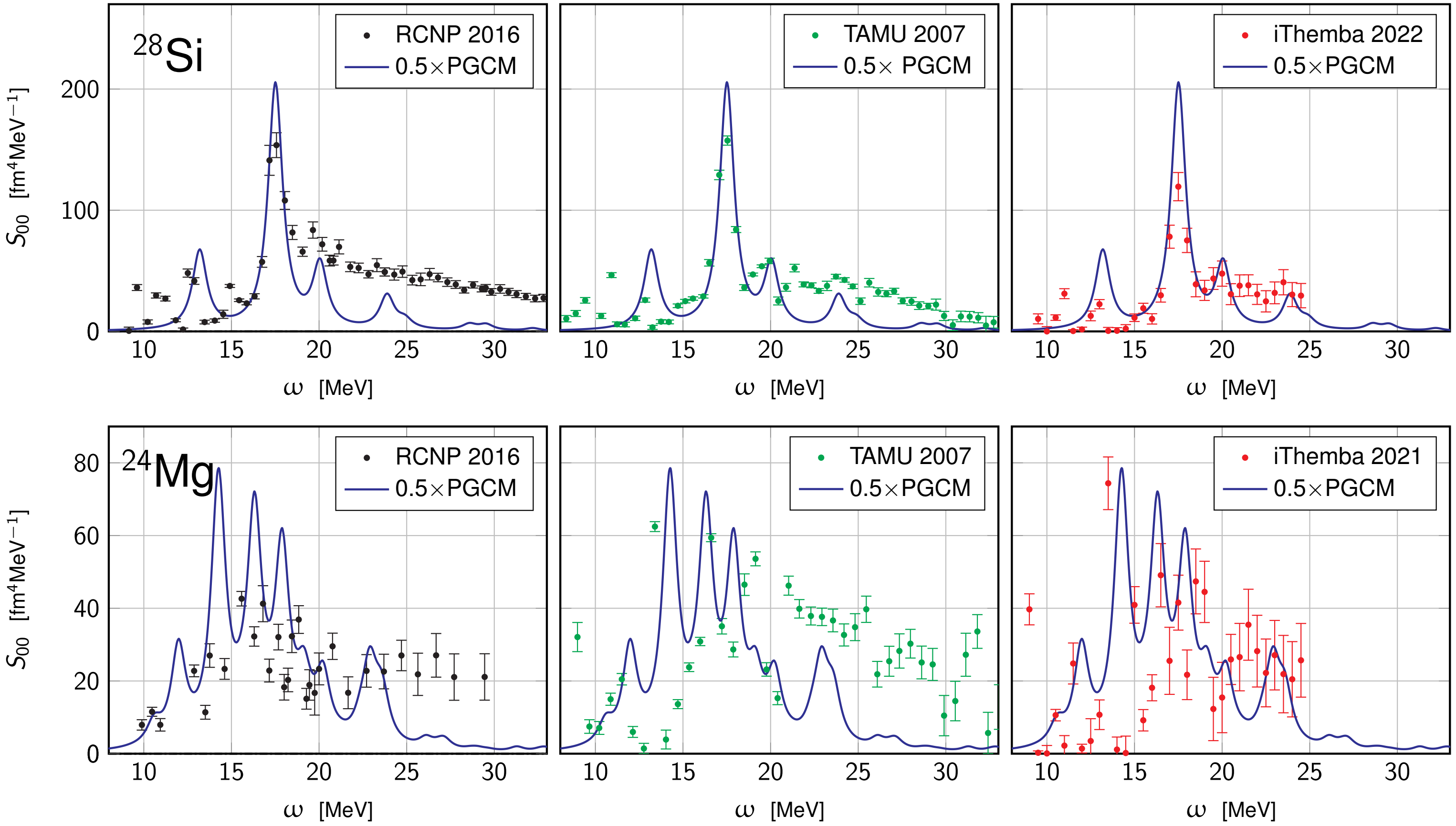

Ab initio PGCM nicely reproduces the experimental data

- Better description of the **main resonance** and **fragmentation**

Experimental data are useful and promising to test different many-body methods

Data are not unambiguous, i.e. higher resolution would be beneficial

Outline

1 Giant Resonances

- Physical introduction
- Existing ab initio theoretical tools

2 Ab initio PGCM

- Formalisms
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- Deformation

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- PAV and VAP strategies
- Rotation-vibration coupling

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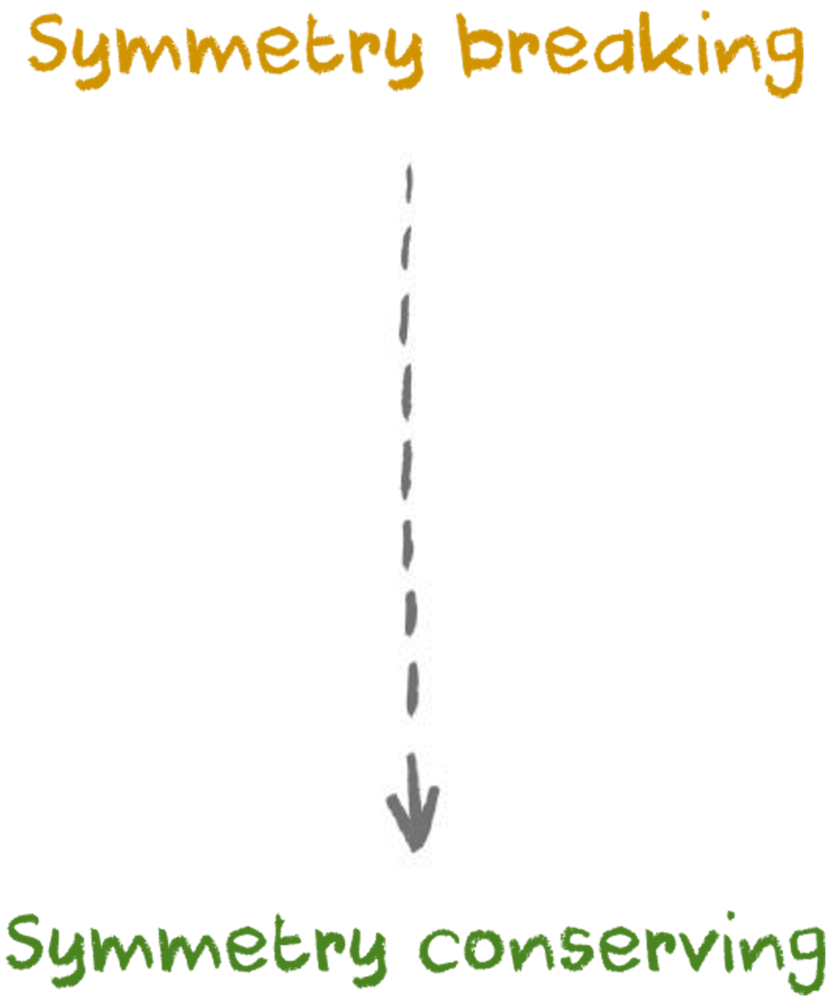
Conclusions and perspectives

Projection in GCM and QRPA

DIFFERENT FLAVOURS OF SYMMETRY BREAKING AND RESTORATION

(Q)RPA

GCM



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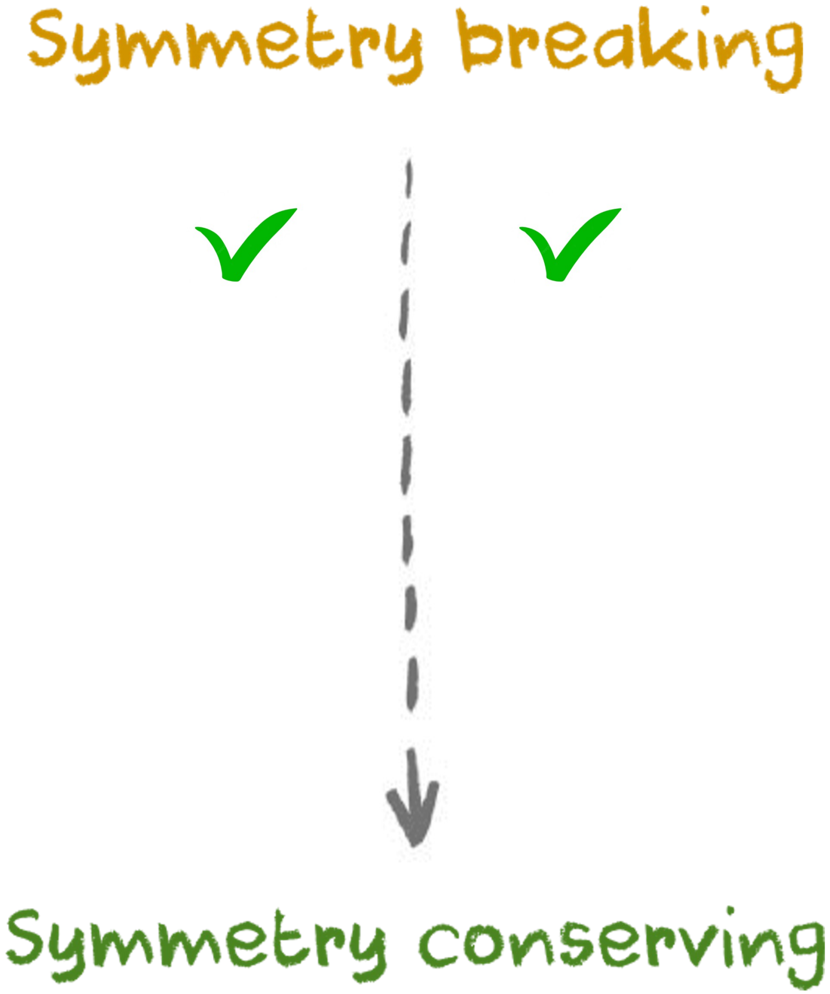
Harmonic fluctuations around deformed HF(B)



GCM

Large amplitudes superposition of def. HF(B) states

Projection in GCM and QRPA

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 PAV RPA [1]	✗	✗	**PROJECTION AFTER DIAGONALIZATION** PAV GCM

Symmetry conserving

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

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PROJECTION BEFORE DIAGONALIZATION P(Q)RPA (2)	✗	✓	**PROJECTION BEFORE DIAGONALIZATION** PGCM

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GMR results — Application (Harmonic fluctuations around deformed HF(B))

GMR results — Application (PGCM)

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Projection in GCM and QRPA

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Symmetry breaking

(Q)RPA

GMR results

Harmonic fluctuations around deformed HF(B) ✓

Application

GMR results

PROJECTION AFTER DIAGONALIZATION

PAV RPA (1) ✓

New implementation

PROJECTION BEFORE DIAGONALIZATION

P(Q)RPA (2) ✗

GCM

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

GMR results

PROJECTION AFTER DIAGONALIZATION

PAV GCM ✓

New implementation

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PROJECTION BEFORE DIAGONALIZATION

PGCM ✓

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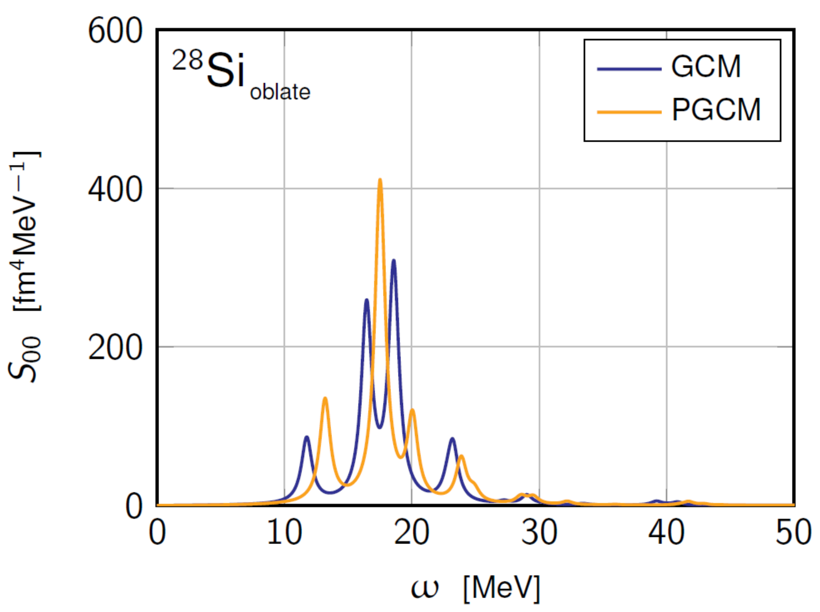
Projection effects in ^{28}Si



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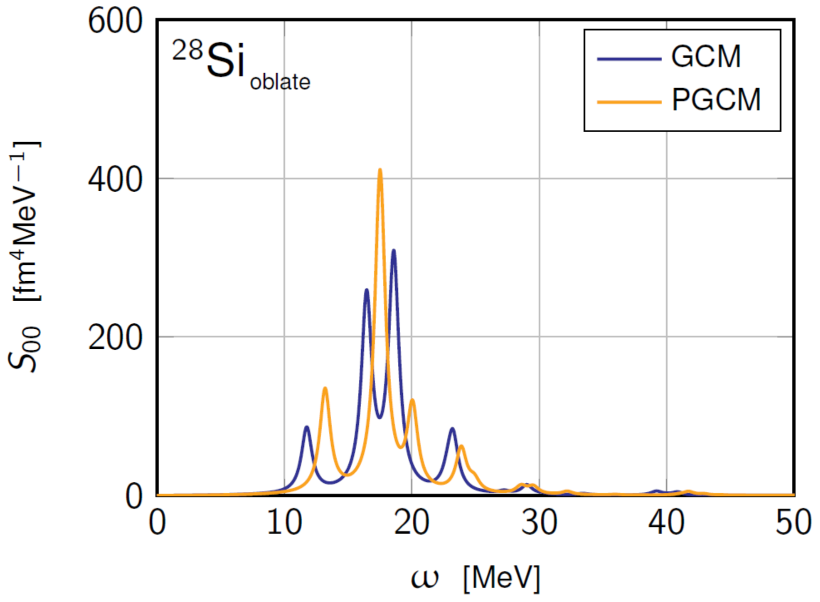

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- Not too dissimilar
- Increased **fragmentation** (e.g. ^{24}Mg)
- More quantitative agreement

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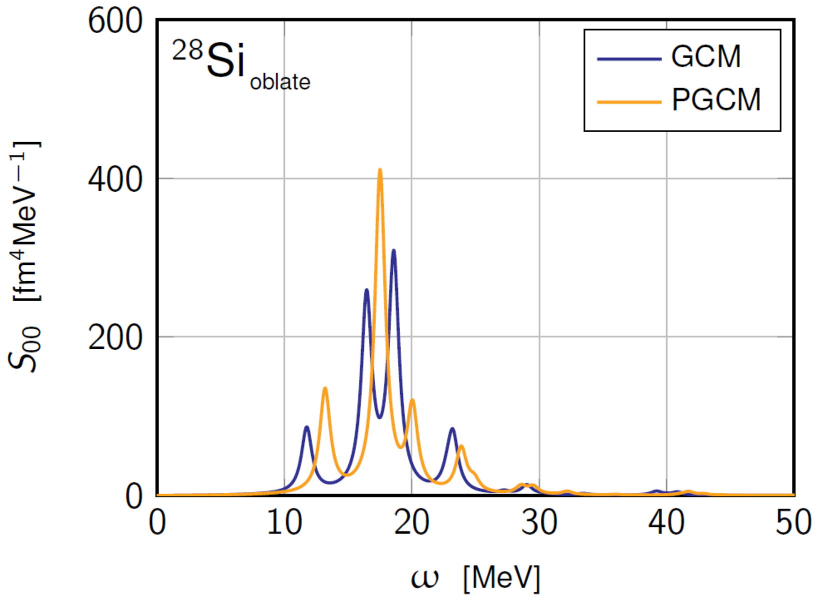

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Can we treat projection a posteriori ?

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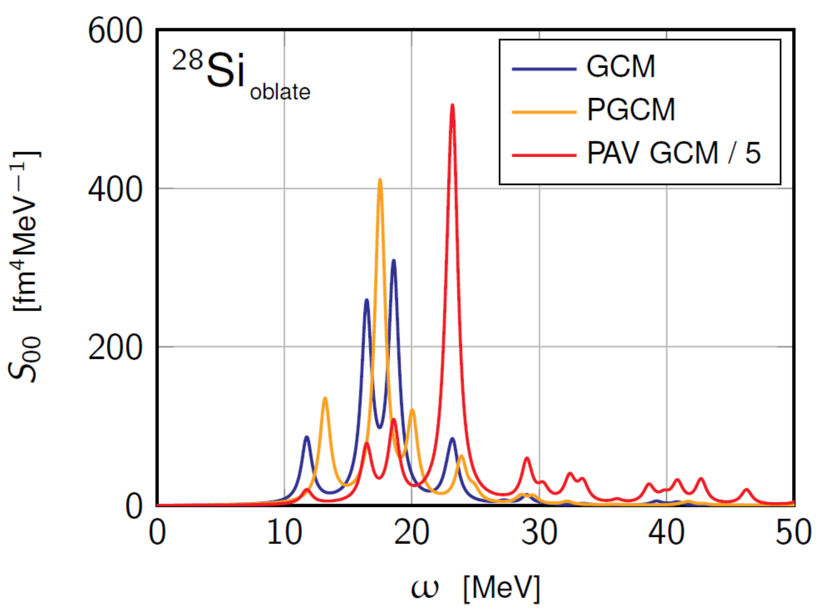

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- Anomalous spectrum
- Zero-frequency rotations (Goldstone modes)
- Born-Oppenheimer-like approximation

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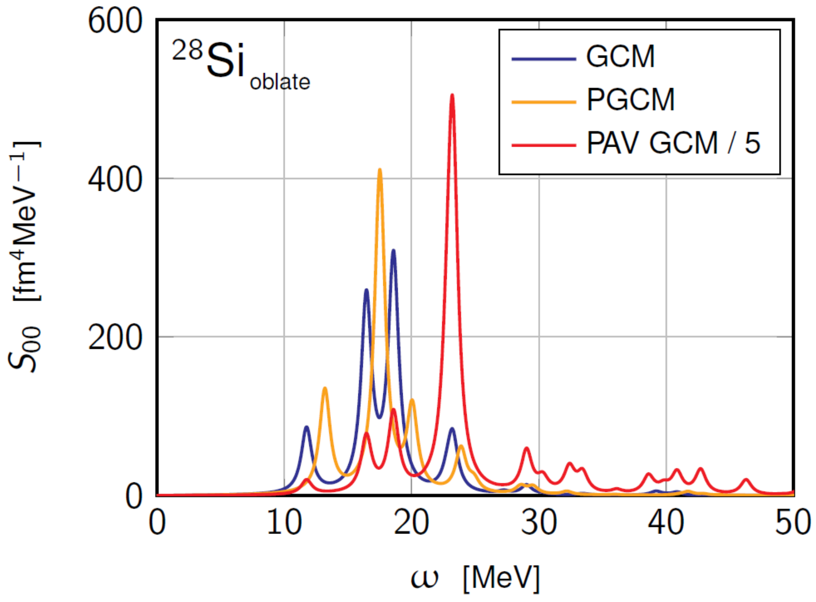

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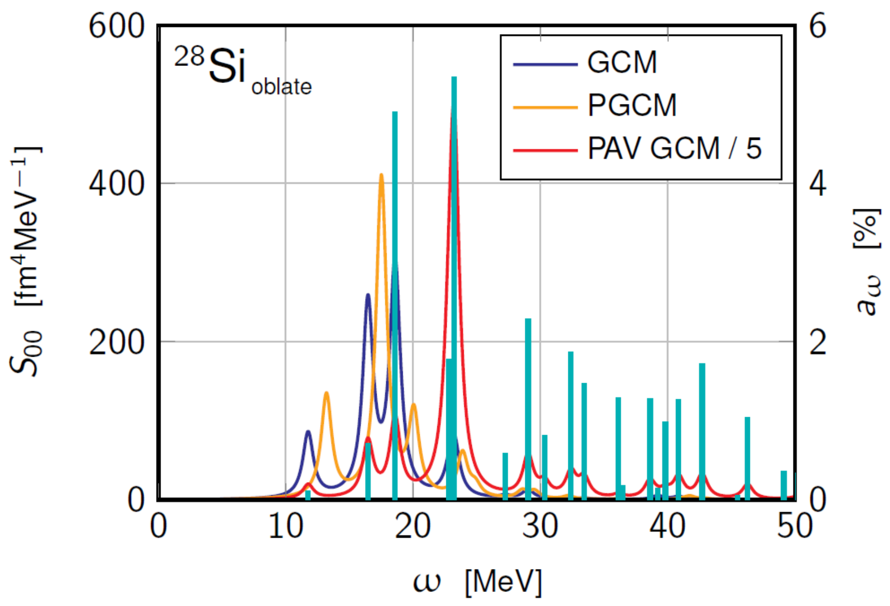

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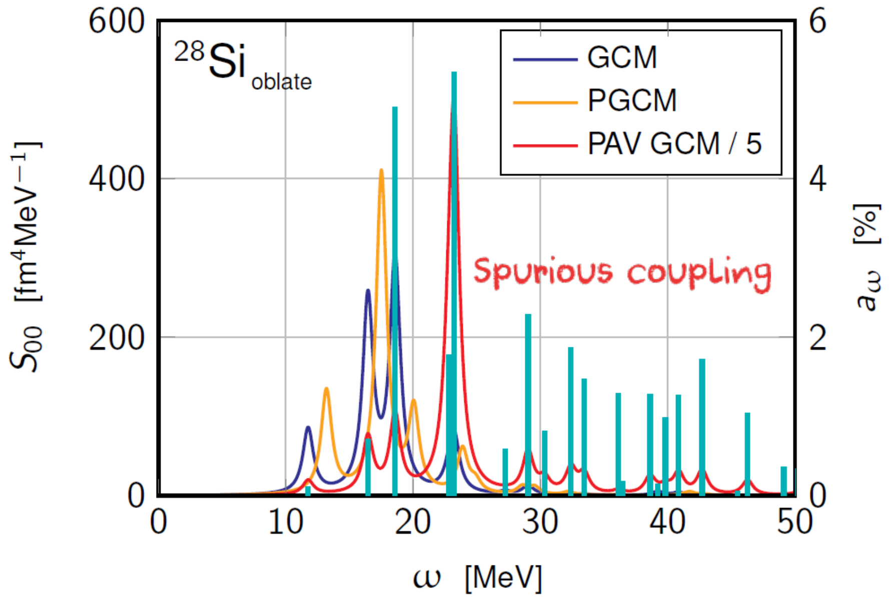

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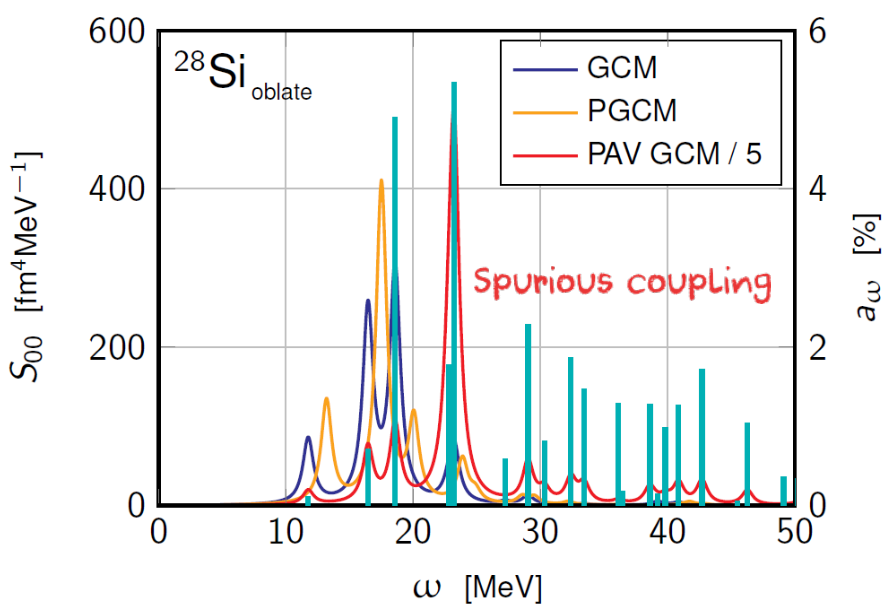

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Can be subtracted !

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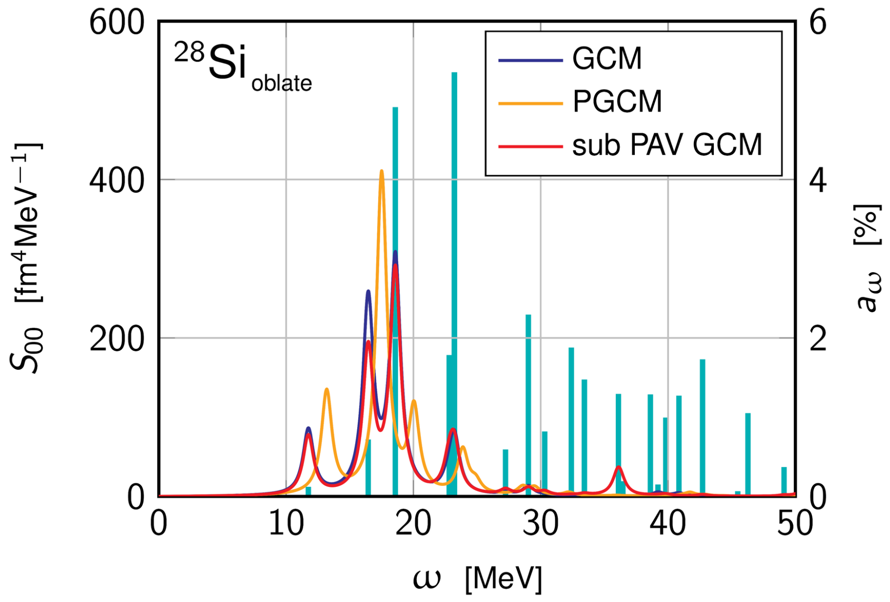

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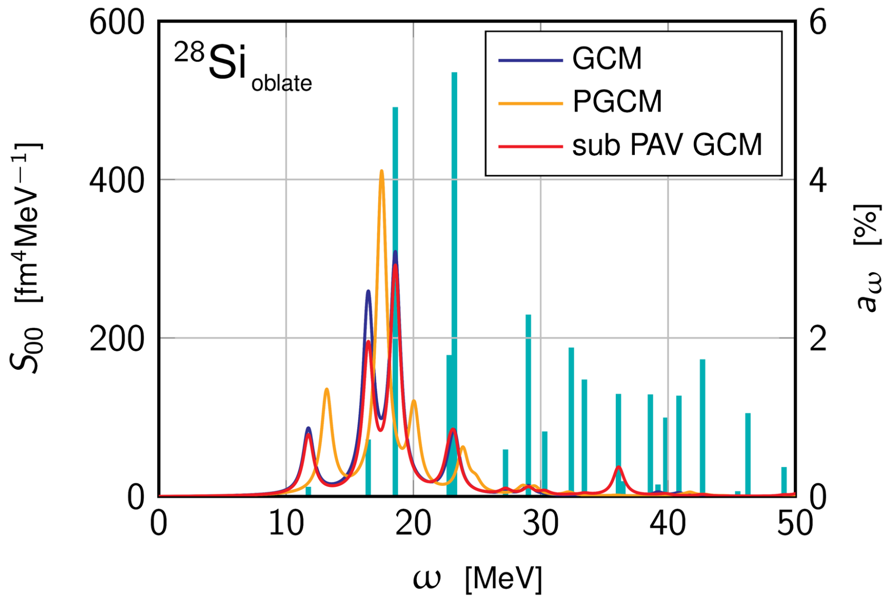

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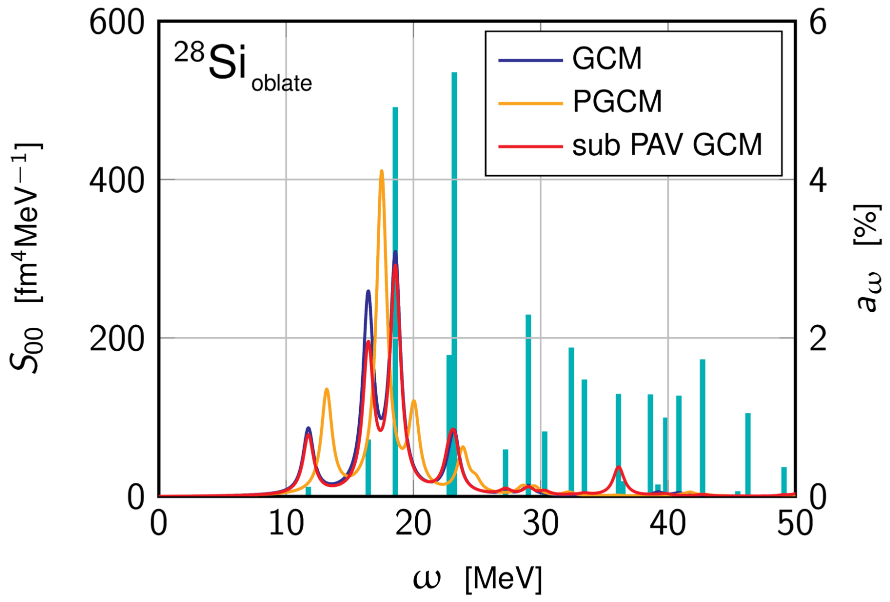

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- Does not depend on the many-body method
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Rotations must be treated variationally

- PGCM already does
- Projected QRPA needed

(1) INFN collaboration, G. Colò and D. Gambacurta

Outline

1 Giant Resonances
- Physical introduction
- Existing ab initio theoretical tools

2 Ab initio PGCM
- Formalisms
- Uncertainty quantification

3 Chosen results

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From finite nuclei to Astrophysics
- Preliminary incompressibility results

Conclusions and perspectives

From finite nuclei to Astrophysics

Symmetry energy

- IV GDR
- Dipole polarizability
- Neutron skin

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Nuclear compressibility

- GMR

$$K_{\mathrm{A}} = (M/\hbar^2)\langle r^2\rangle E_{\mathrm{GMR}}^2$$

$$\tilde{E}_k = \sqrt{\frac{m_{\mathrm{k}}}{m_{k-2}}} \qquad \bar{E}_1 = \frac{m_1}{m_0}$$

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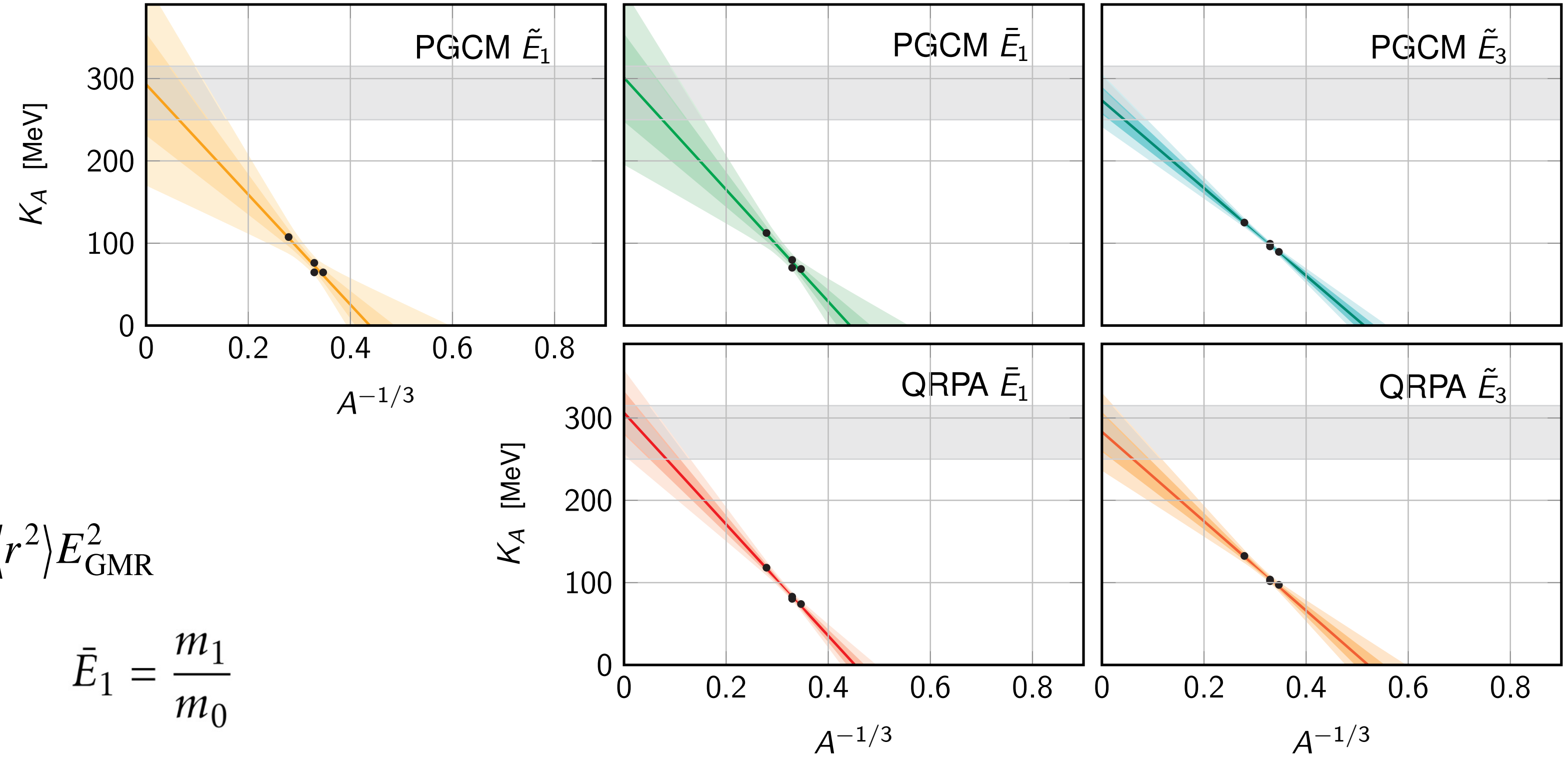


Preliminary evaluation of K_∞

- Starting from deformed systems
- Extrapolation in agreement with commonly accepted values
- Systematic investigation in heavier systems (Sn, Mo isotopic chains, neutron rich)

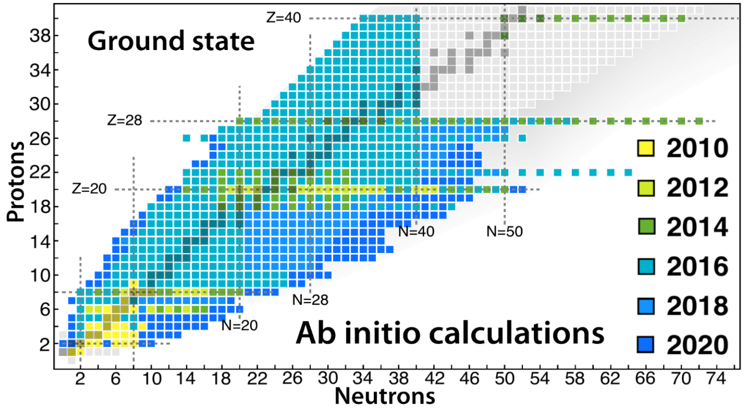
Outline

Current frontiers

SPECTROSCOPY

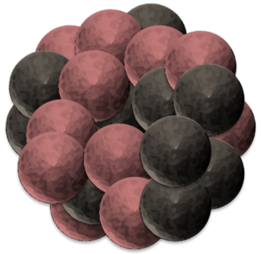
- Single-particle
- Collective excitations

OPEN-SHELL



[Hergert, Front. Phys, 2020]

HEAVY-MASS SYSTEMS



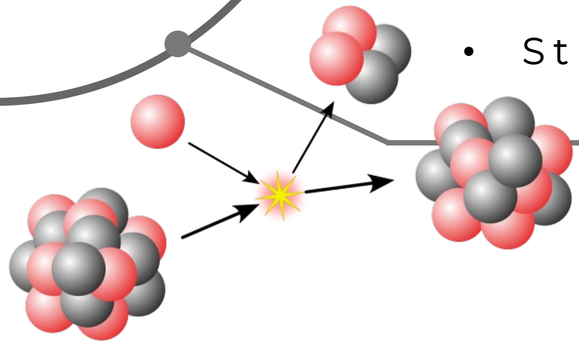
ACCURACY

$$H = T + V_{\mathrm{LO}} + V_{\mathrm{NLO}} + V_{\mathrm{N^2LO}} + \dots$$

$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

UNCERTAINTIES

- Systematic uncertainties
  - Hamiltonian
  - A-body solution
  - Basis representation
- Statistical uncertainties



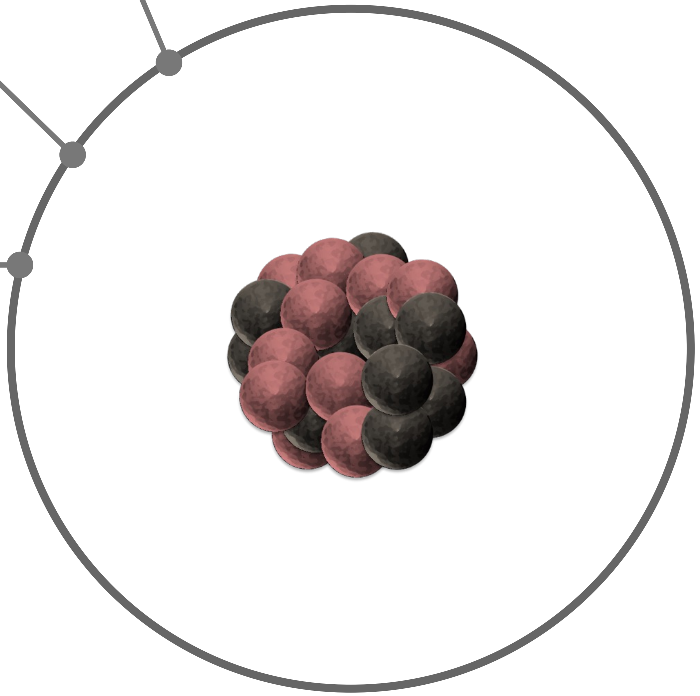
REACTIONS

Conclusions and perspectives

SPECTROSCOPY

OPEN-SHELL

UNCERTAINTIES

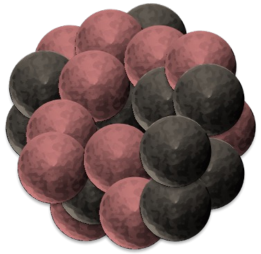


Conclusions and perspectives

S P E C T R O S C O P Y

O P E N - S H E L L

U N C E R T A I N T I E S



Take-away messages

- PGCM reliable tool for *ab initio** spectroscopy
- Access to new observables and phenomena in *ab initio*
- Different levels of symmetry breaking and restoration reveal new physical insights

Conclusions and perspectives

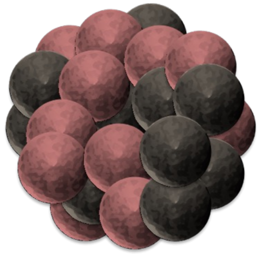
Perspectives

- Systematic comparison to new and existing exp data
- Deeper uncertainty quantification (EC)

SPECTROSCOPY

OPEN-SHELL

UNCERTAINTIES



Take-away messages

- PGCM reliable tool for *ab initio** spectroscopy
- Access to new observables and phenomena in *ab initio*
- Different levels of symmetry breaking and restoration reveal new physical insights

Conclusions and perspectives

Perspectives

Systematic comparison to new and existing exp data

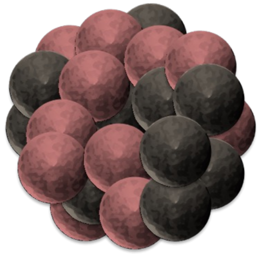
Deeper uncertainty quantification (EC)

Develop full symmetry-conserving QRPA

S P E C T R O S C O P Y

O P E N - S H E L L

U N C E R T A I N T I E S



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SPECTROSCOPY

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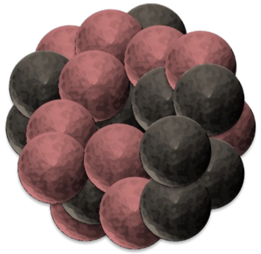

Perspectives

- Systematic comparison to new and existing exp data
- Deeper uncertainty quantification (EC)
- Develop full symmetry-conserving QRPA

HEAVY-MASS SYSTEMS

- Large-scale calculations with VS-IMSRG
- Finite-nuclei constraints for Astrophysics

Take-away messages

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- Access to new observables and phenomena in *ab initio*
- Different levels of symmetry breaking and restoration reveal new physical insights

Thanks for the attention

Technische Universität Darmstadt

Alexander Tichai
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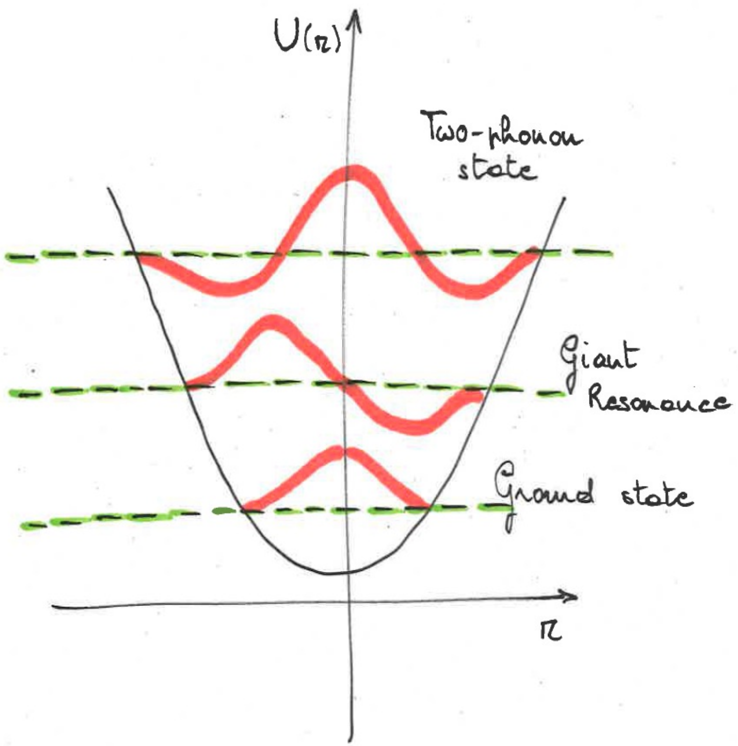
Mikael Frosini
Benjamin Bally
Jean-Paul Ebran
Alberto Scalesi

INFN

Gianluca Colò
Danilo Gambacurta

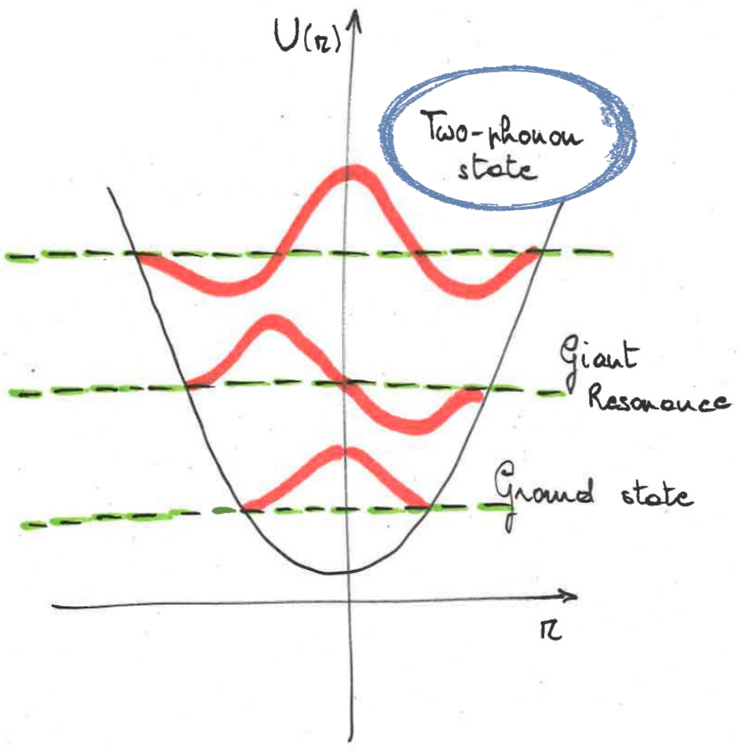
Backup slides

Multi-phonon states in ^{46}Ti



- **GRs** can be interpreted as the first phonon of a collective excitation

Multi-phonon states in ^{46}Ti



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- Higher phonons also exist ! Multi-phonon states

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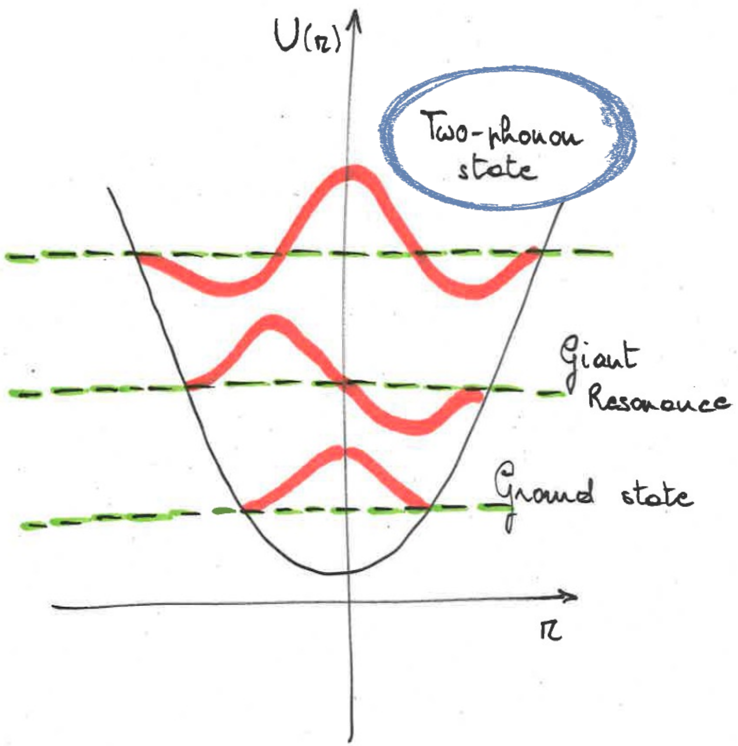

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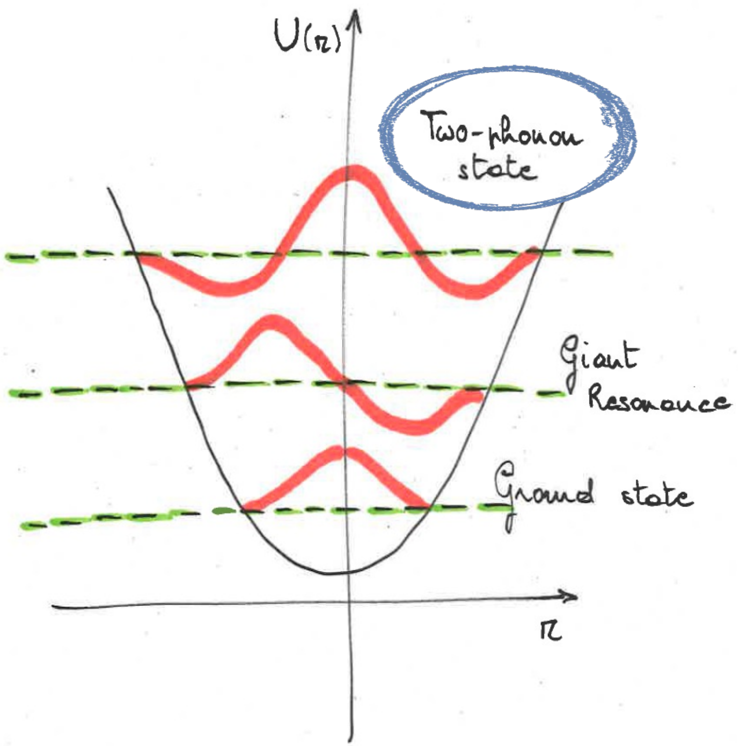

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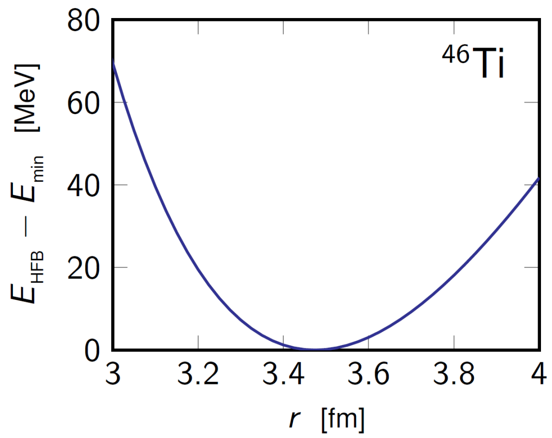
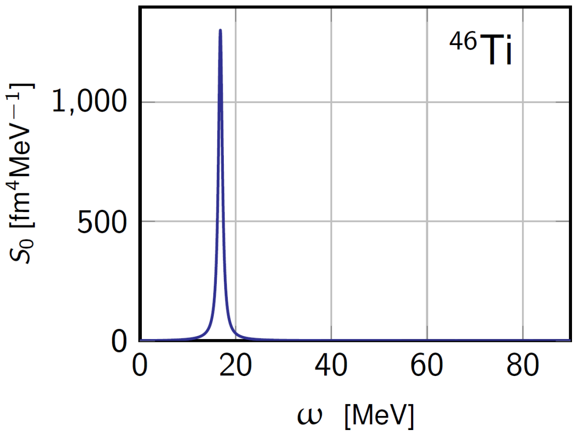
One-dimensional PGCM calculation





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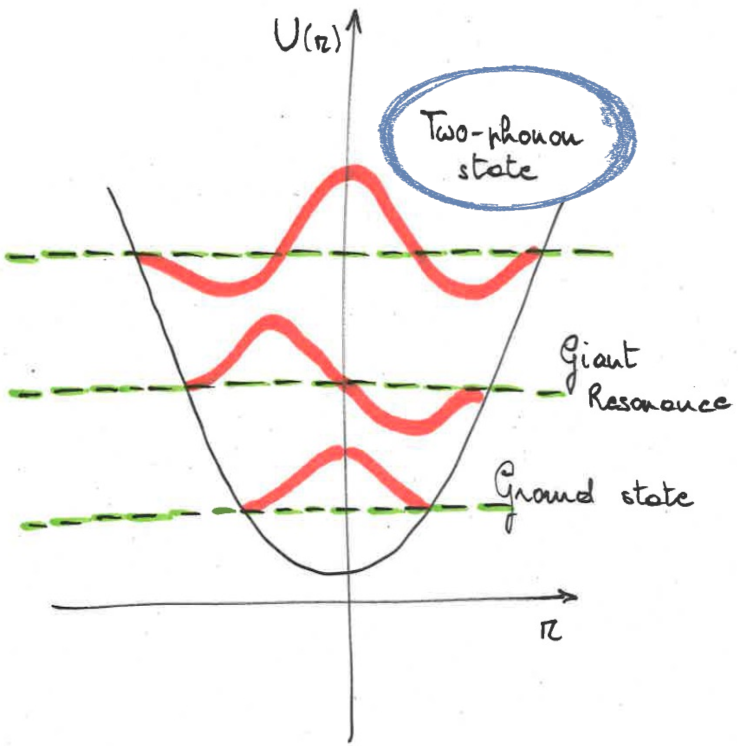

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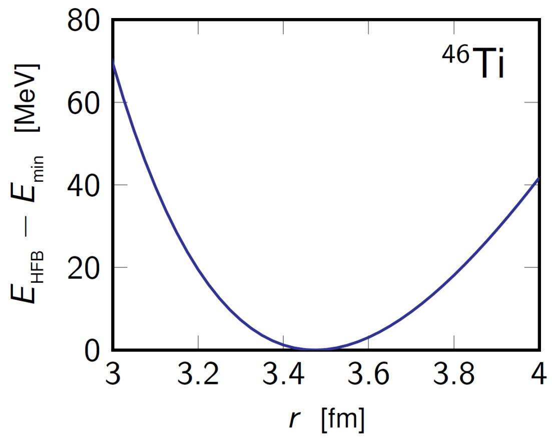

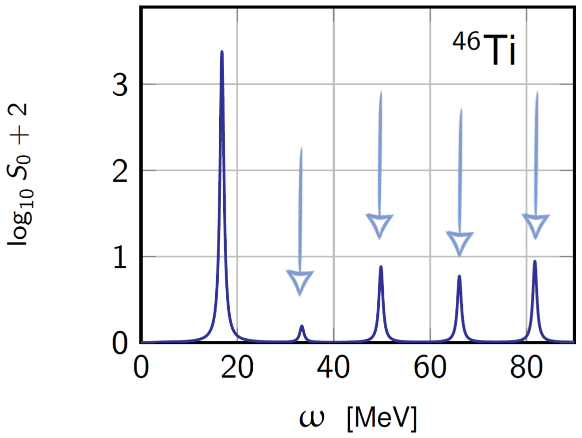

- PGCM predicts high-lying states

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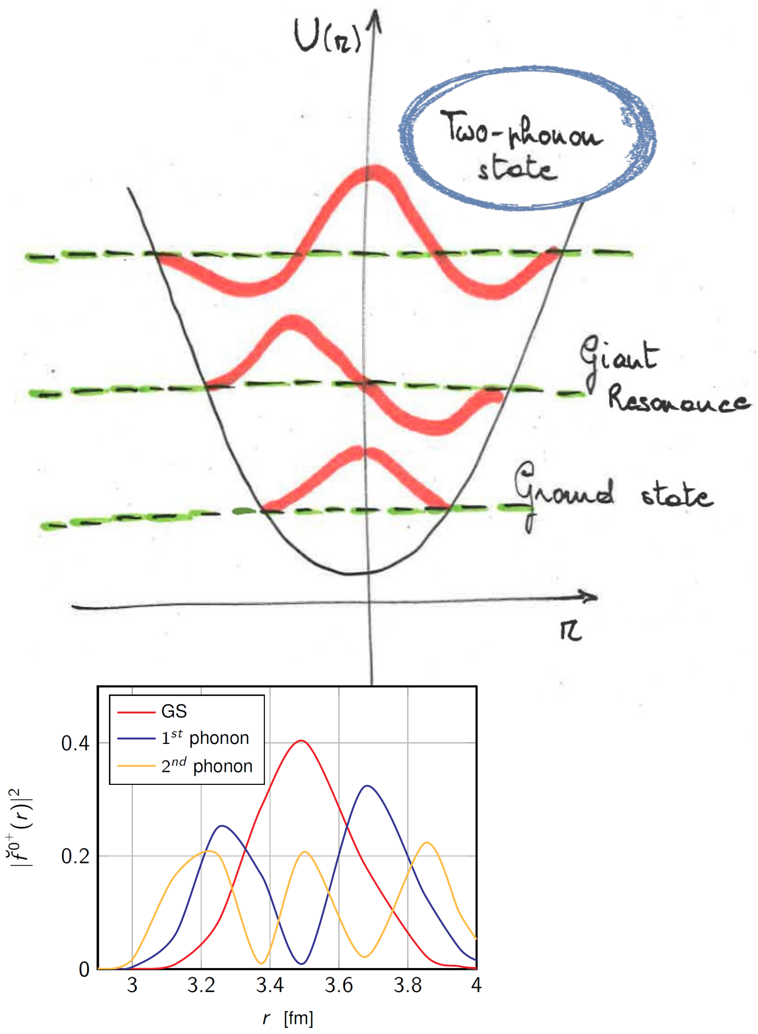

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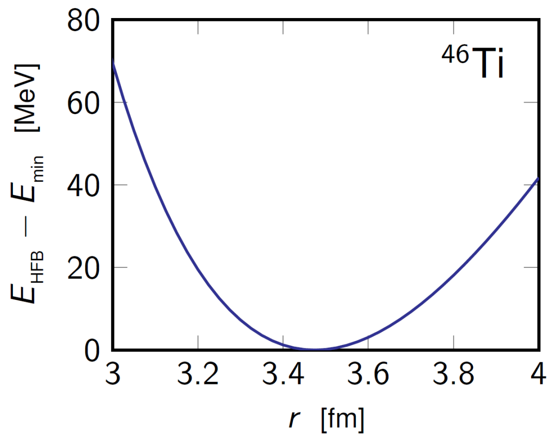

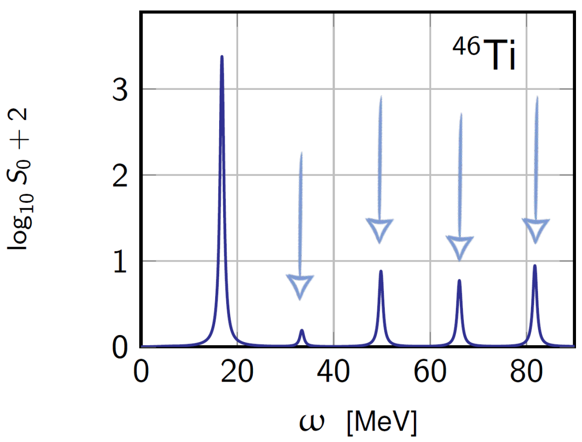

- PGCM predicts high-lying states
- Close to the harmonic oscillator eigen-solutions

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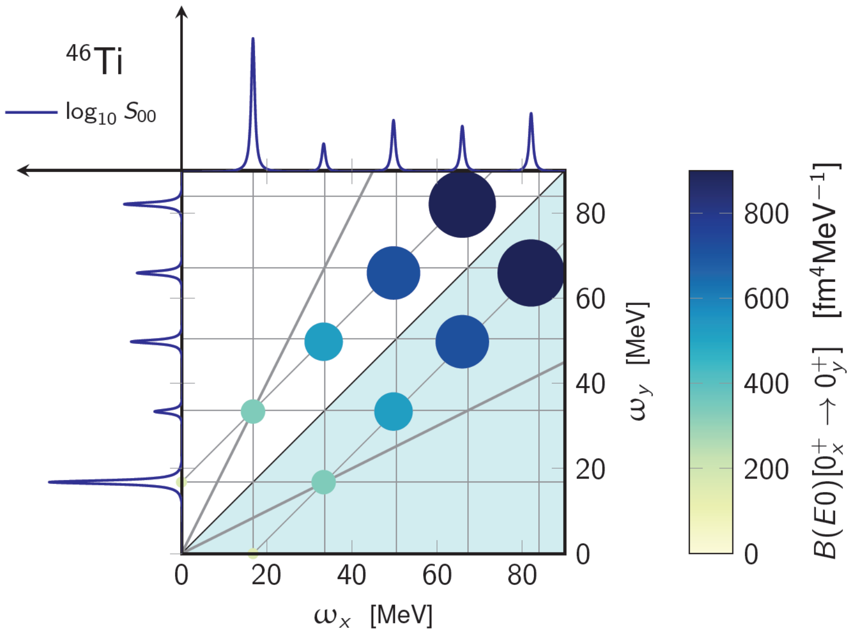

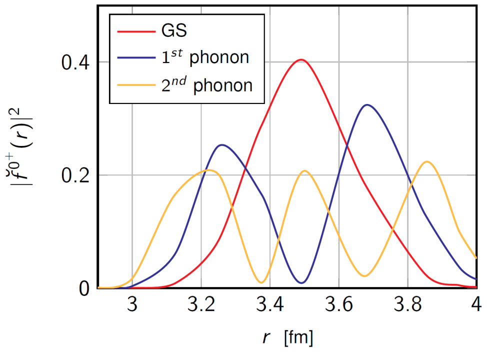

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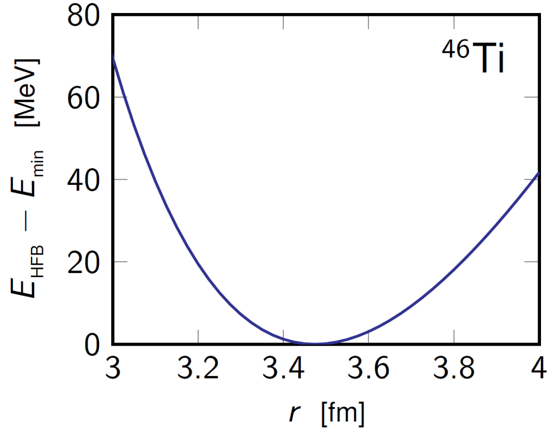

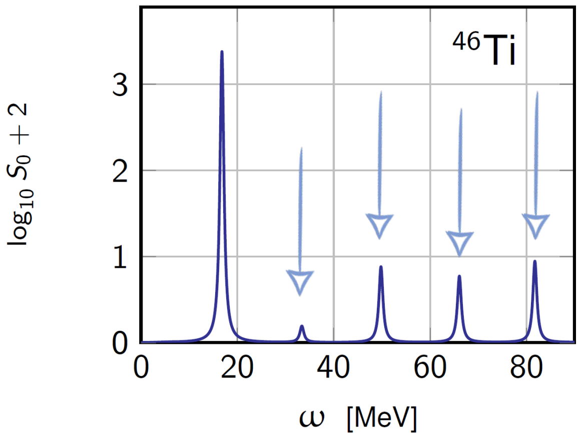

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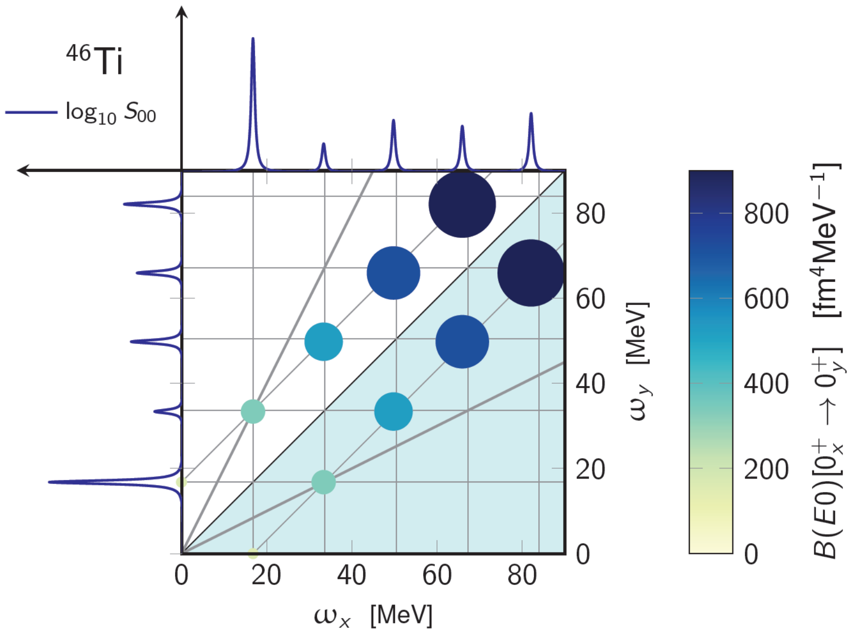

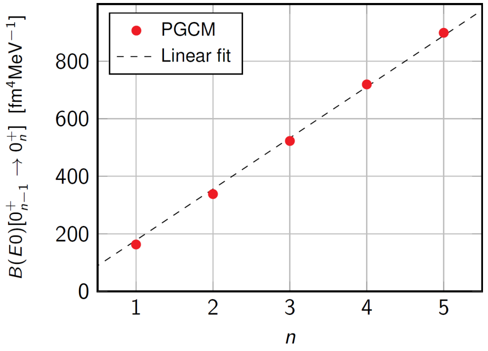

$$|\langle n-1|r^2|n\rangle|^2 = \frac{\hbar}{2m\omega} n$$

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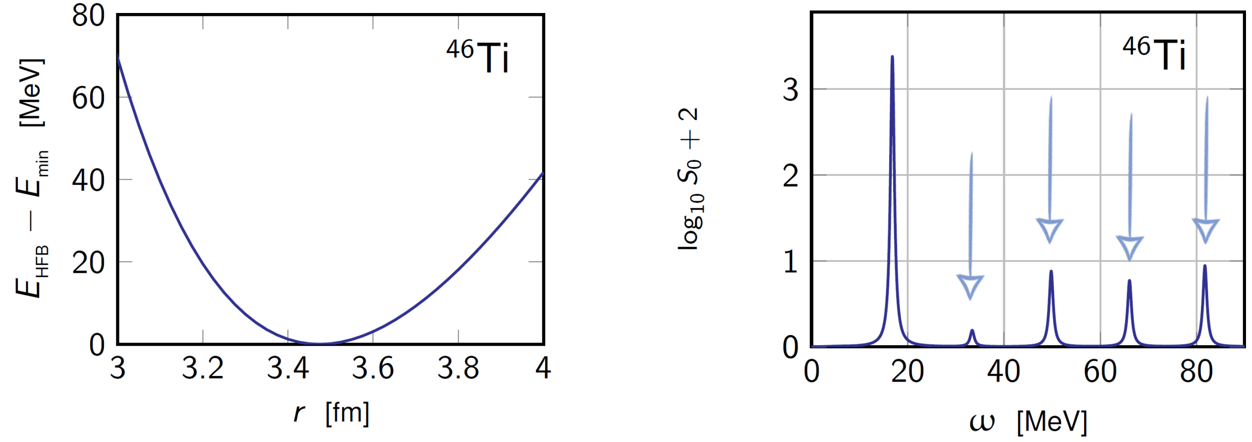

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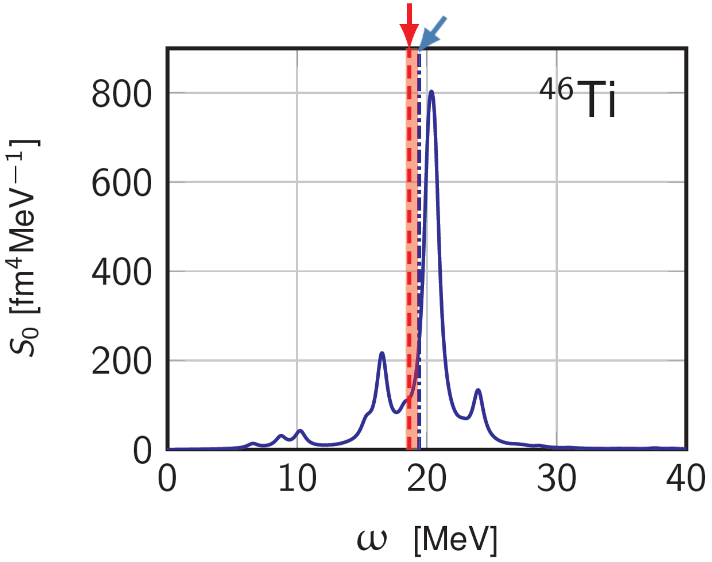
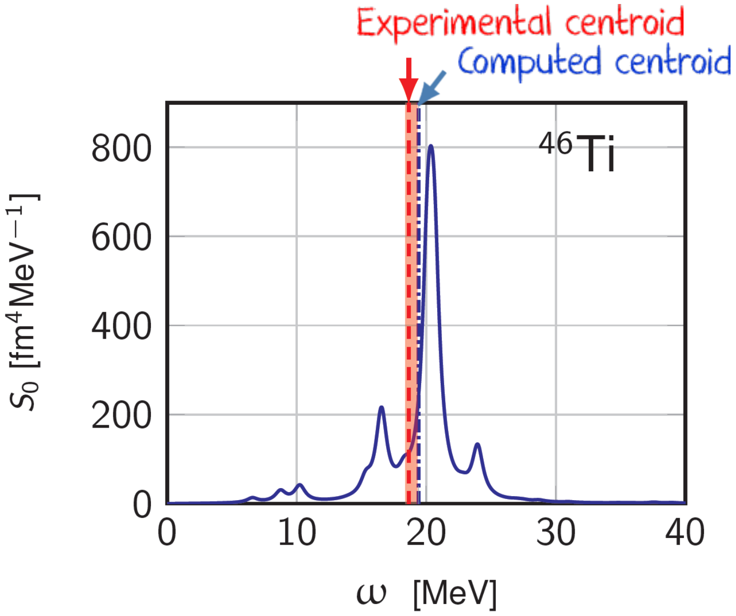
x Linear trend in the transition strength

Two-dimensional calculations



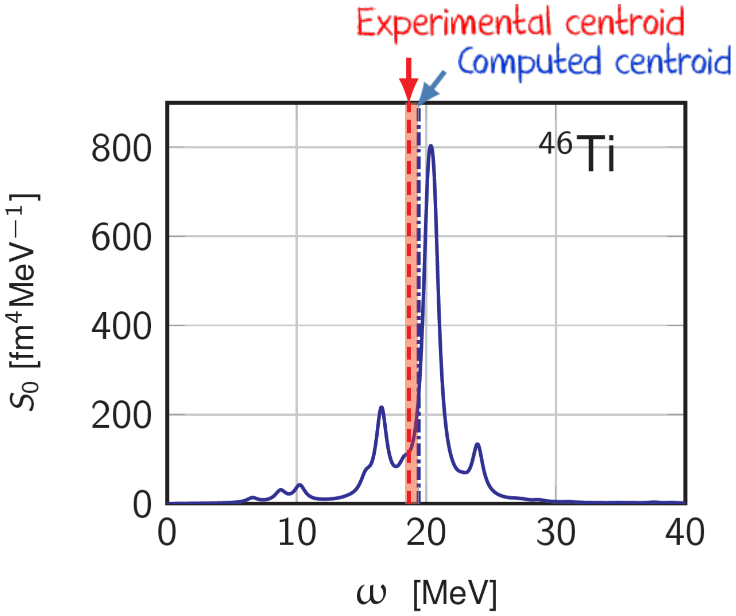
- 2-D PGCM in the (r, β_2) plane

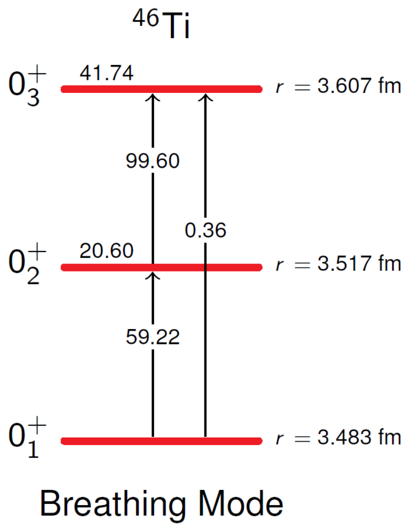
Two-dimensional calculations



- 2-D PGCM in the (r, β_2) plane
- Good agreement with experiment

Two-dimensional calculations





- 2-D PGCM in the (r, β_2) plane
- Good agreement with experiment
- Multi-phonon states observed

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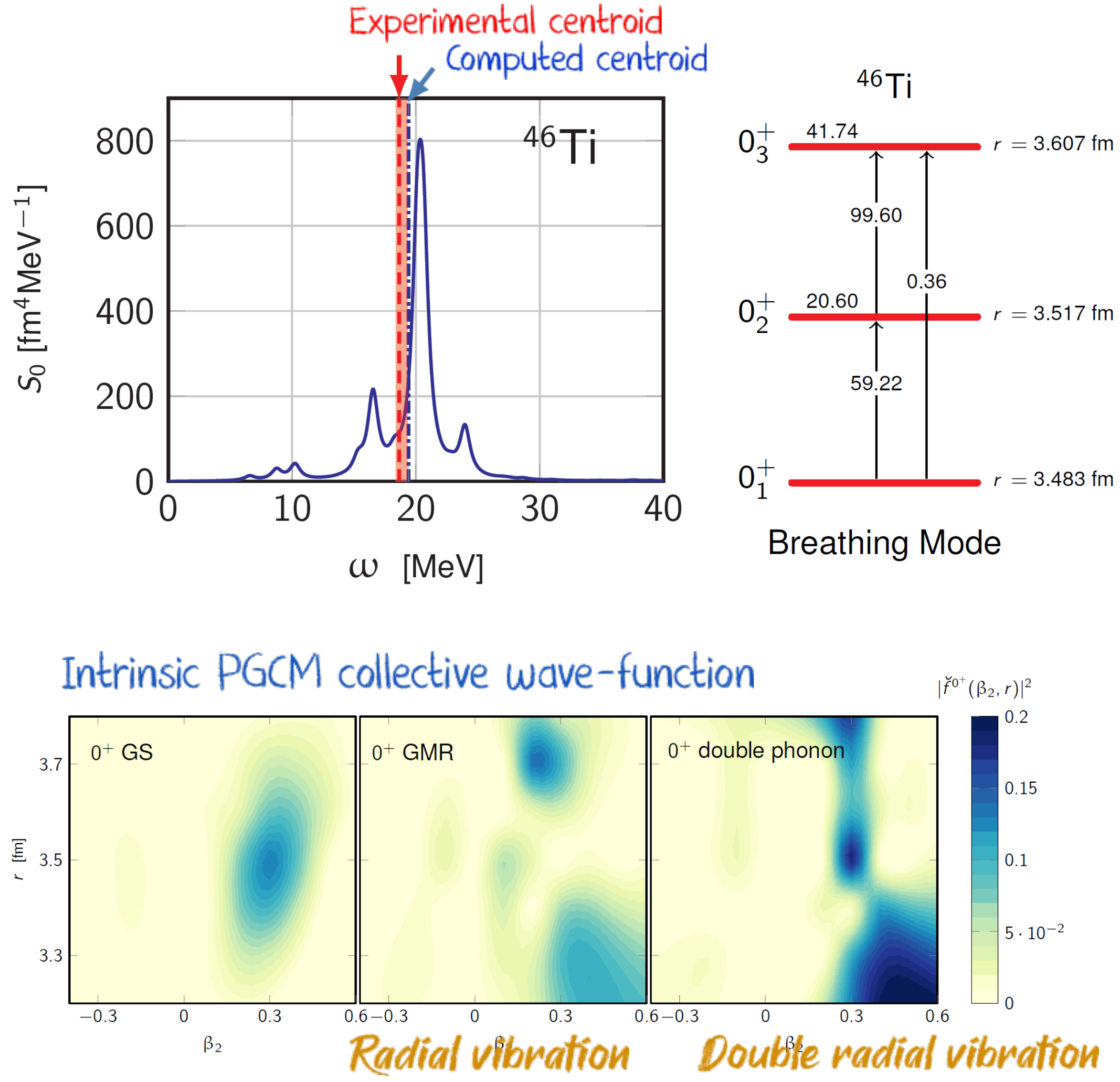

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- Harmonicity well confirmed

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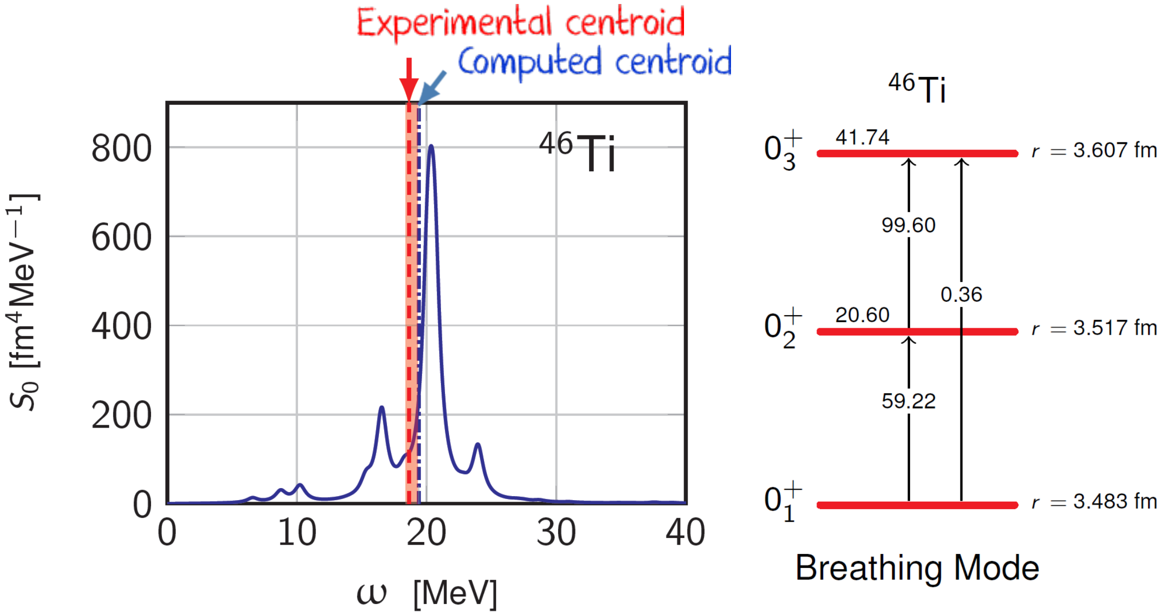

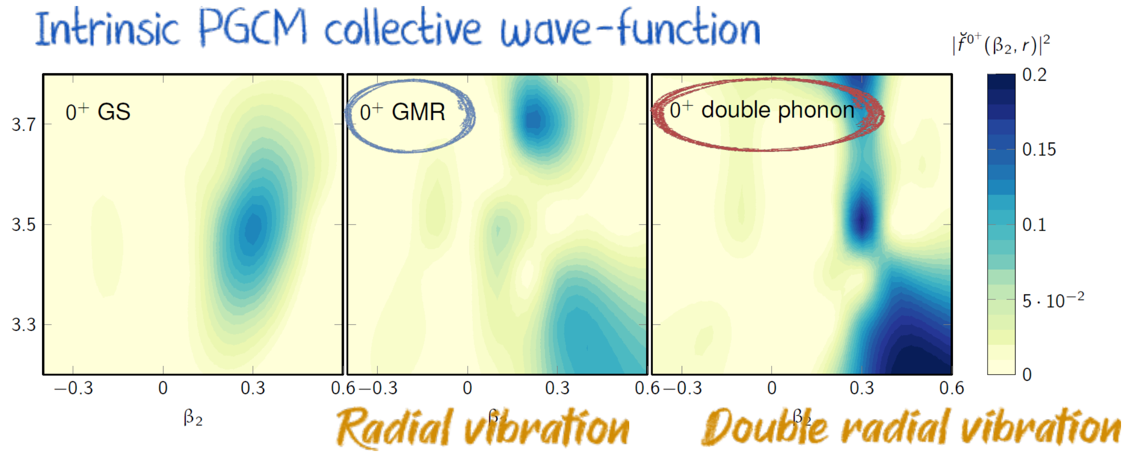

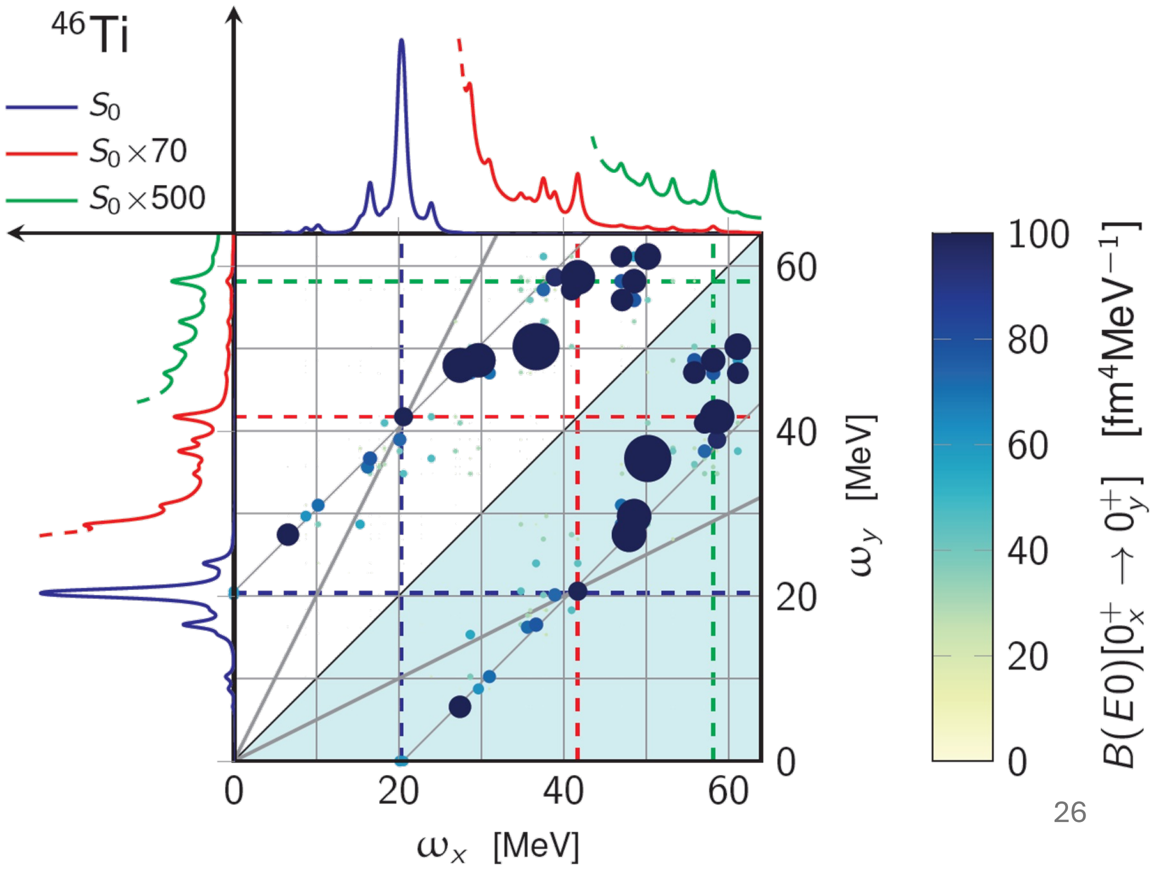

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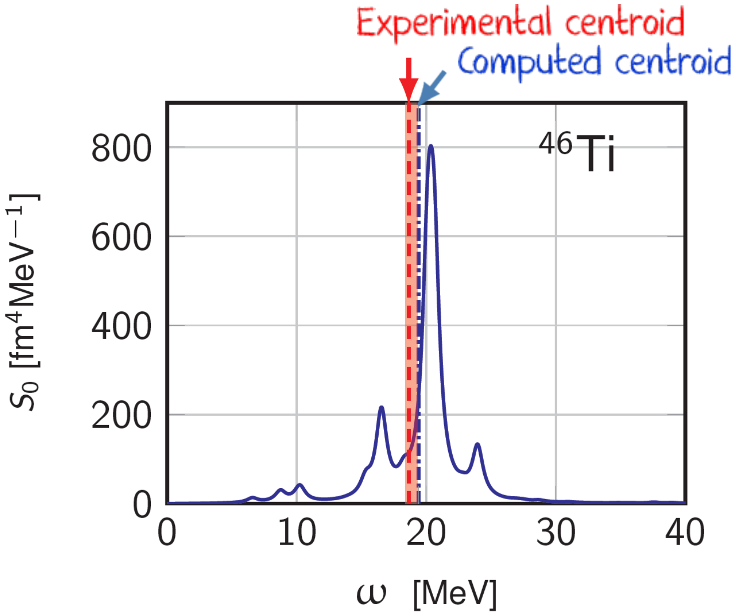

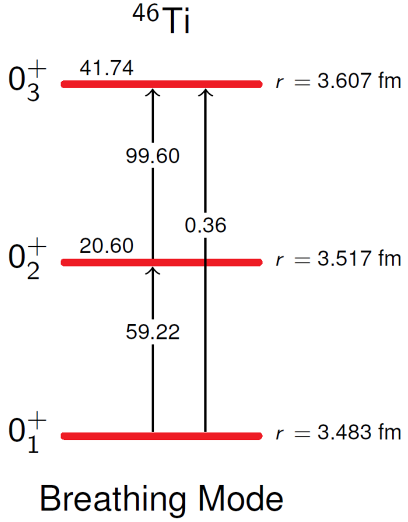

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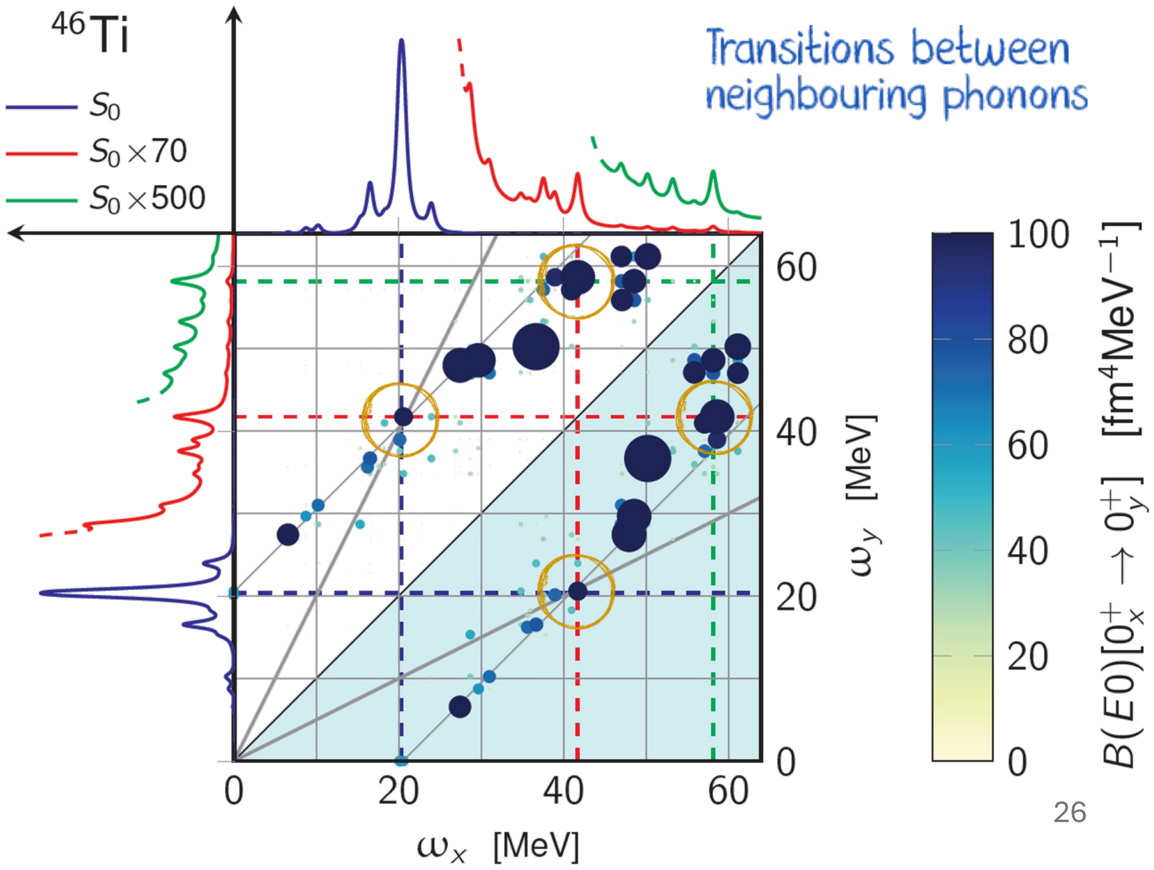

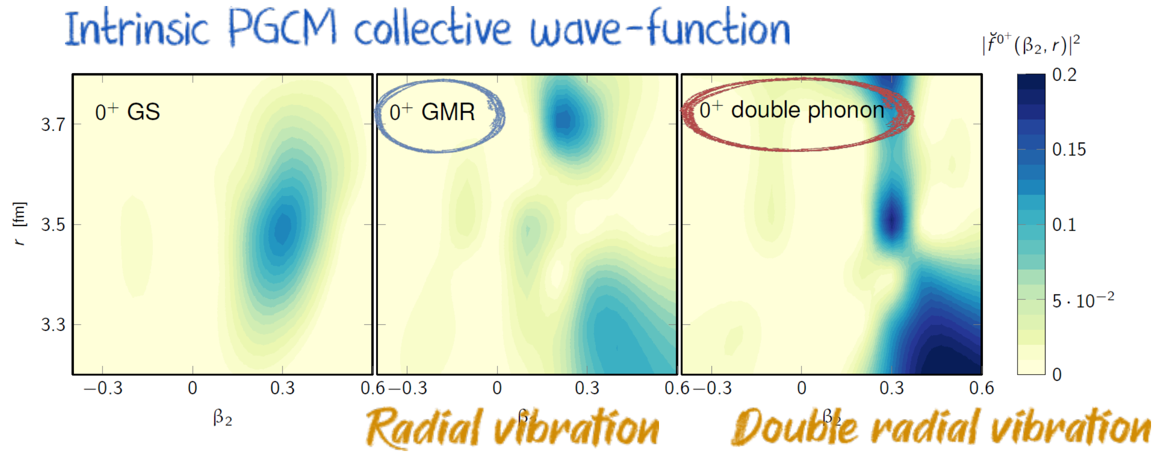

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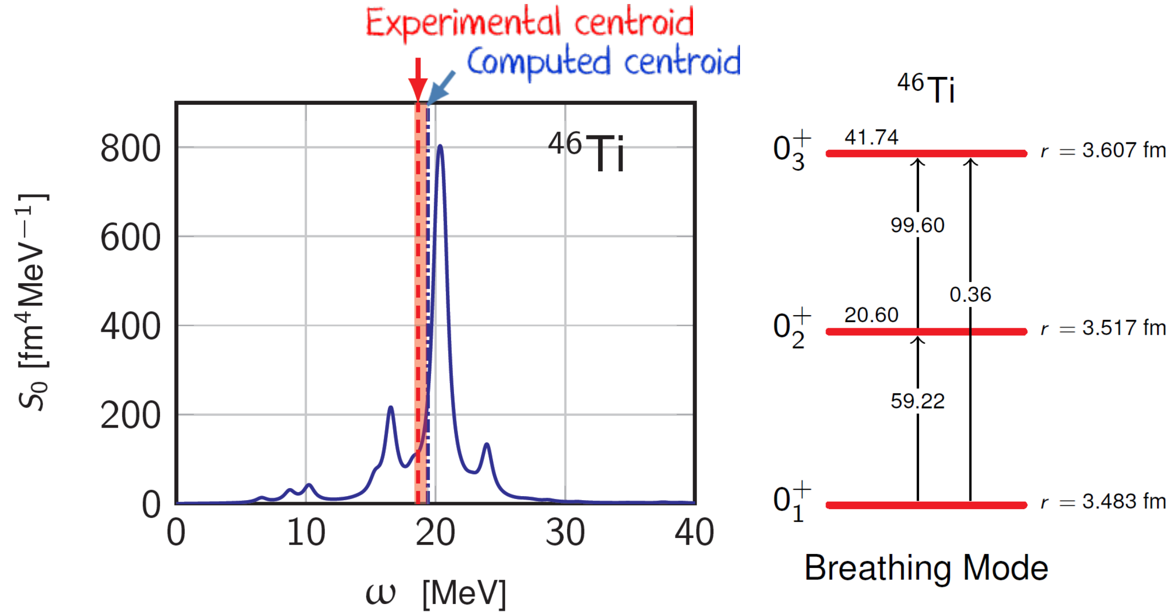
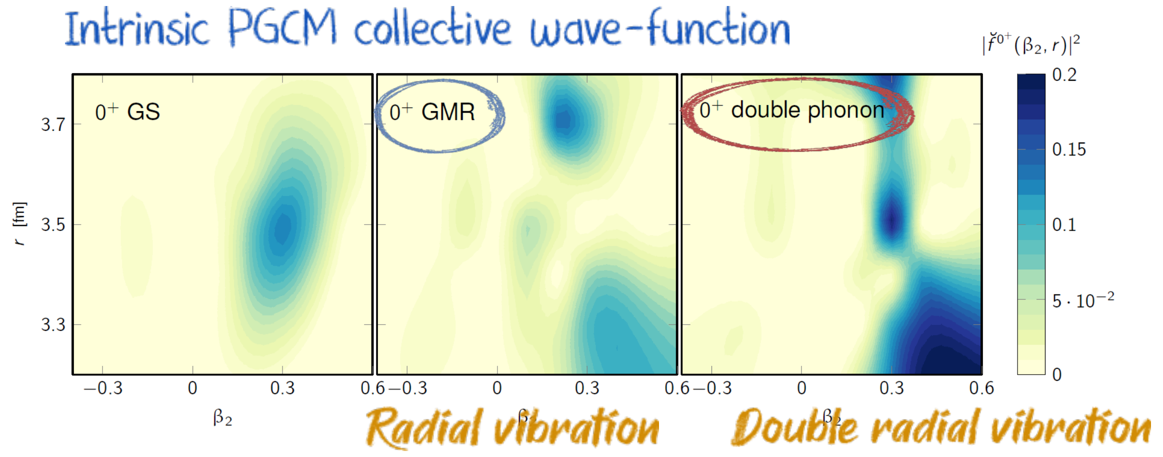
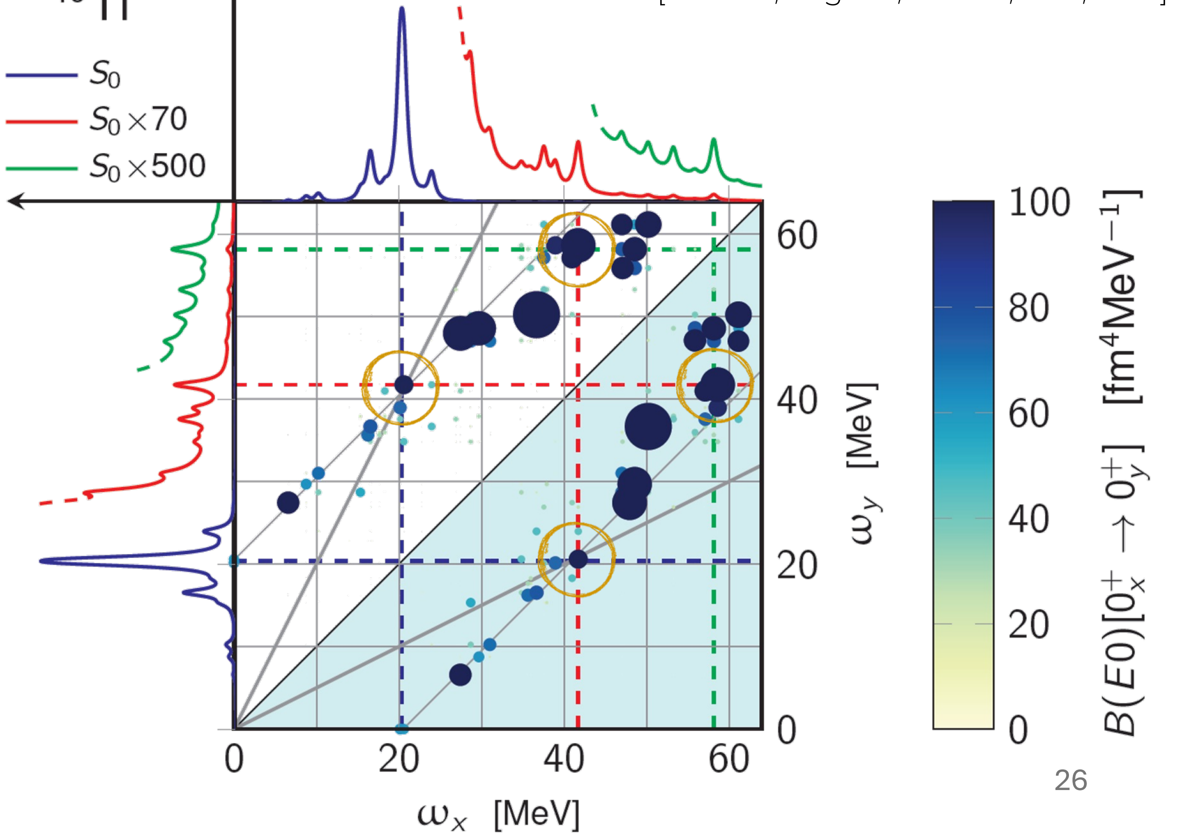
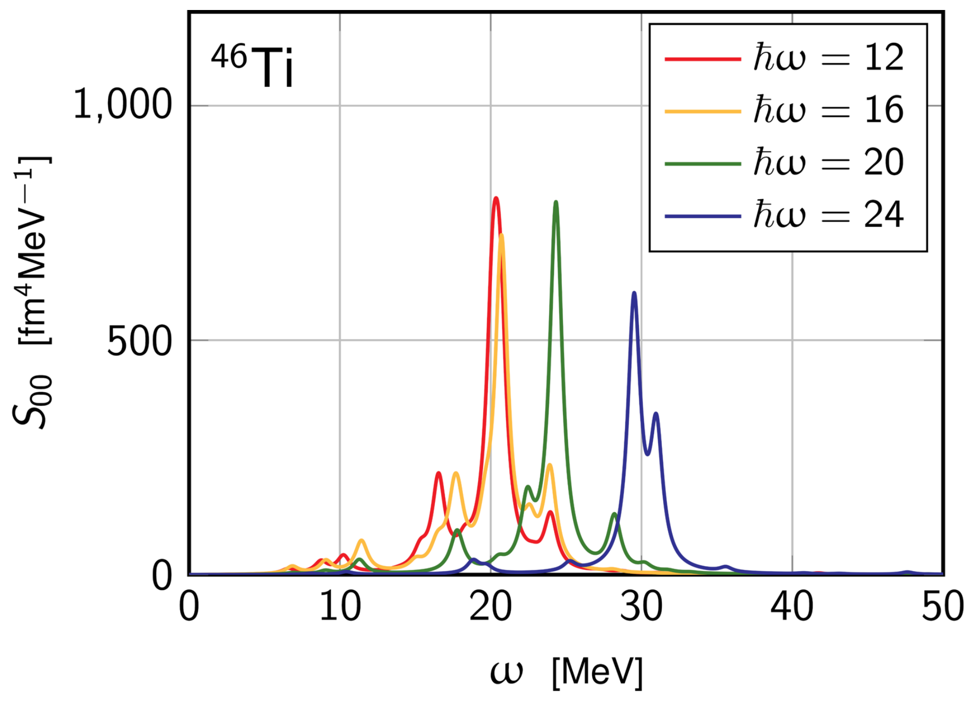


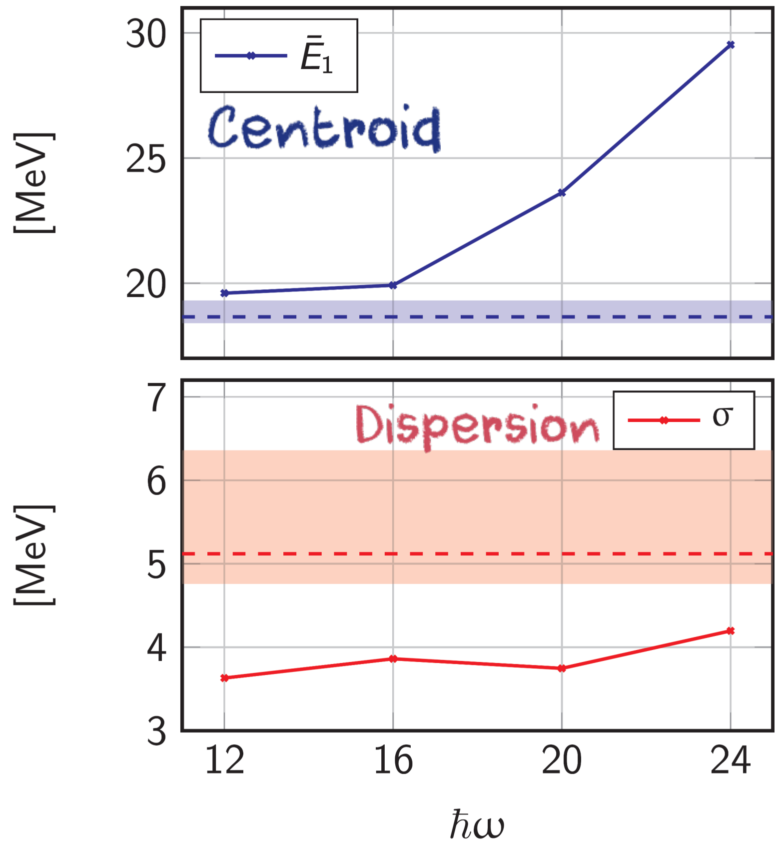


[Marevic, Regnier, Lacroix, PRC, 2023]



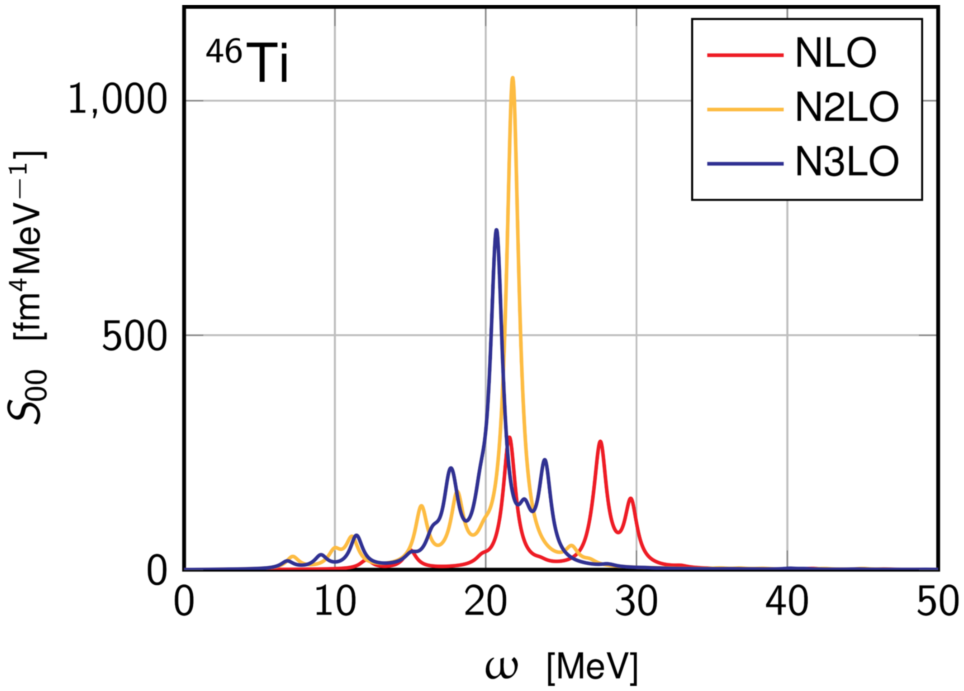
Harmonic Oscillator width

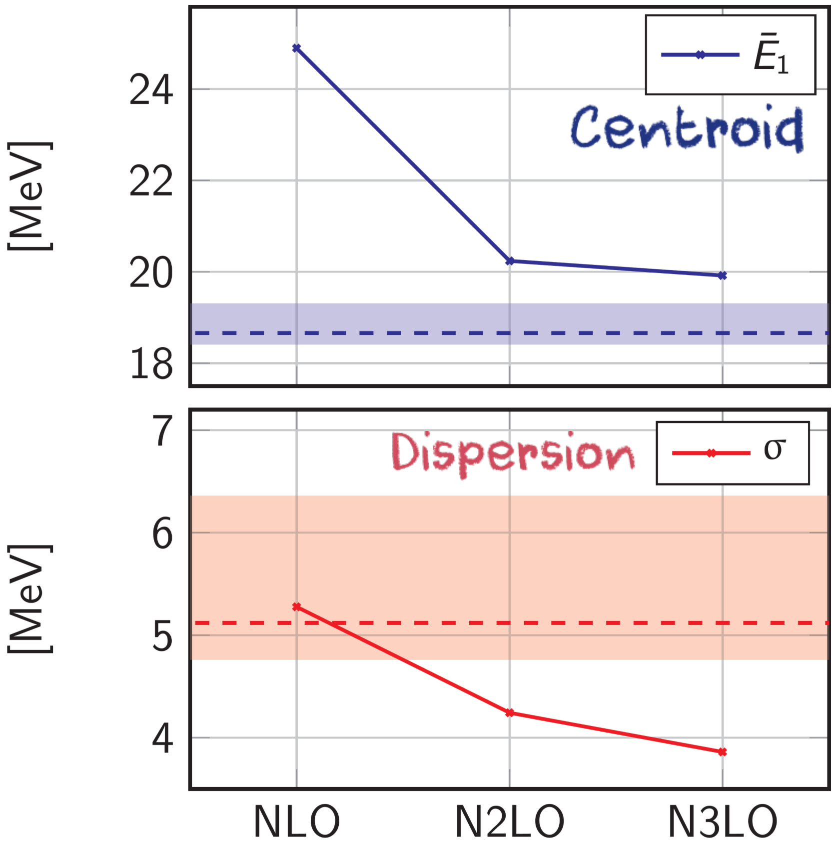




- Good overall convergence ✓
- Centroid relative error ~ 1,6 % ✓
- Dispersion relative error ~ 6 % ✓

Chiral Order





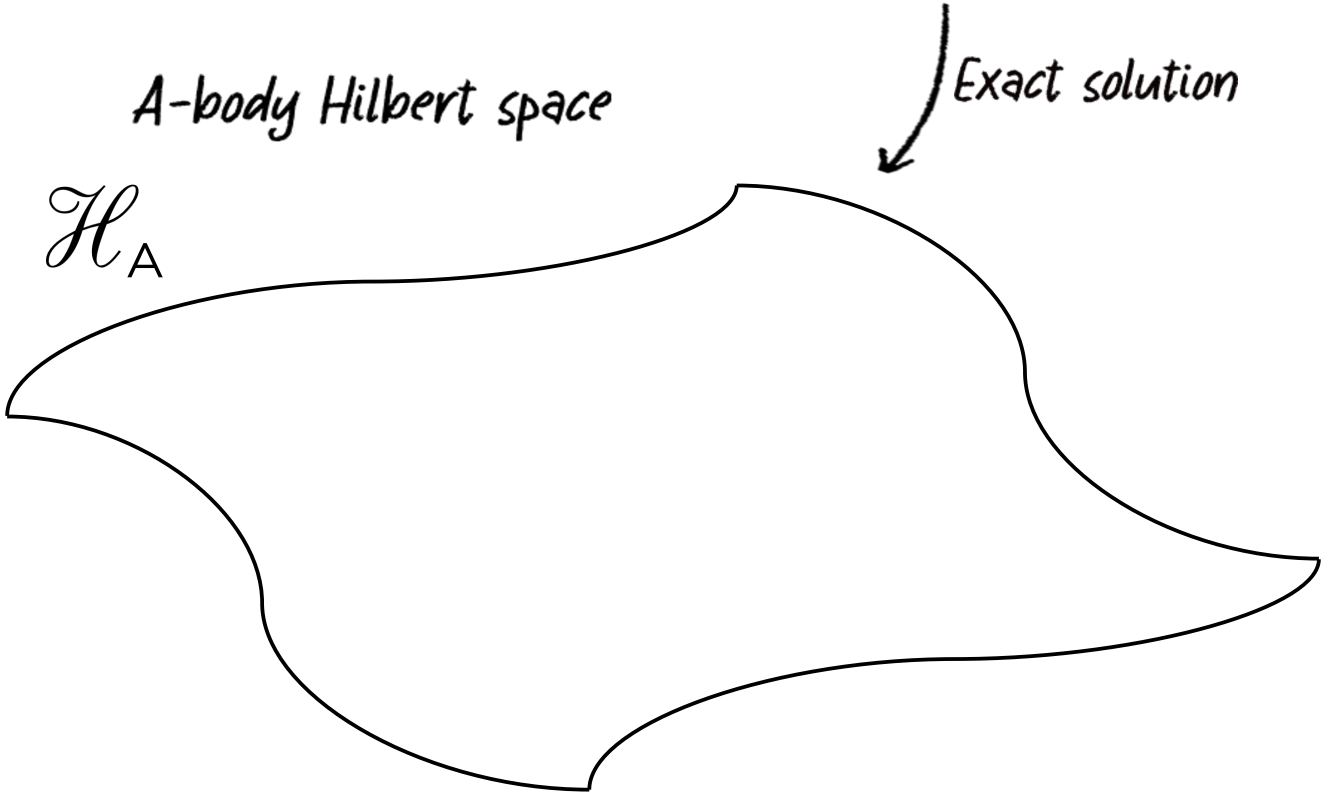
- Good overall convergence ✓
- Centroid relative error ~ 1,6 % ✓
- Dispersion relative error ~ 9,8 % ~

Pattern present but slowly converging

[Epelbaum, Krebs, Meissner, EPJA, 2015]

Many-body truncation

Schrödinger equation $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$



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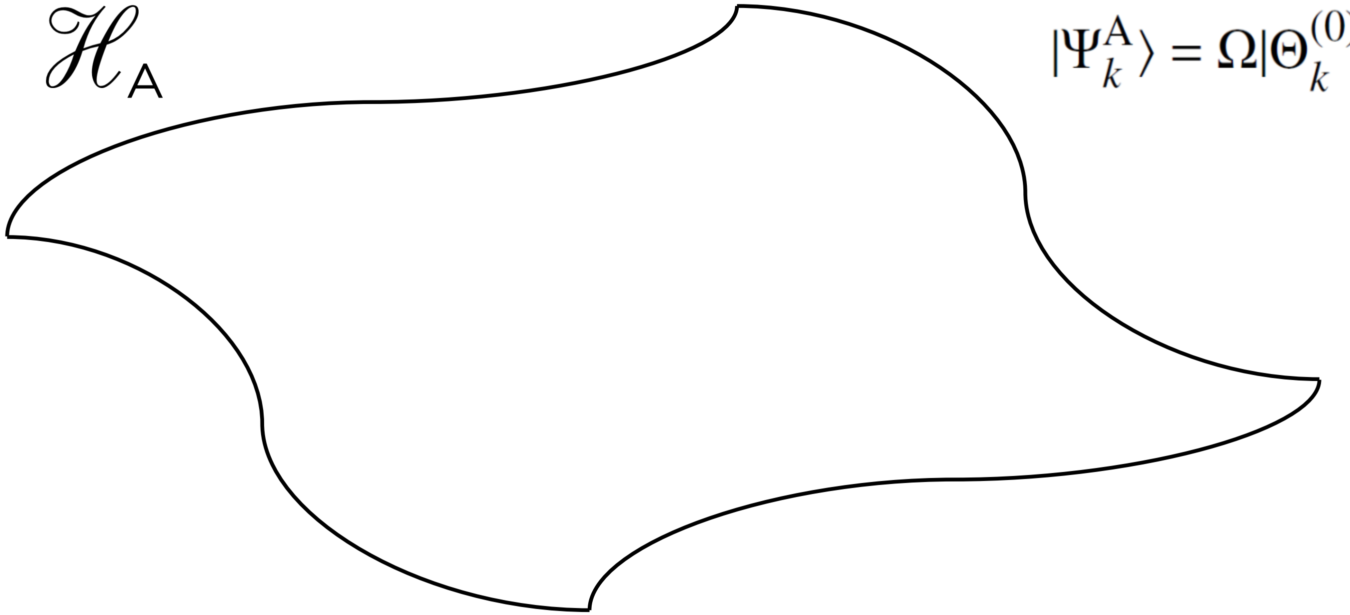
Exact solution

A-body Hilbert space

$\mathcal{H}_A$



$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle$

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PGCM : multi-reference unperturbed state

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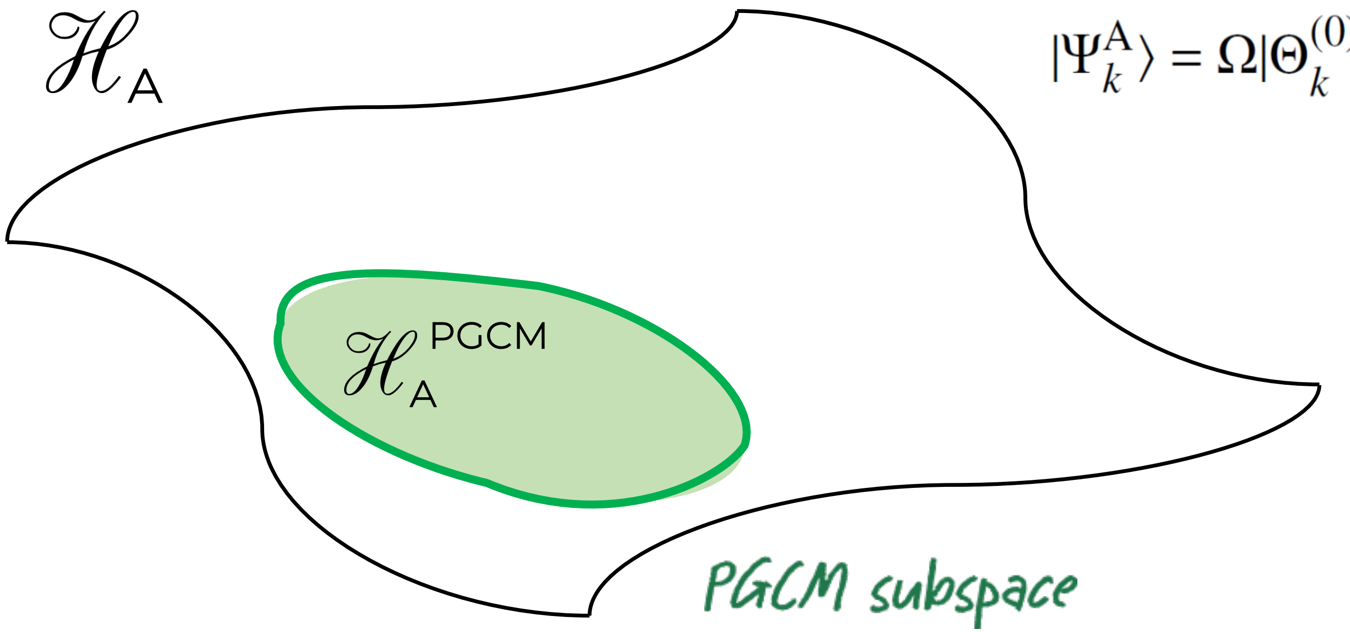

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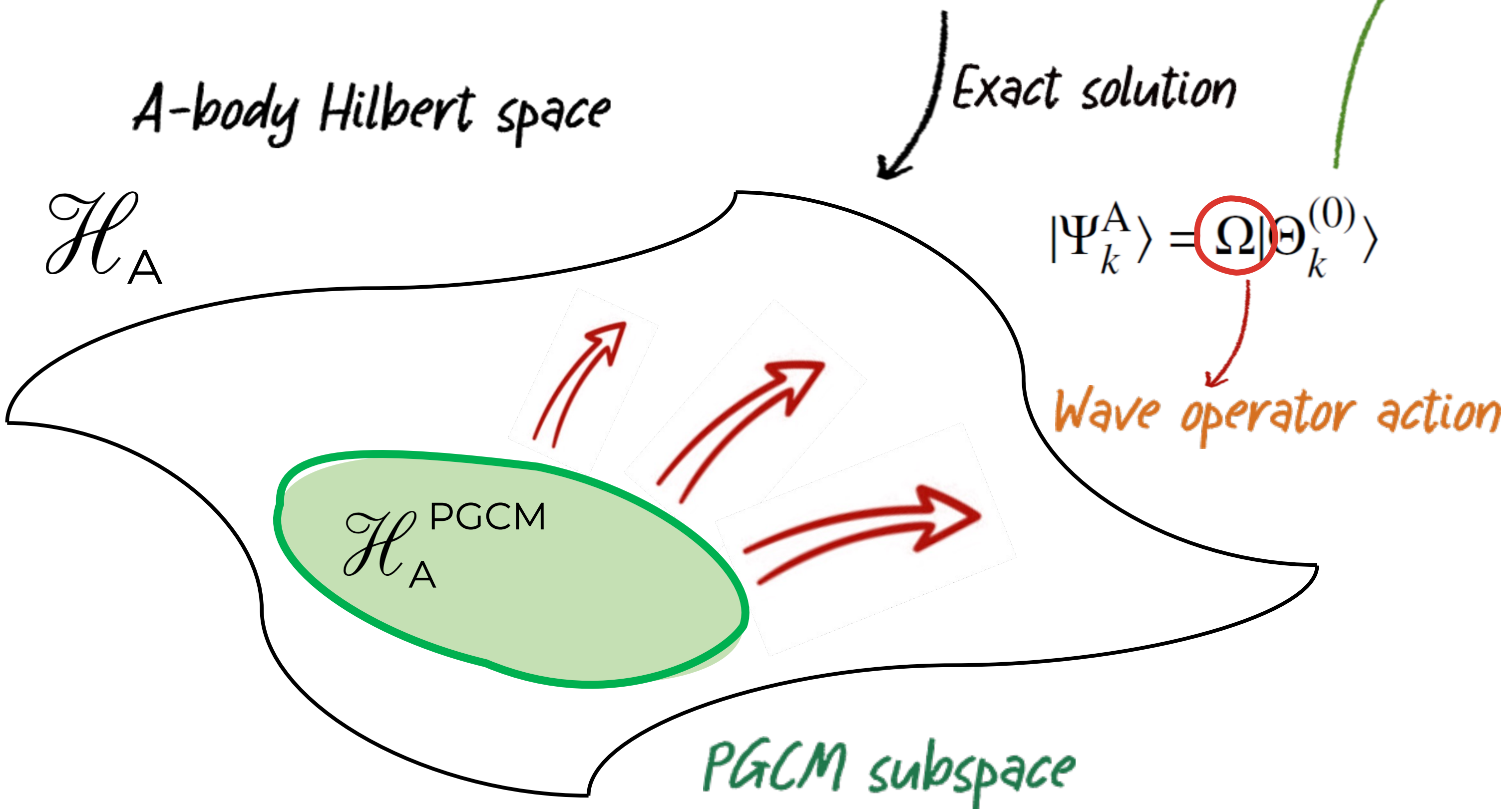

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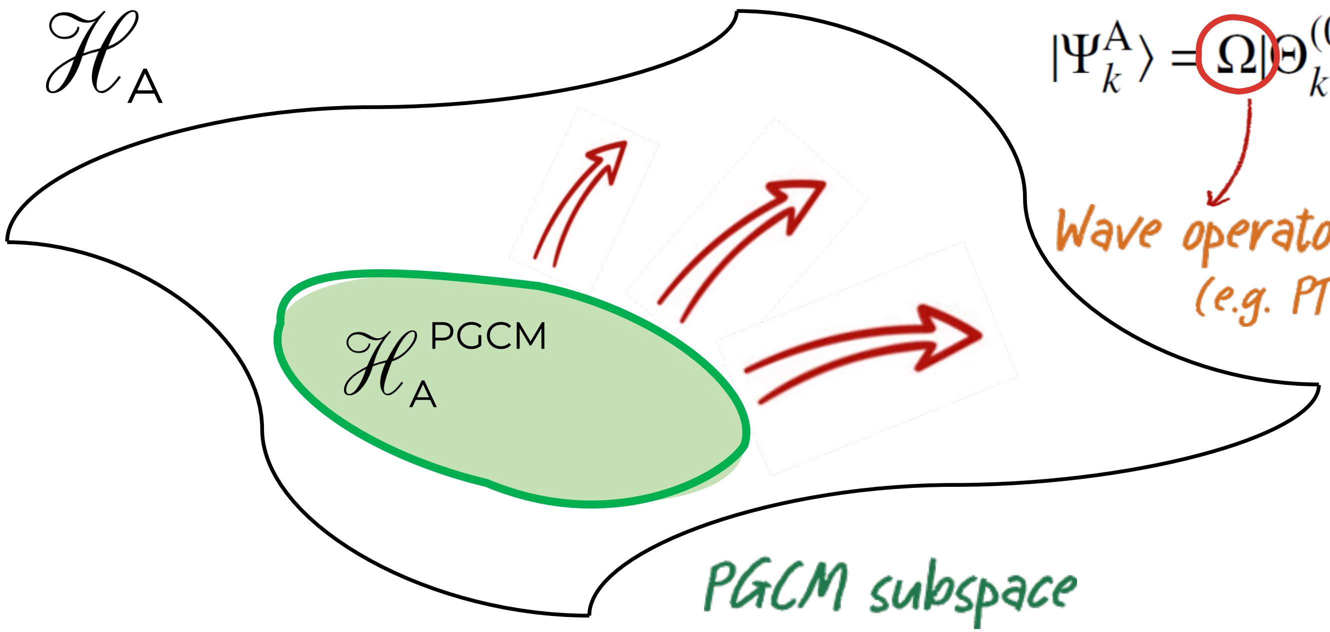
PGCM-PT : *ab initio* expansion method(1)

A-body Hilbert space

Exact solution

$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \ldots$$

Wave operator action (e.g. PT)



(1) [Frosini, Duguet, Ebran and Somà, EPJA 58(62), 2022]

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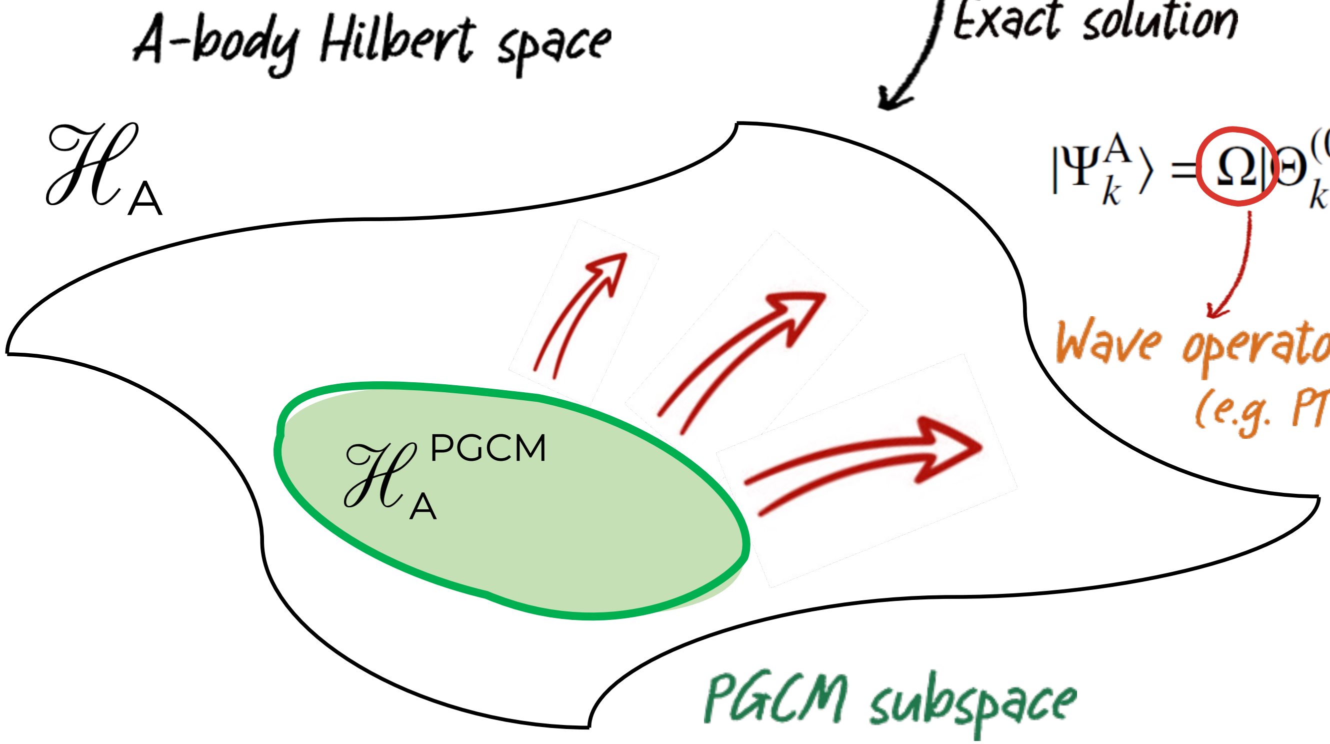

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PGCM-PT : ab initio expansion method[1]

PGCM-PT(2) up to 2nd order so far[2]

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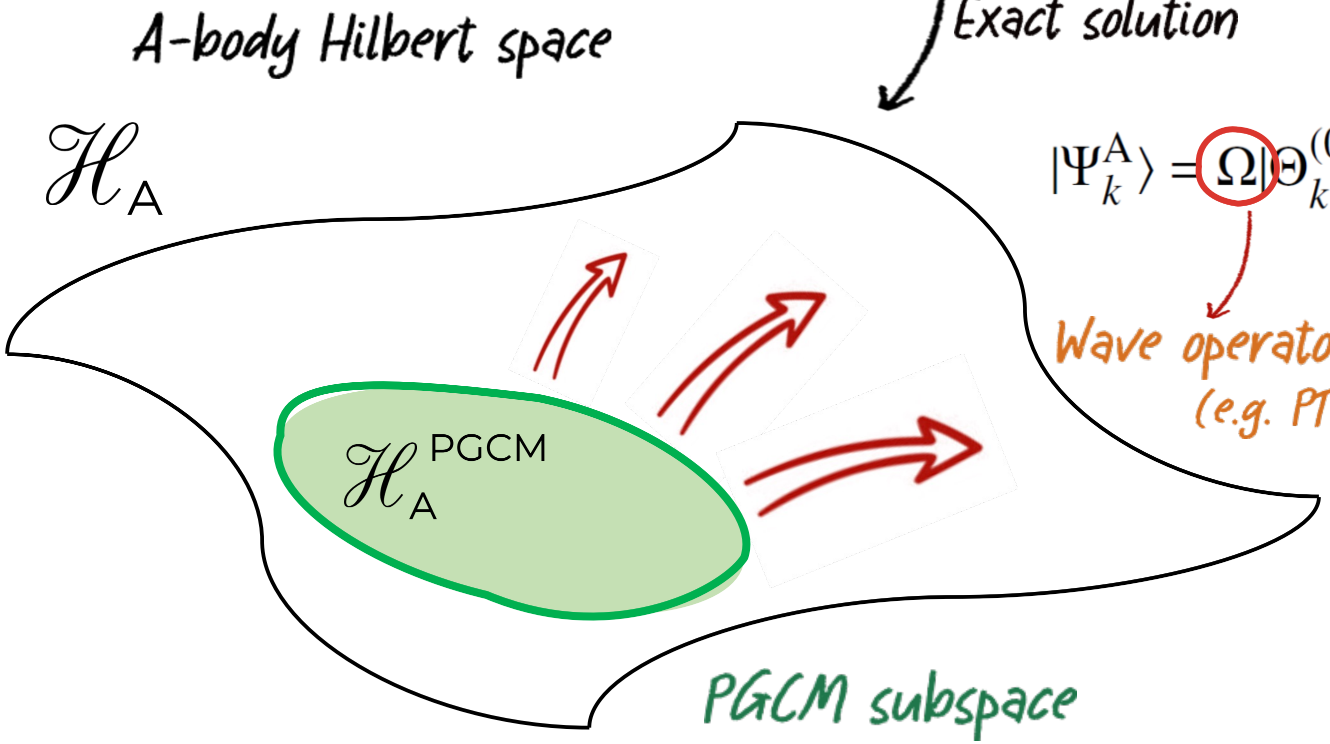

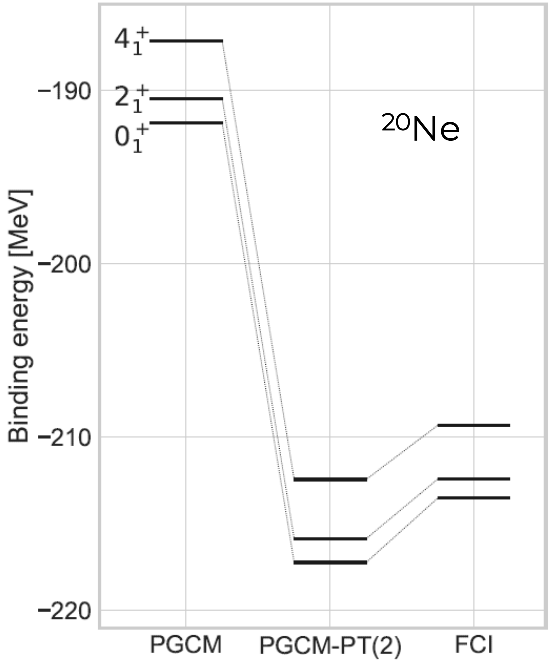

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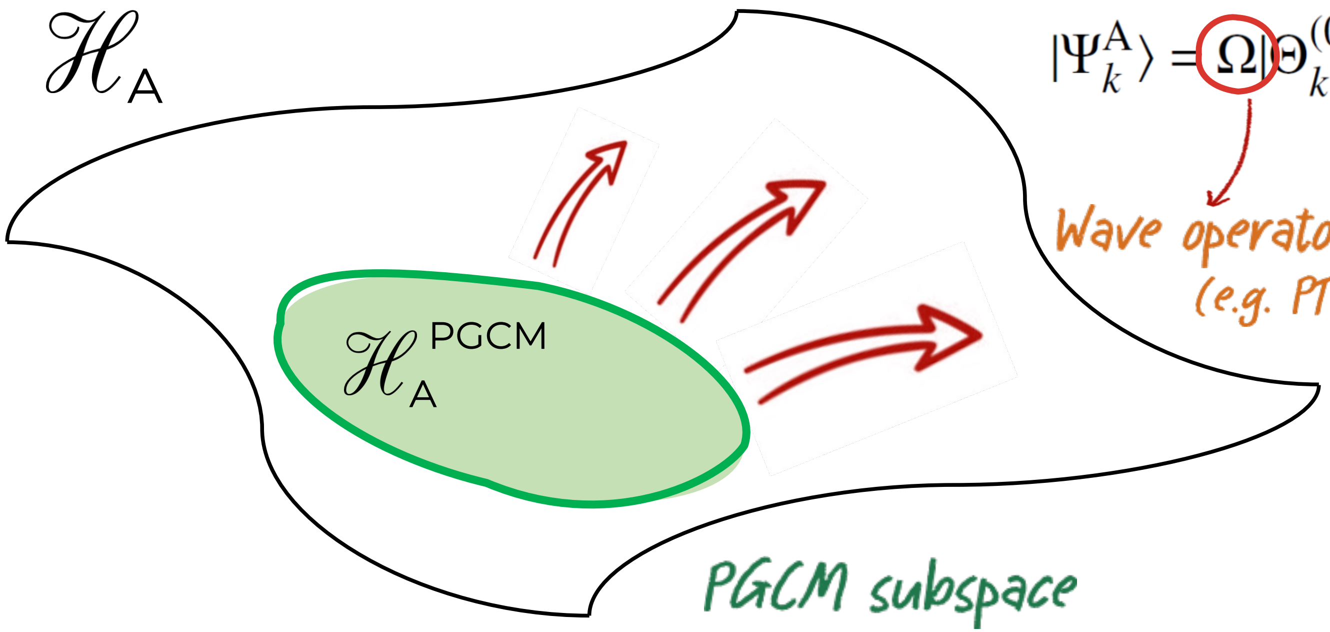

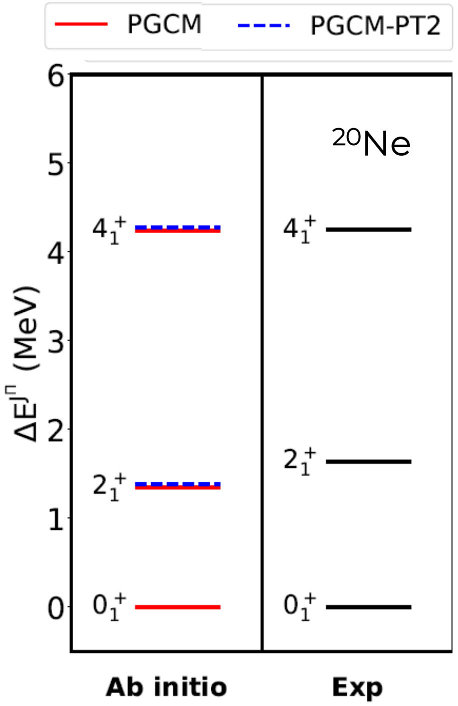

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Many-body truncation

Schrödinger equation $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$

Exact solution

Dynamical correlations mostly cancel out

PGCM reliable for low-lying collective spectroscopy

$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \ldots$$

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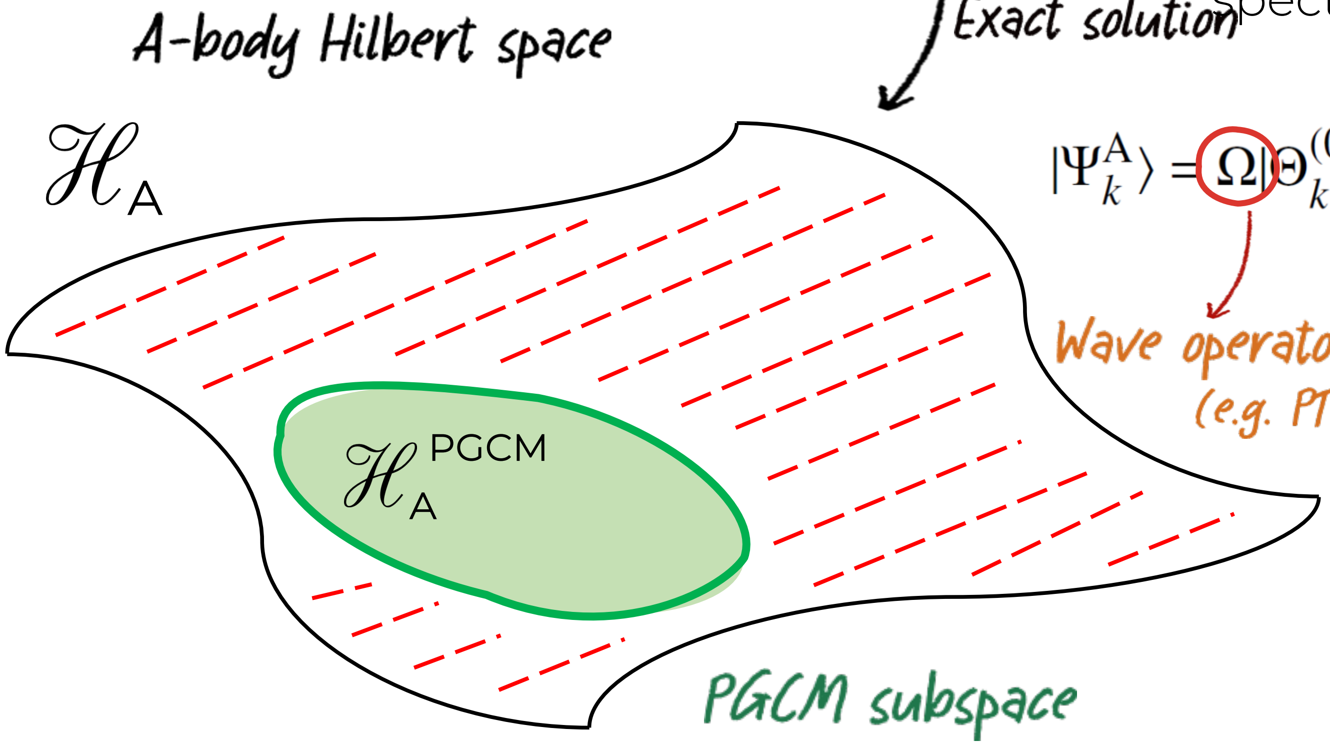
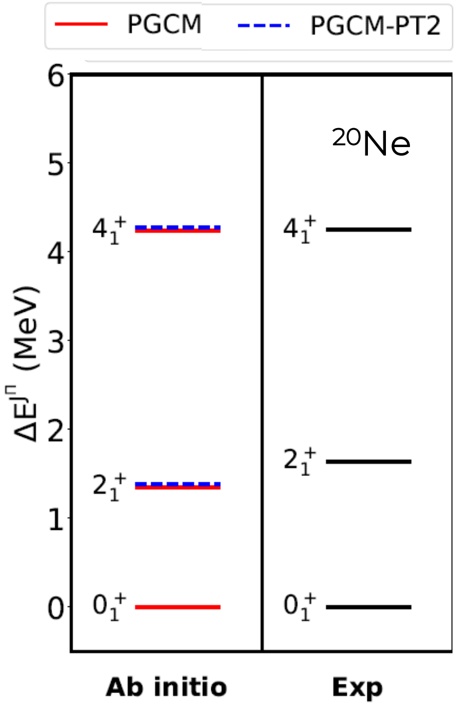


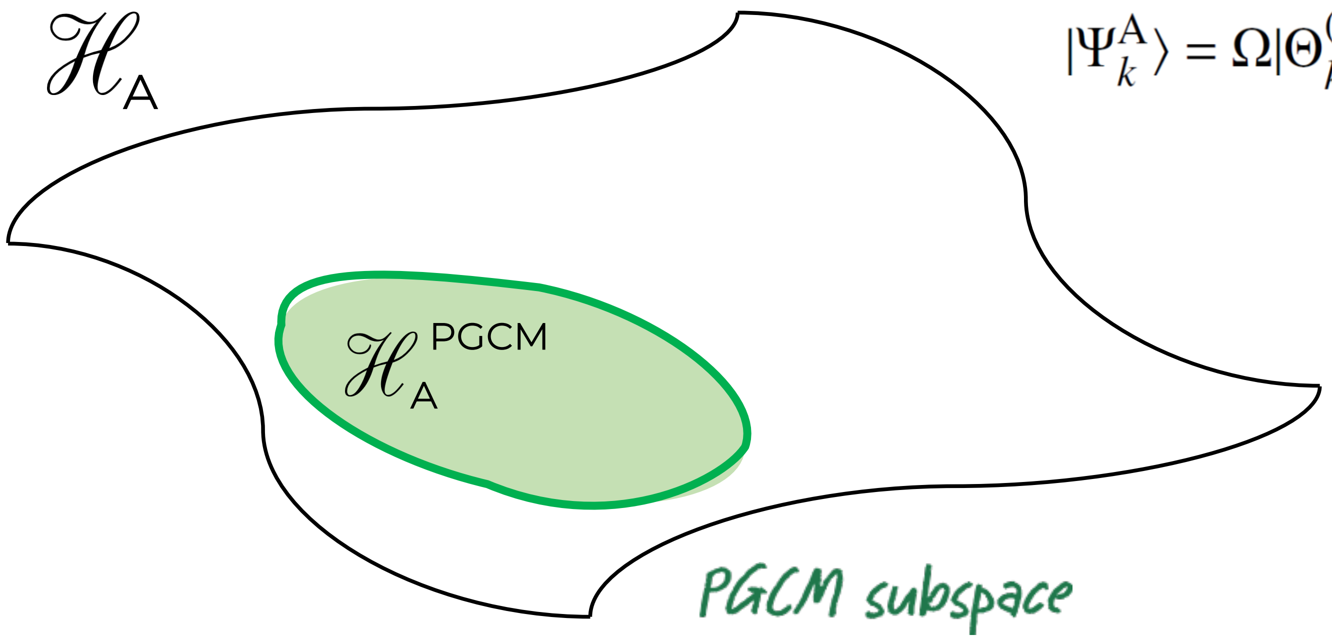


(1) [Frosini, Duguet, Ebran and Somà, EPJA 58(62), 2022]

(2) [Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao and Somà, EPJA 58(64), 2022]

SRG dependence

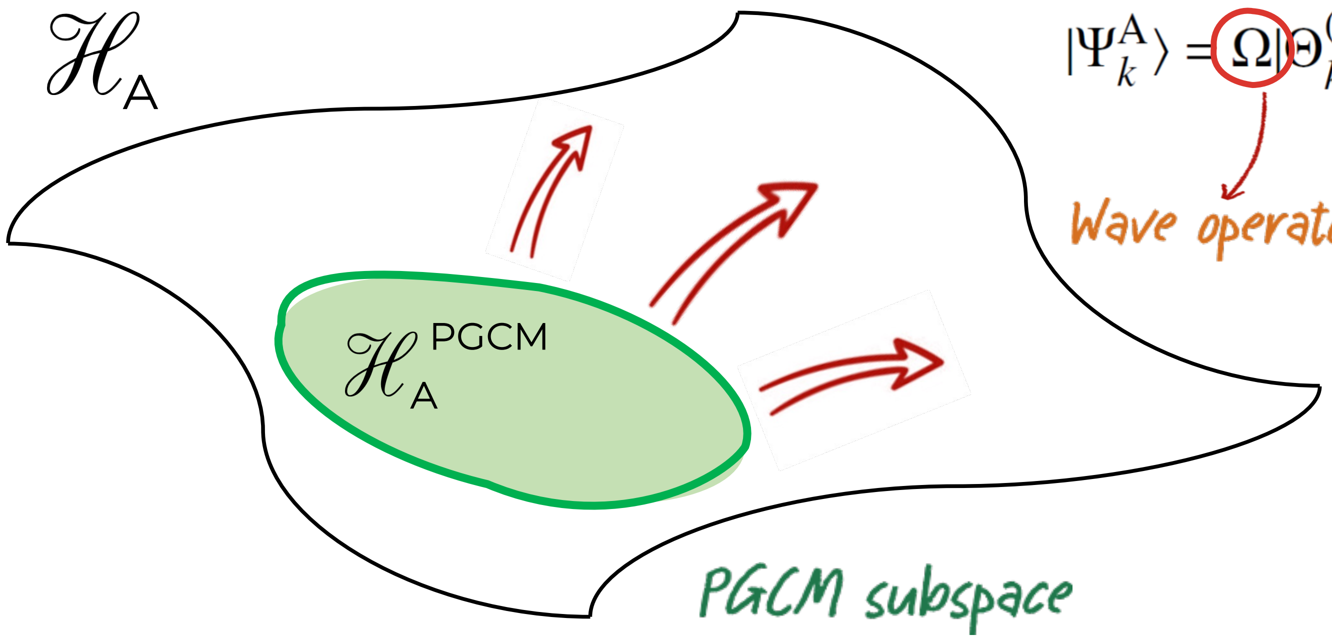
A-body Hilbert space



$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle$$

SRG dependence

A-body Hilbert space

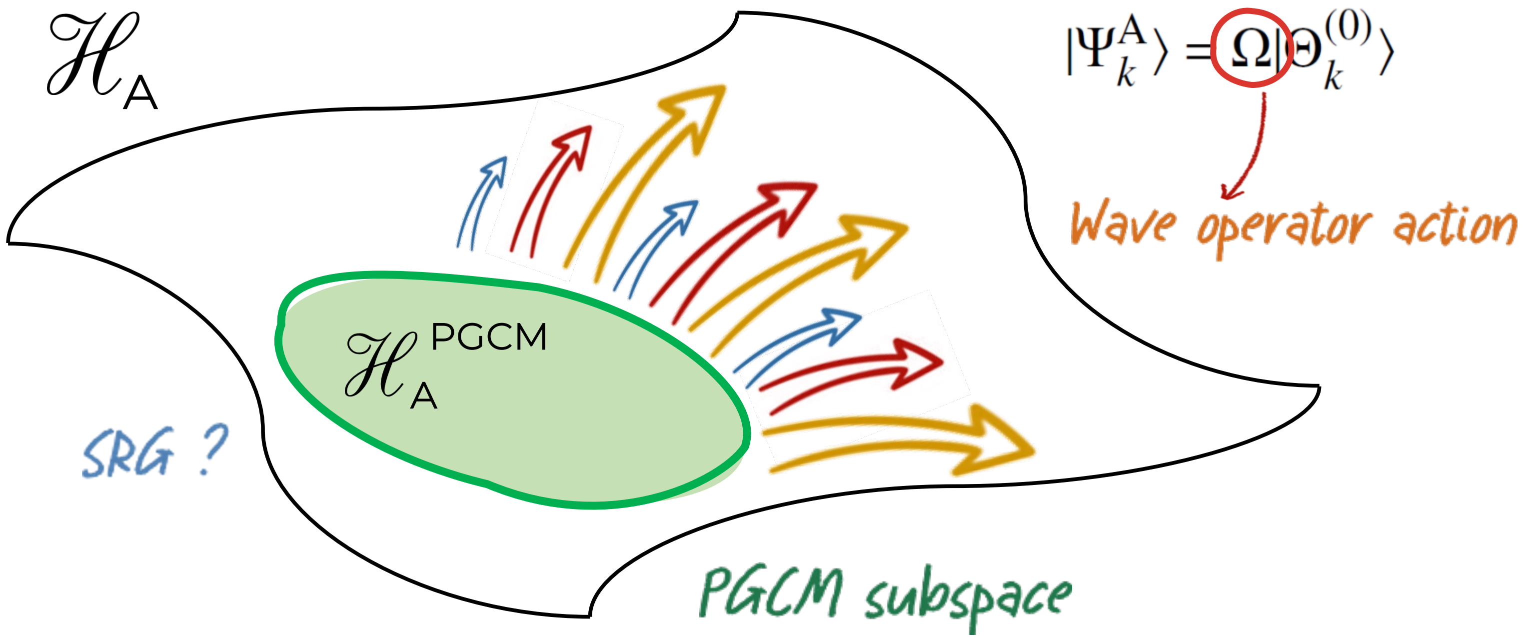


$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle$$

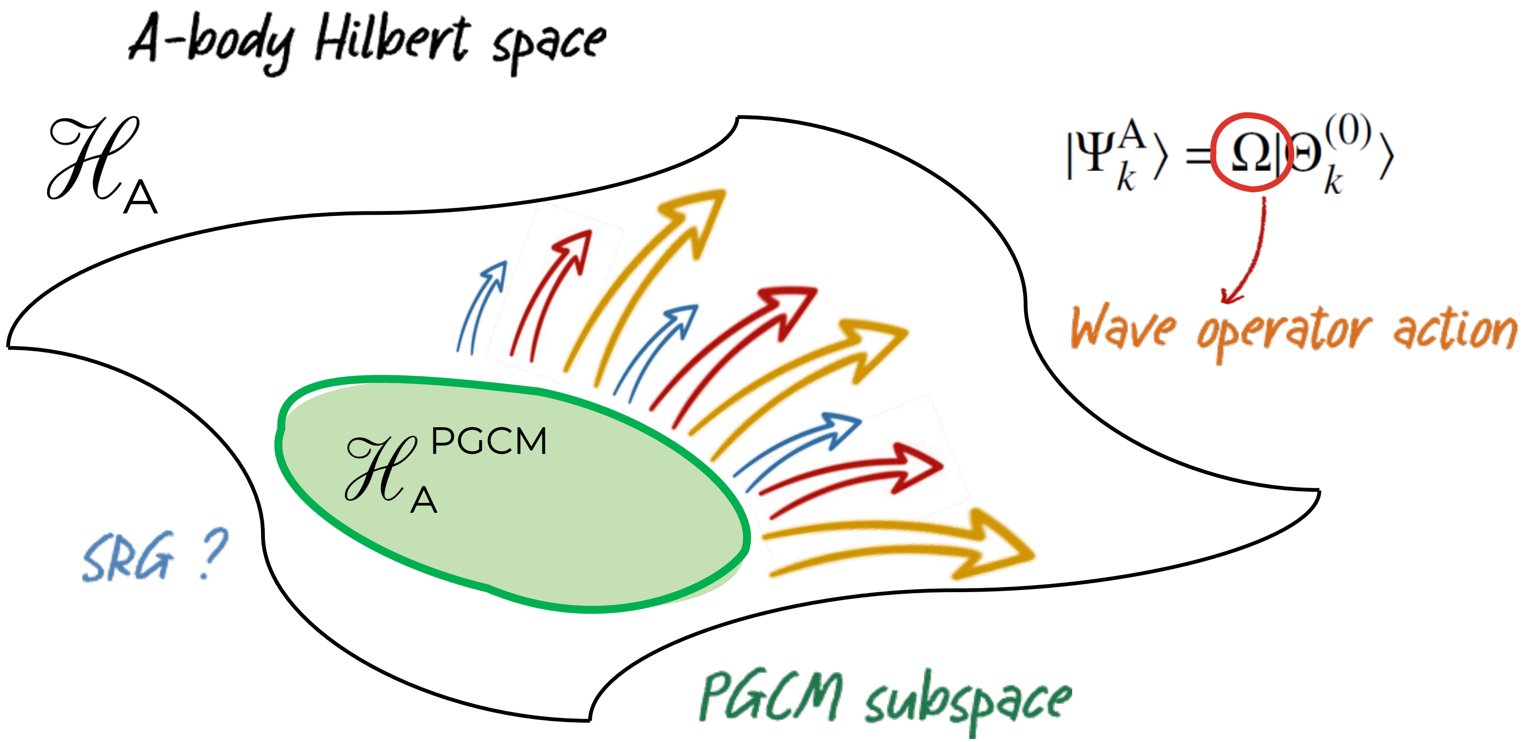
Wave operator action

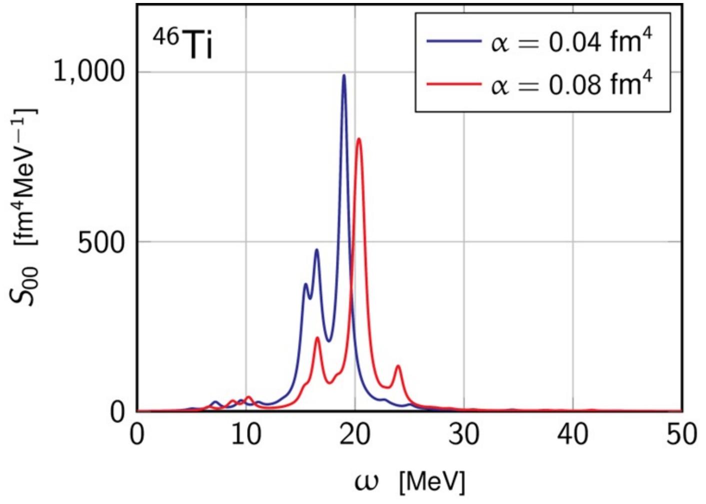
SRG dependence

A-body Hilbert space

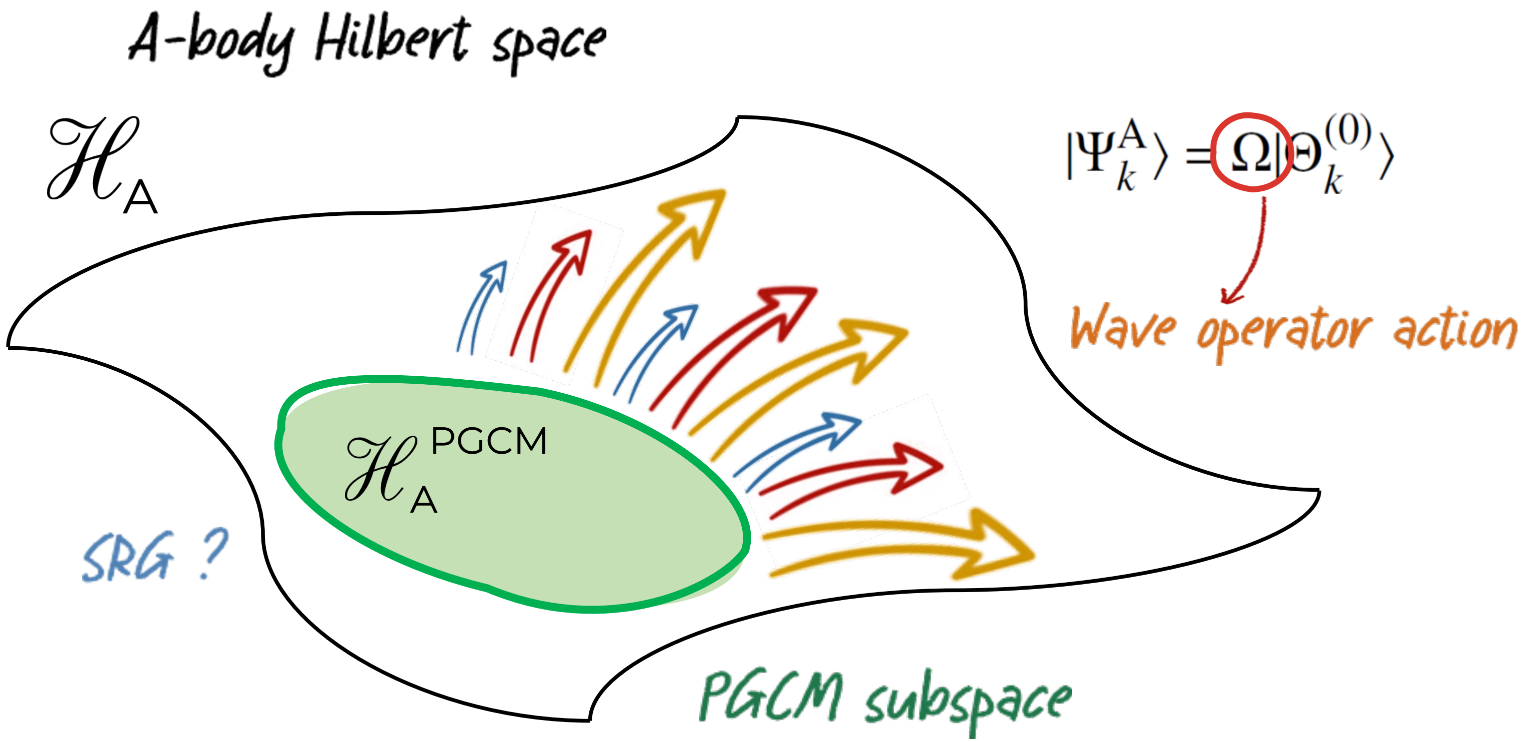


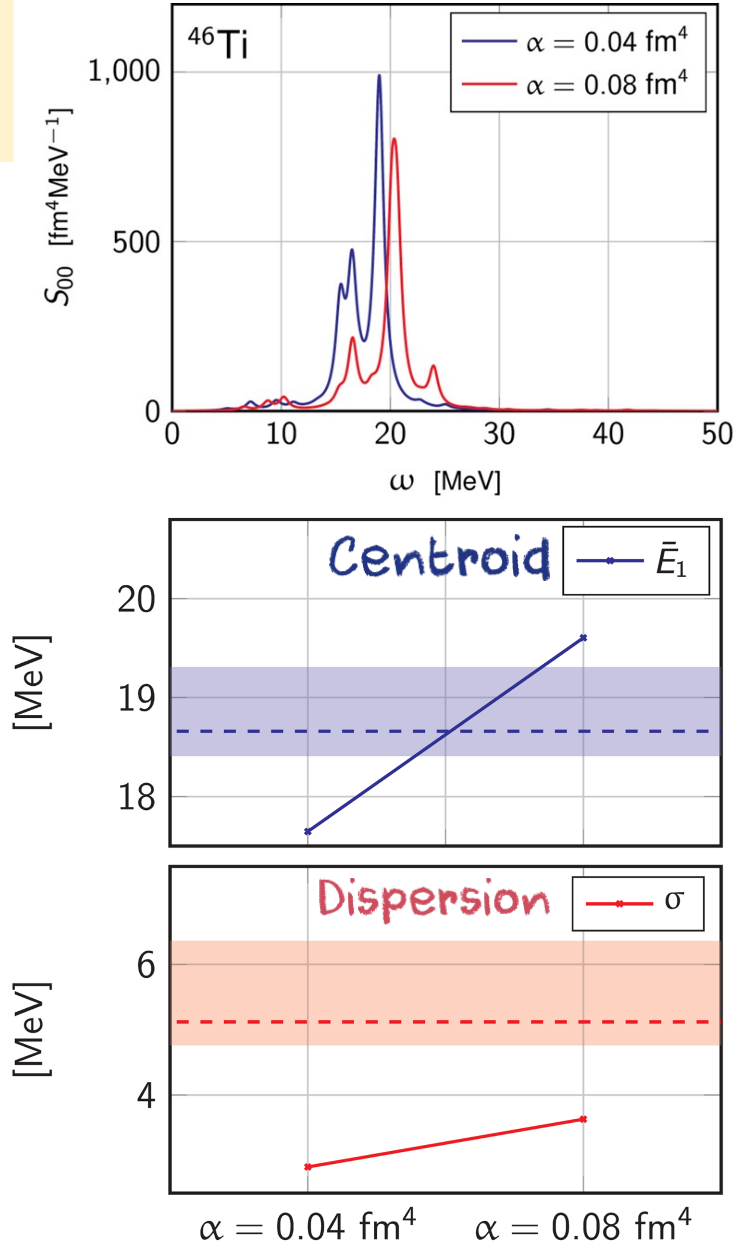
SRG dependence





SRG dependence

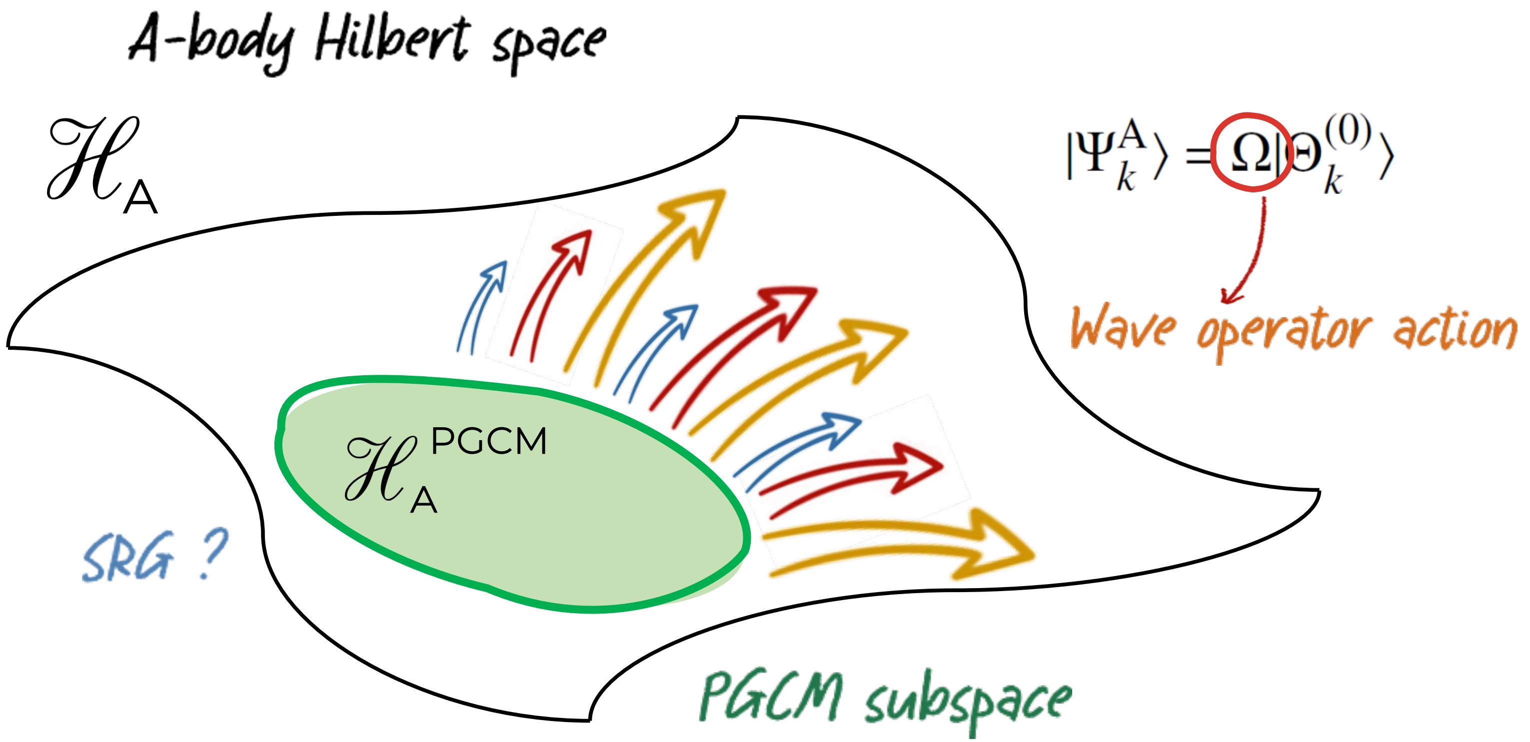




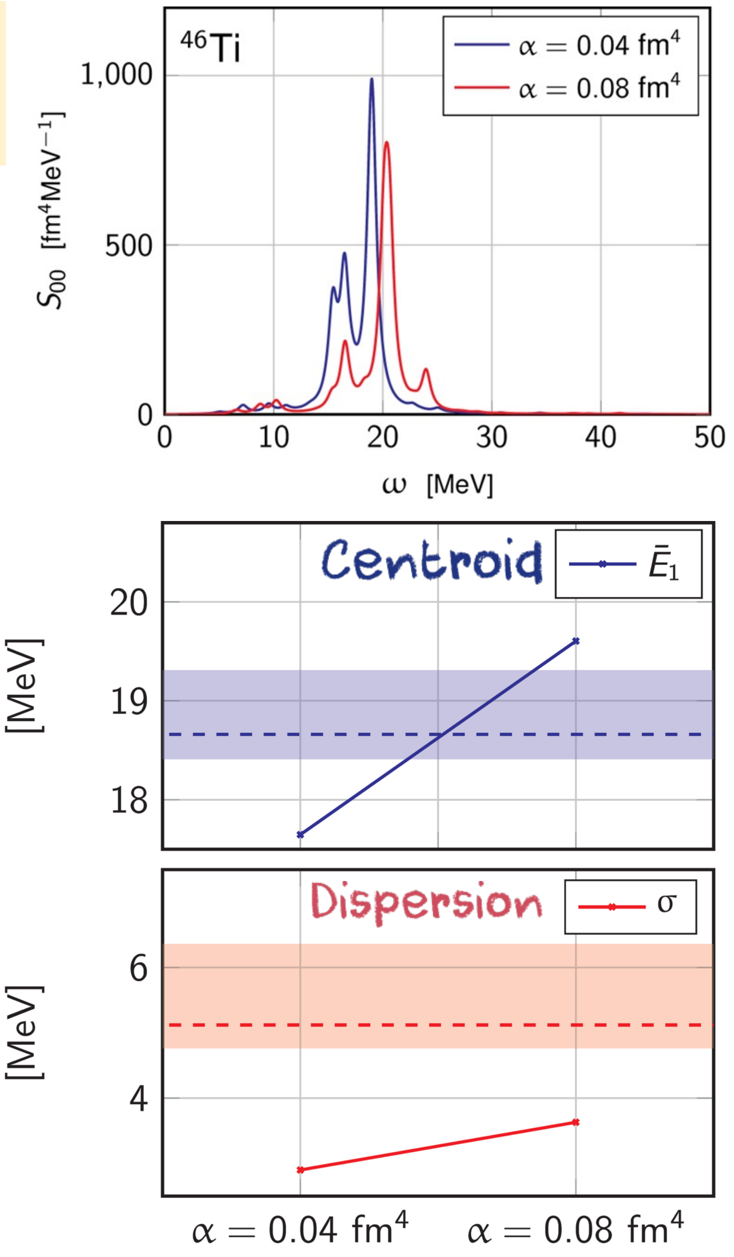
- Centroid variation ~ 10 %

~

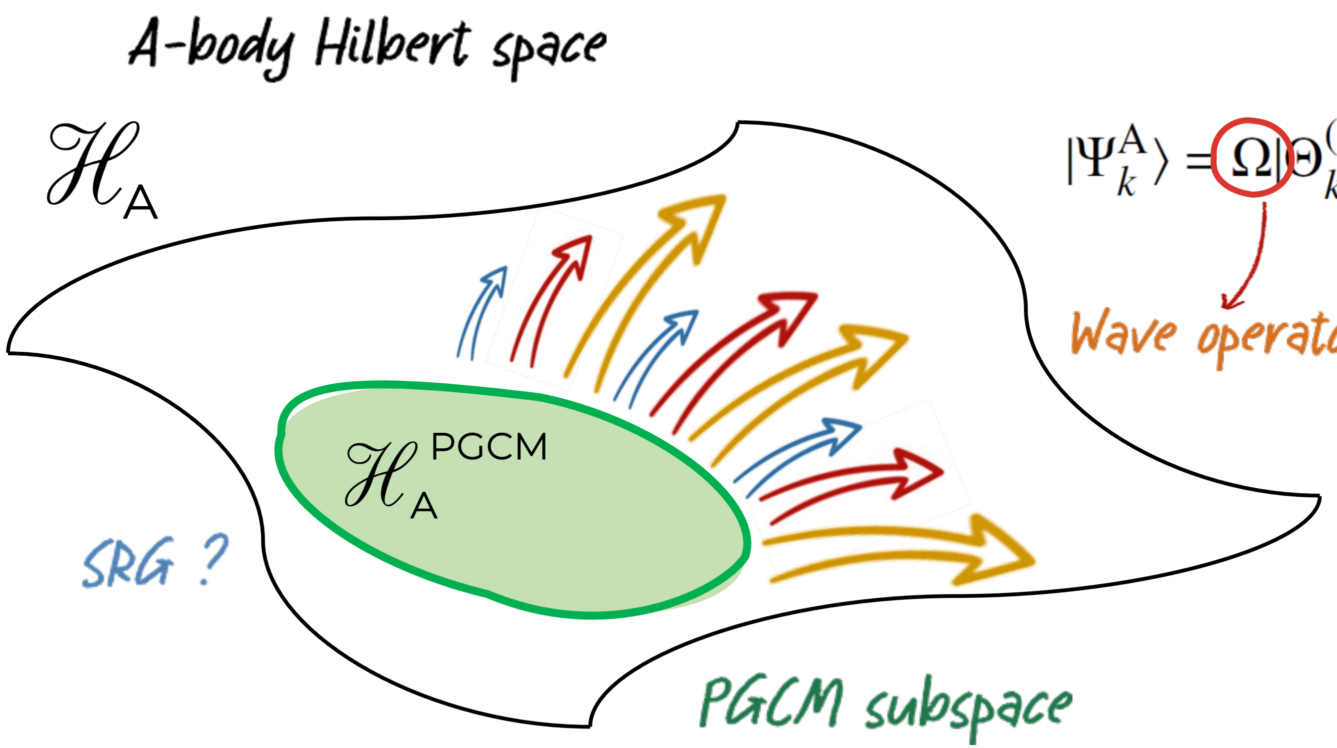
SRG dependence



- Centroid variation ~ 10 %
- Dispersion variation ~ 20 %

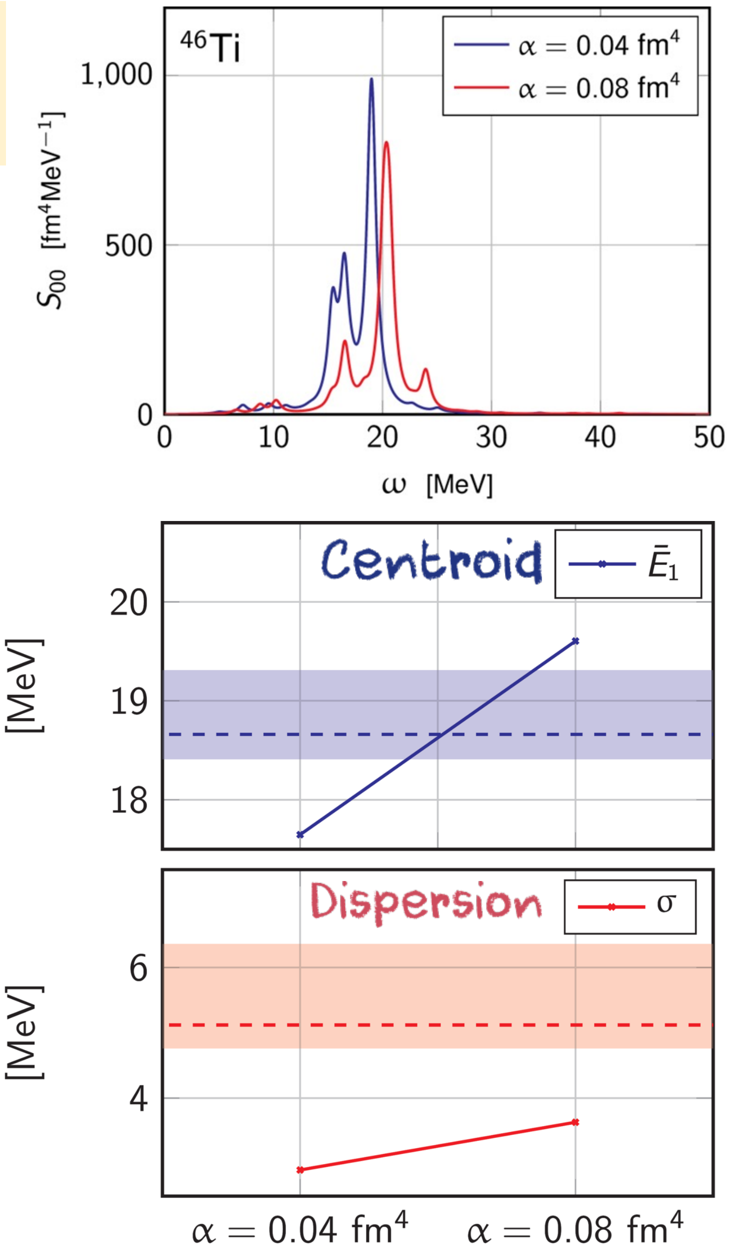


SRG dependence



$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle$$

Wave operator action

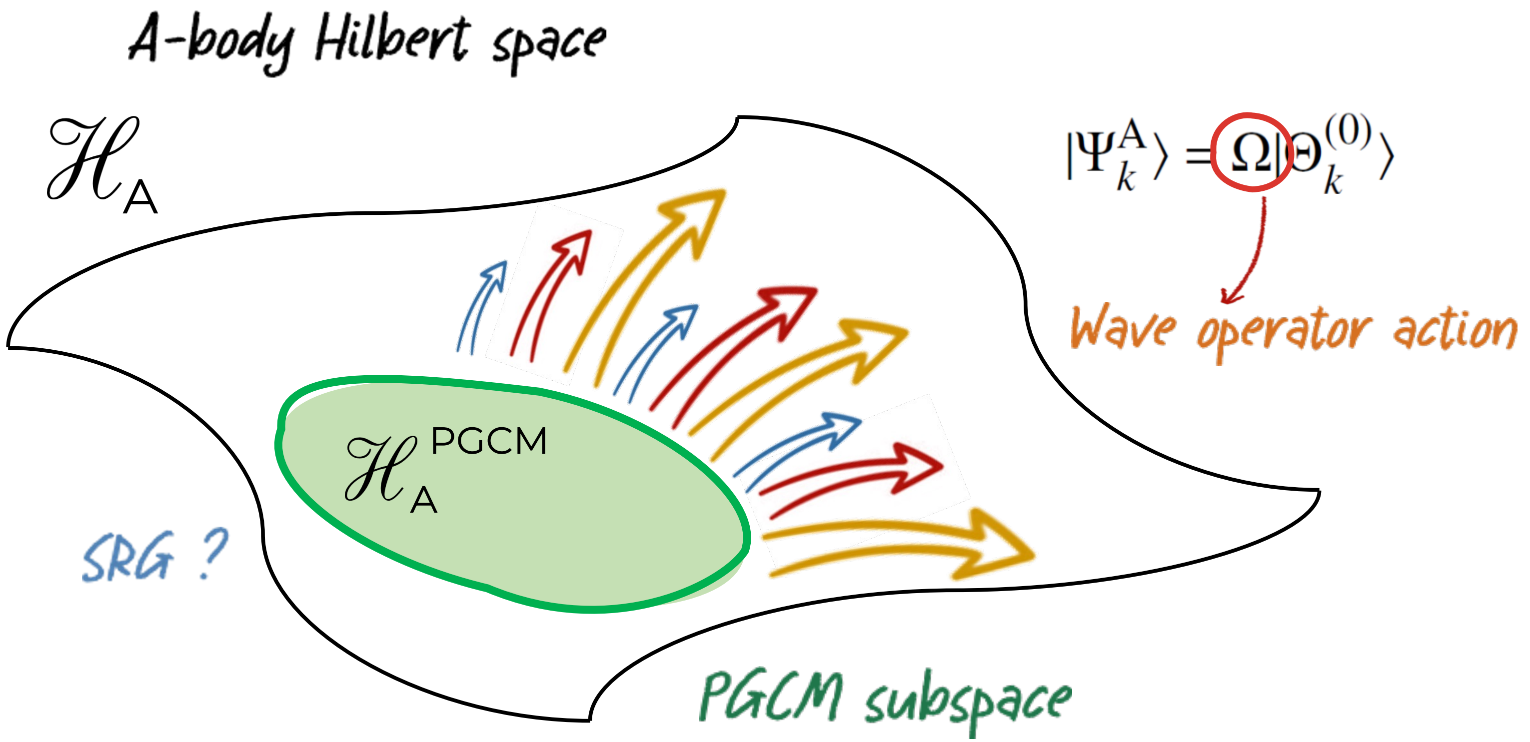


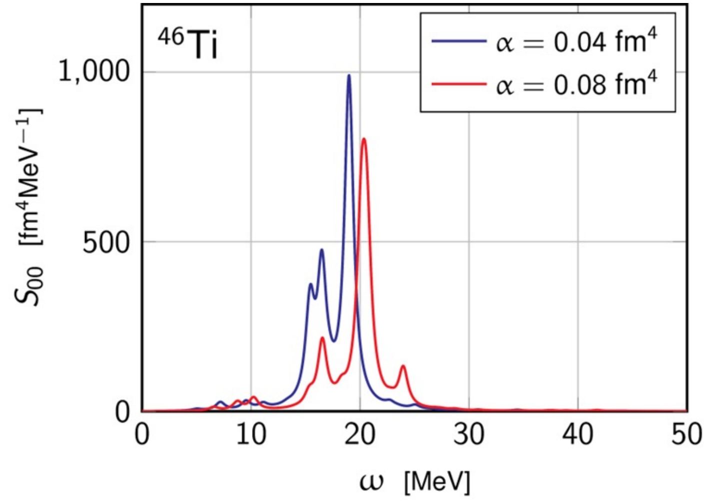
- Centroid variation ~ 10 %
- Dispersion variation ~ 20 %
- Consistent with ab initio RPA

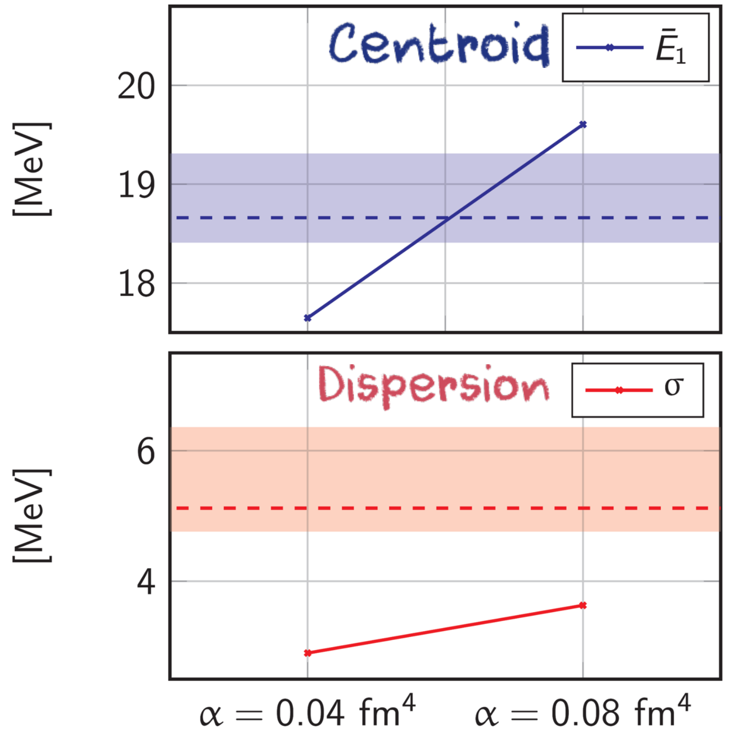
≈
≈

[Trippel, PhD Thesis, 2016]

SRG dependence





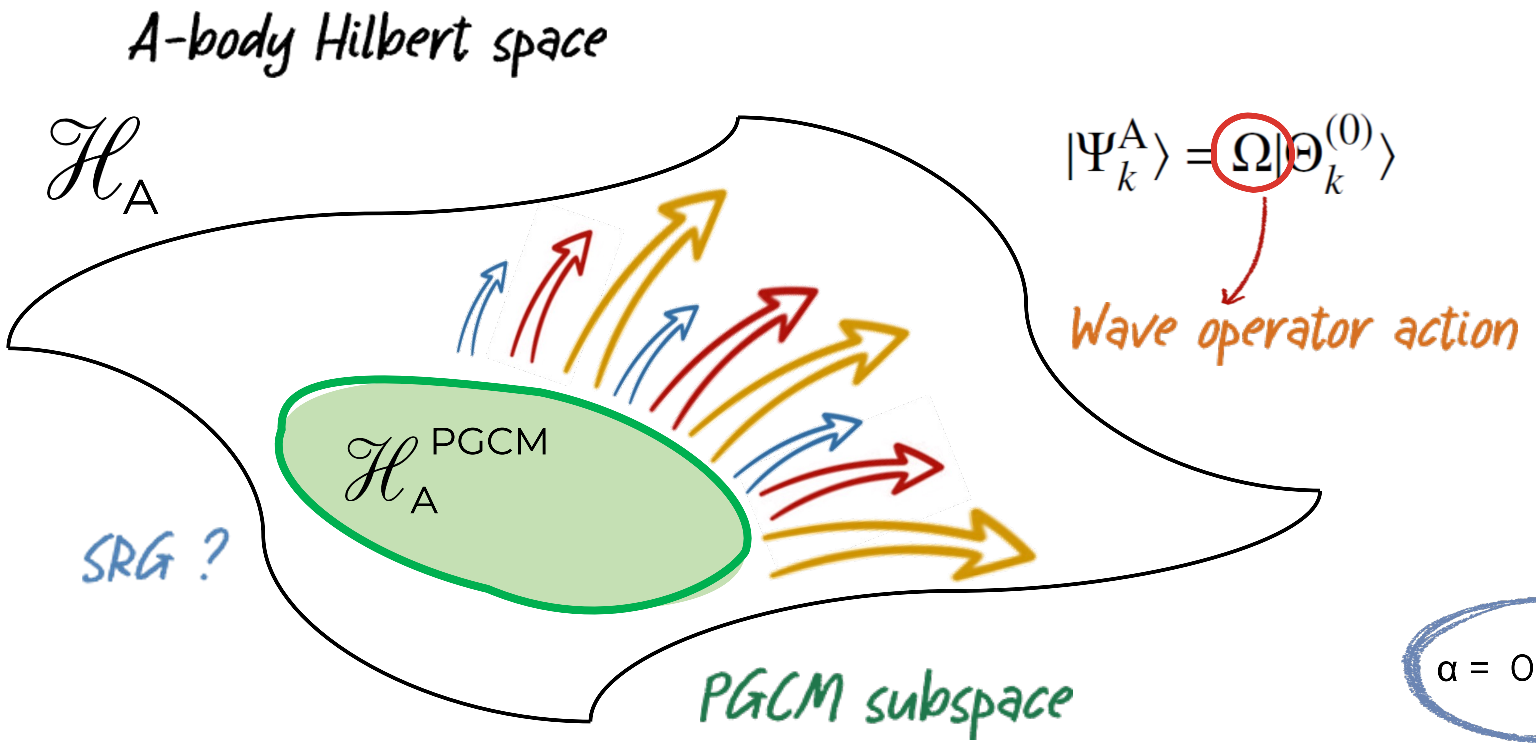


- Centroid variation ~ 10 %
- Dispersion variation ~ 20 %
- Consistent with ab initio RPA
- Entangles H and many-body truncations

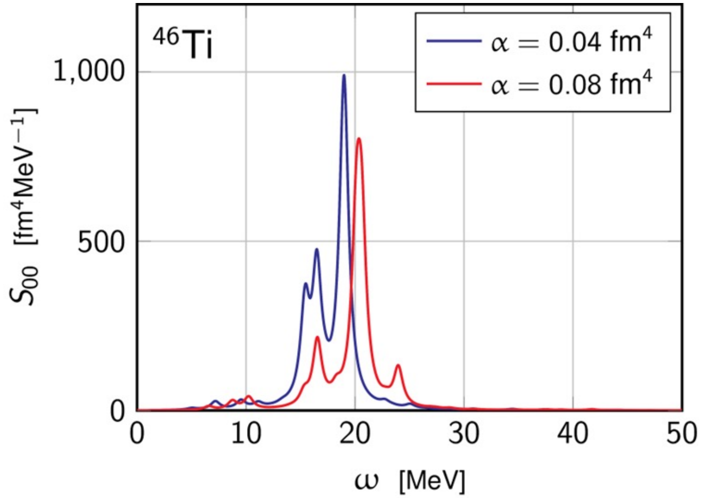
≈

[Trippel, PhD Thesis, 2016]

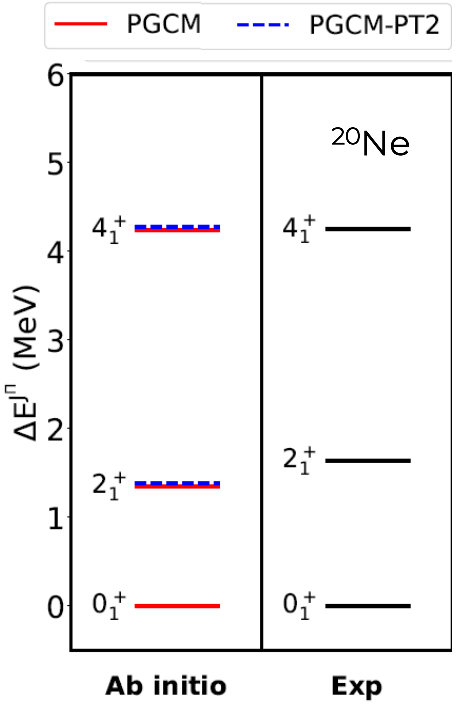
SRG dependence



α = 0,08 fm⁴



[Trippel, PhD Thesis, 2016]

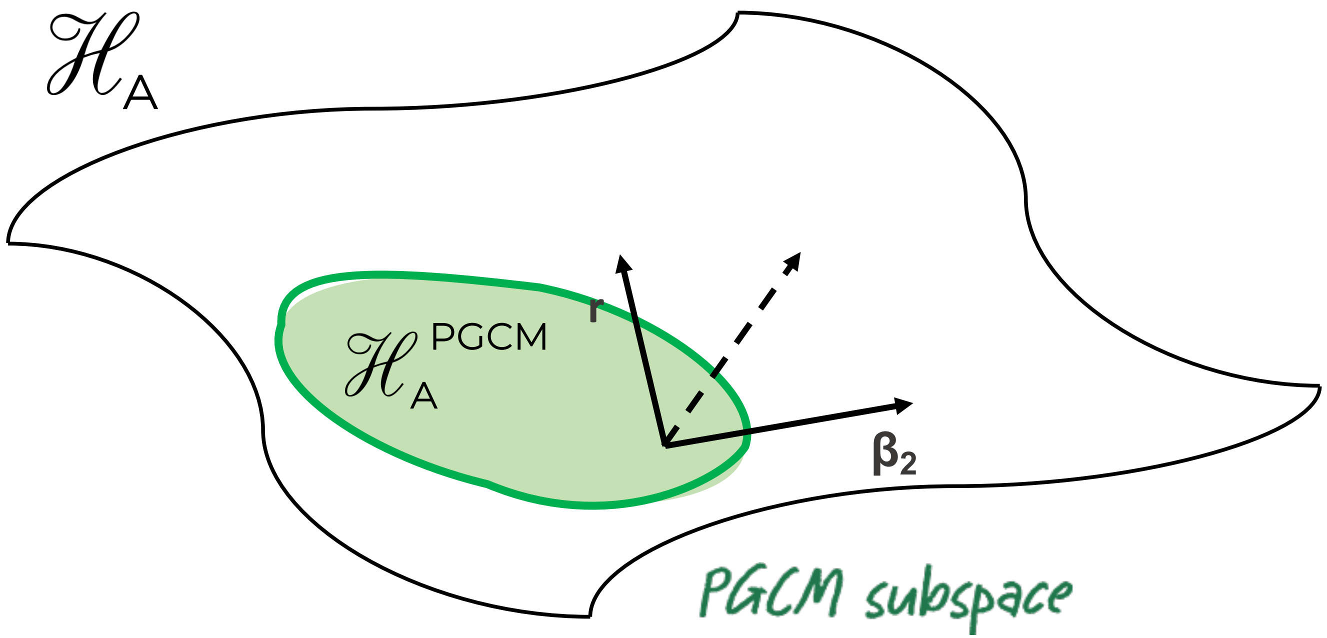


- Centroid variation ~ 10 %
- Dispersion variation ~ 20 %
- Consistent with ab initio RPA
- Entangles H and many-body truncations
- Comparison to PGCM-PT needed (S. Bofos PhD)

[Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao and Somà, EPJA 58(64), 2022]

Generator coordinates choice

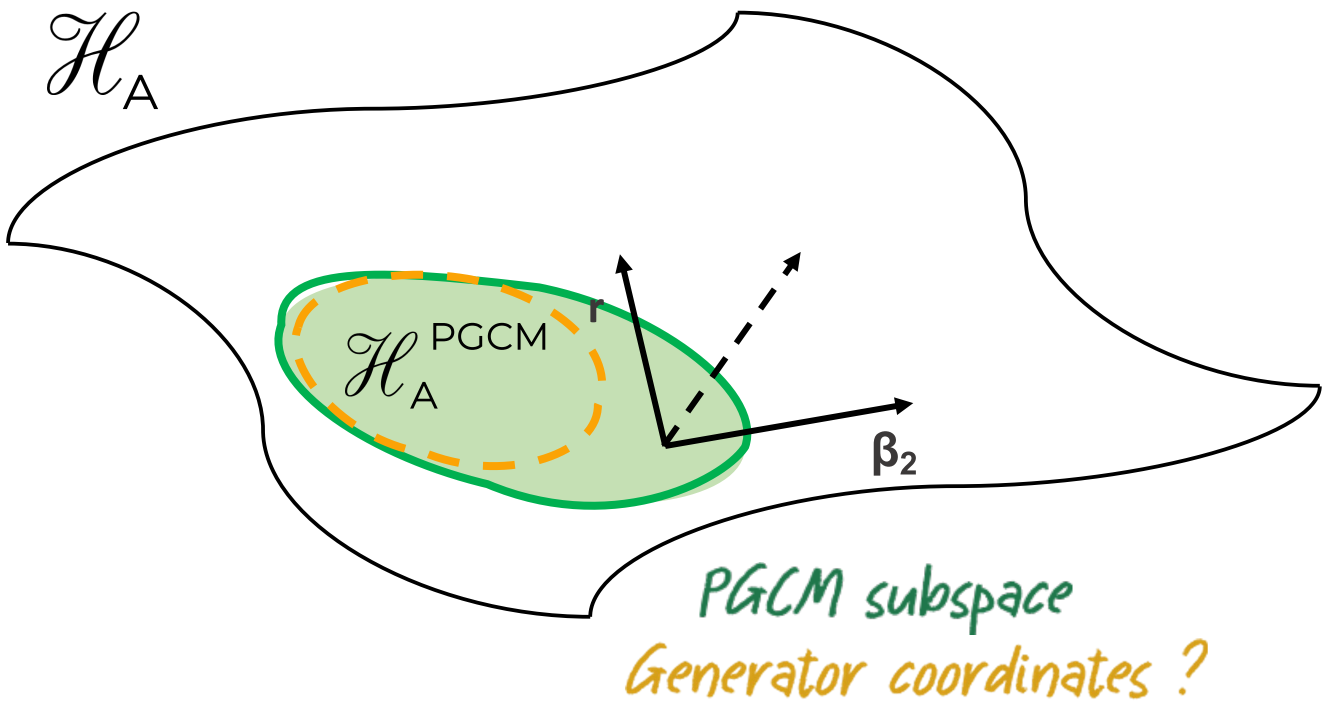
A-body Hilbert space



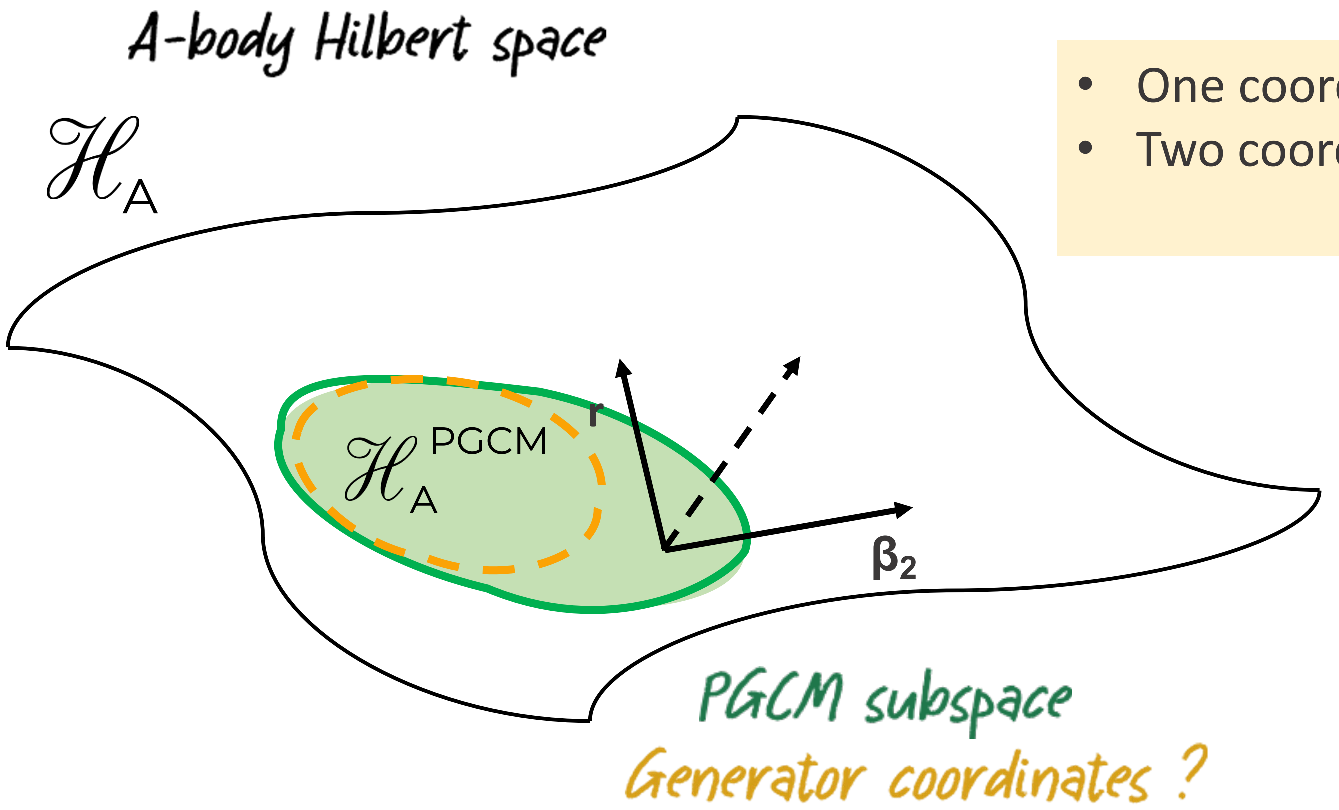
PGCM subspace

Generator coordinates choice

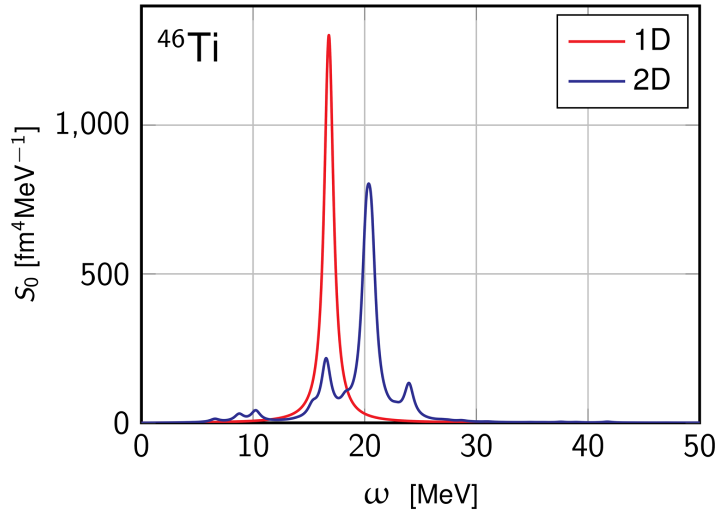
A-body Hilbert space



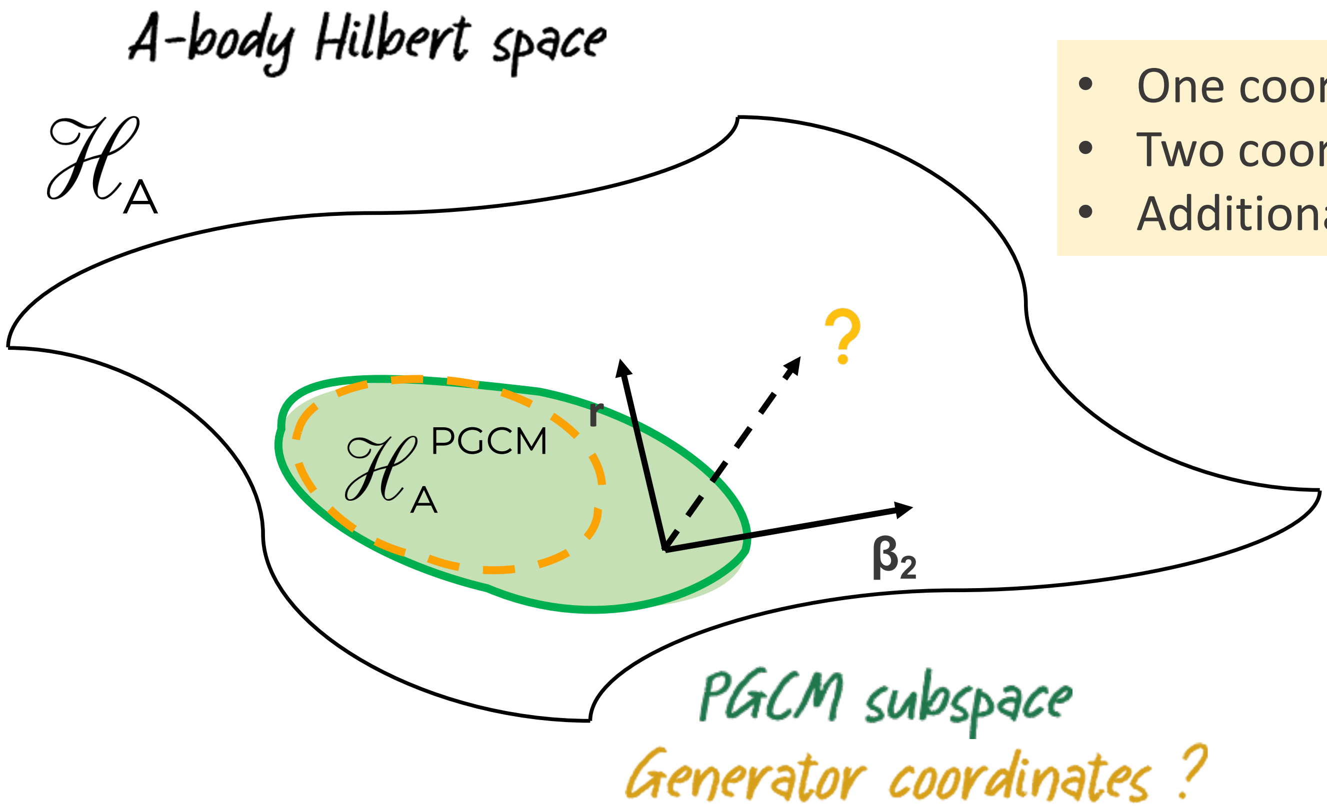
Generator coordinates choice



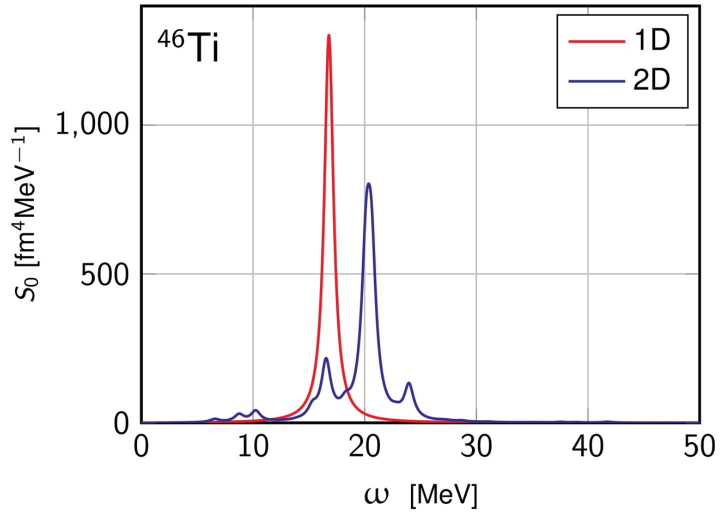
- One coordinate insufficient (deformed systems)
- Two coordinates necessary: empirical knowledge **r** and $\boldsymbol{\beta_2}$



Generator coordinates choice

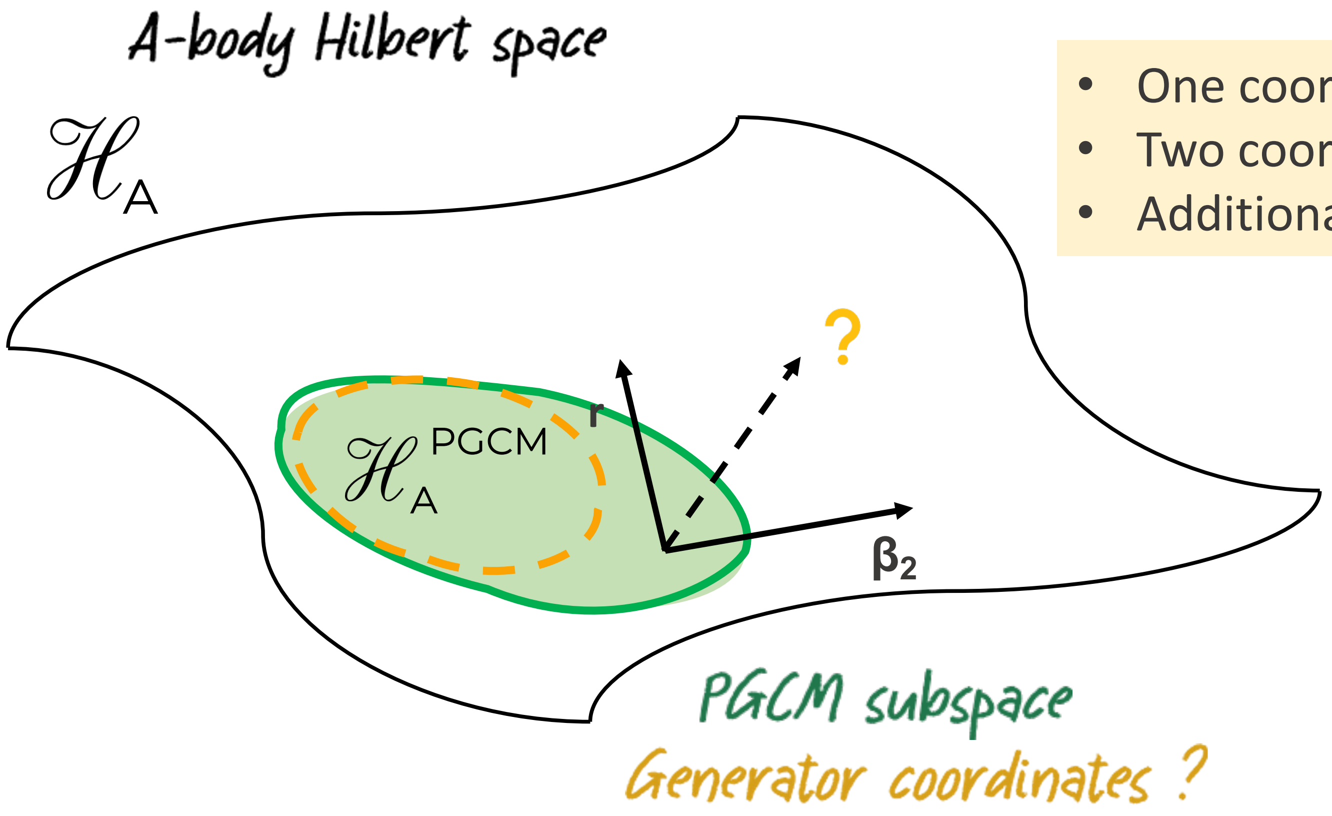


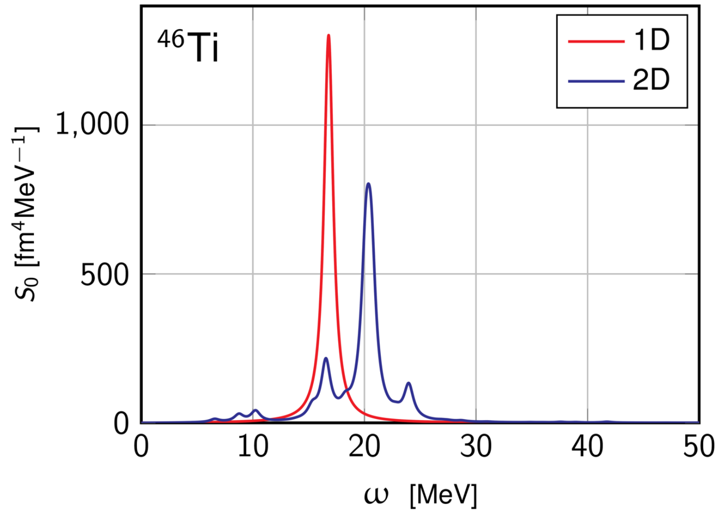
- One coordinate insufficient (deformed systems)
- Two coordinates necessary: empirical knowledge **r** and $\boldsymbol{\beta_2}$
- Additional coordinates ?



Generator coordinates choice

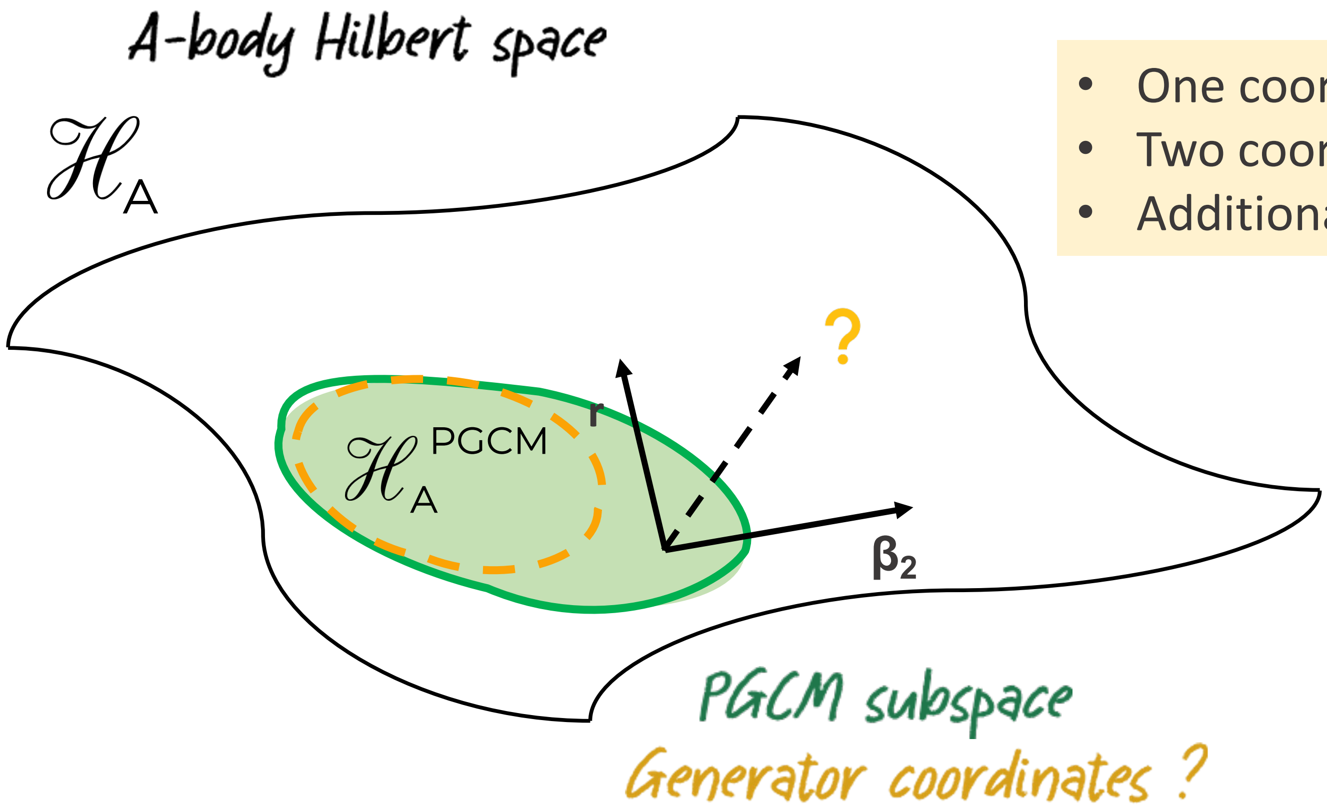
- One coordinate insufficient (deformed systems)
- Two coordinates necessary: empirical knowledge **r** and $\boldsymbol{\beta_2}$
- Additional coordinates ?



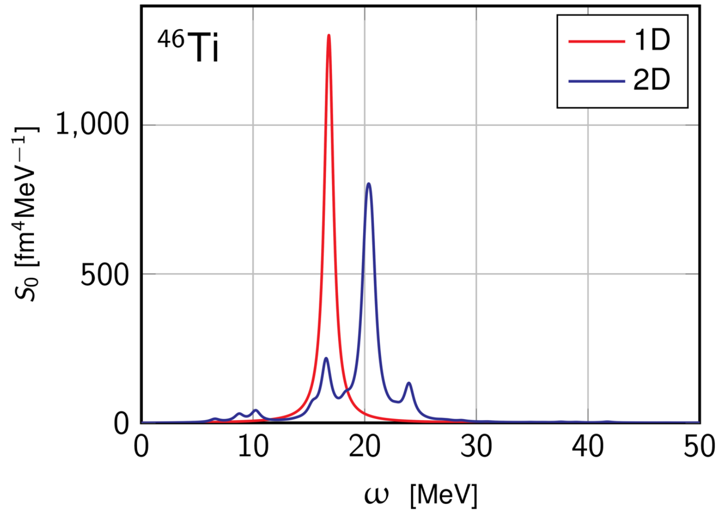


PGCM alone suited for ab initio ?

Generator coordinates choice



- One coordinate insufficient (deformed systems)
- Two coordinates necessary: empirical knowledge **r** and $\boldsymbol{\beta_2}$
- Additional coordinates ?



PGCM alone suited for ab initio ?

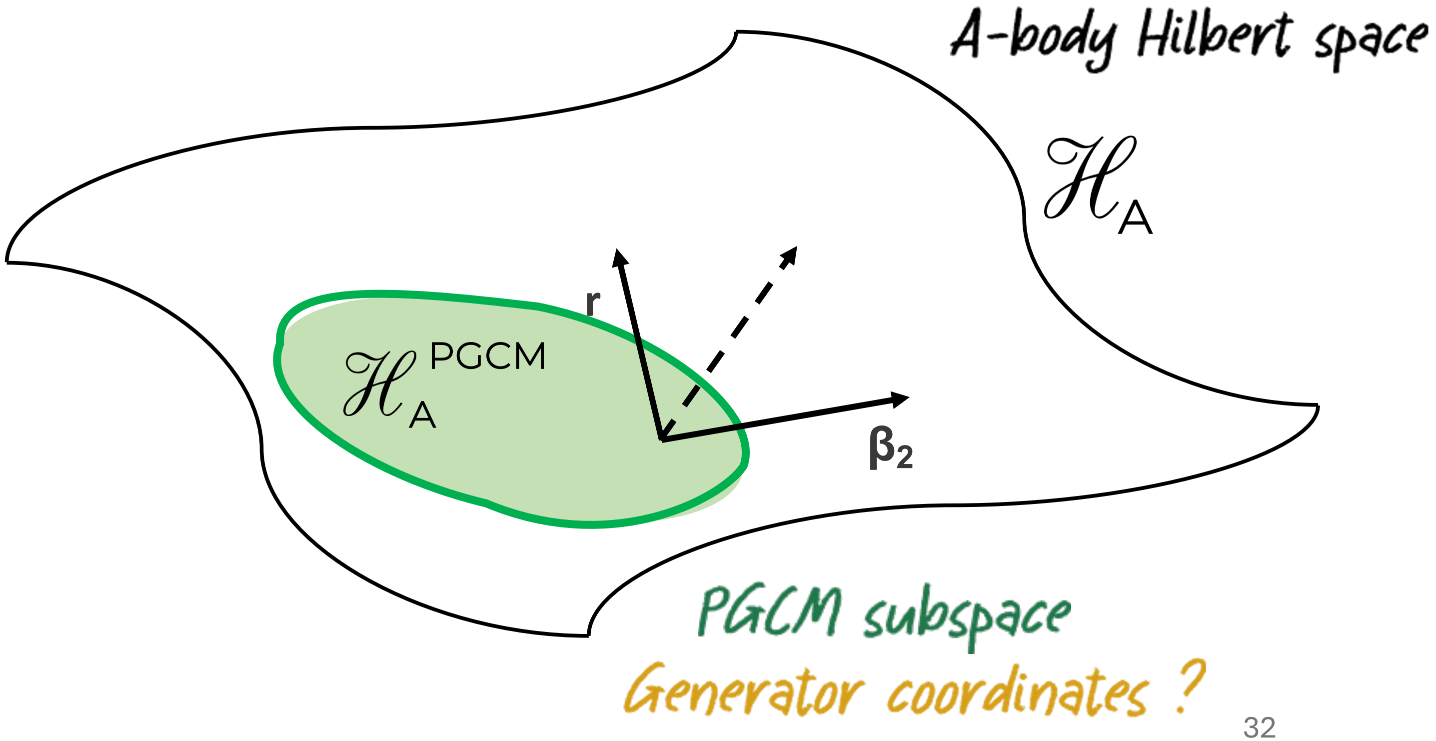
[S. Bofos, ongoing] Systematic **VS-PGCM** study

Many possible directions

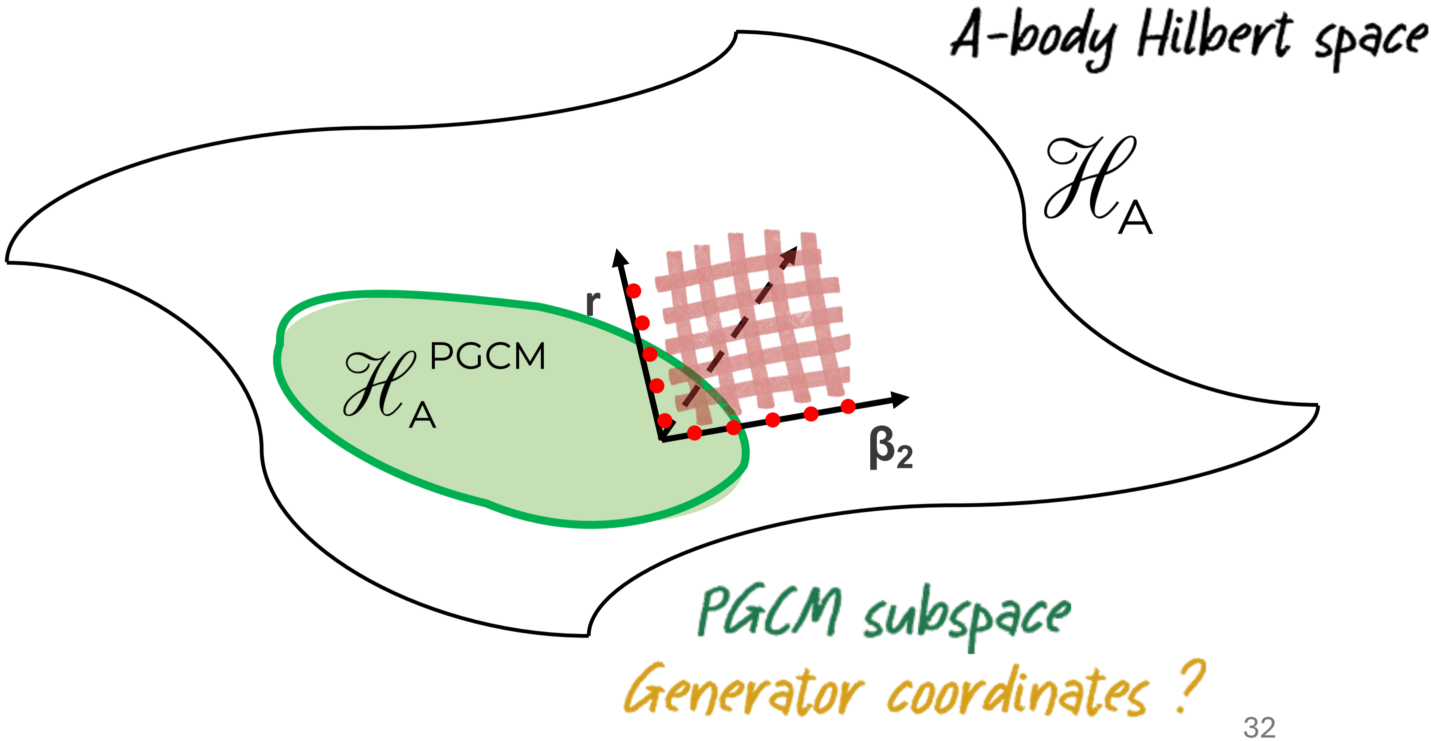
MCSM-like calculations (greedy algorithm)

Momentum-like coordinates (**DGCM**)

HFB vacua selection

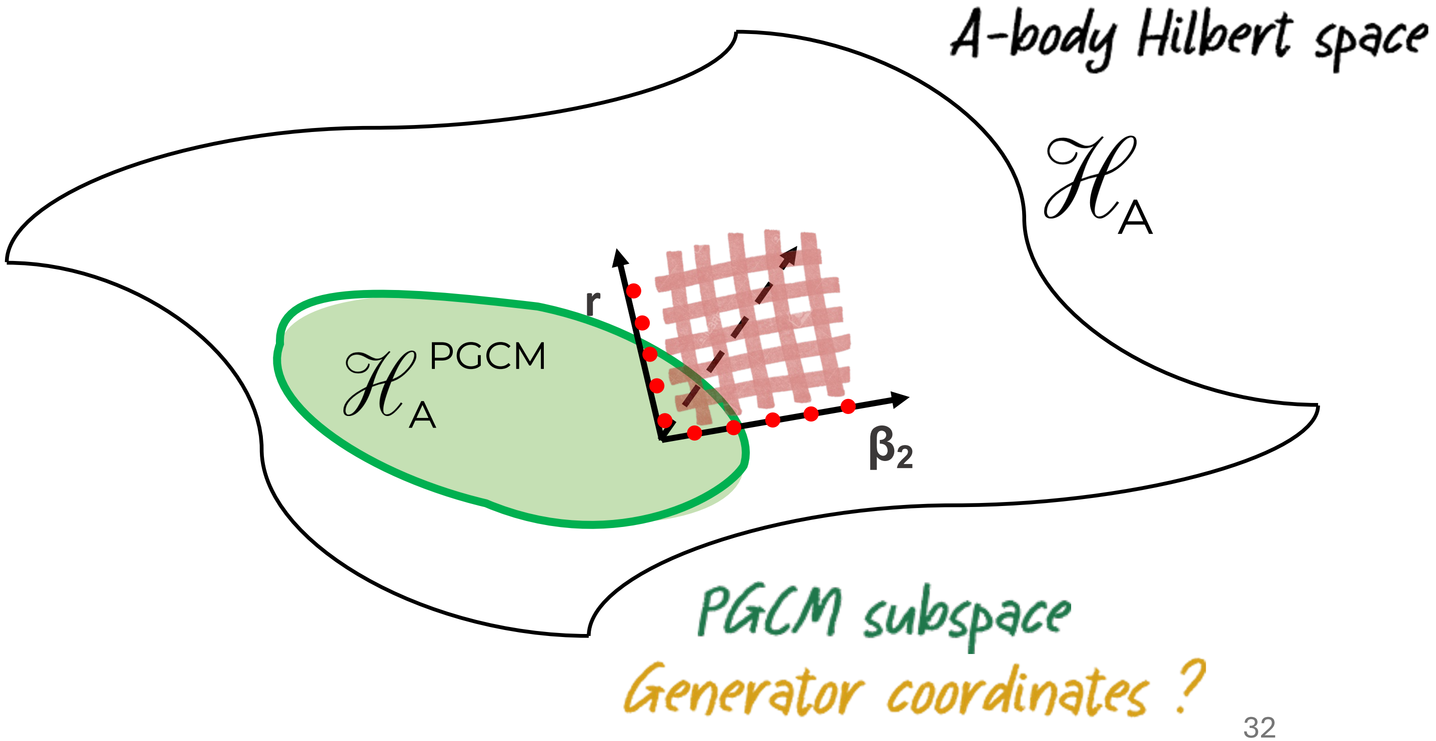


HFB vacua selection



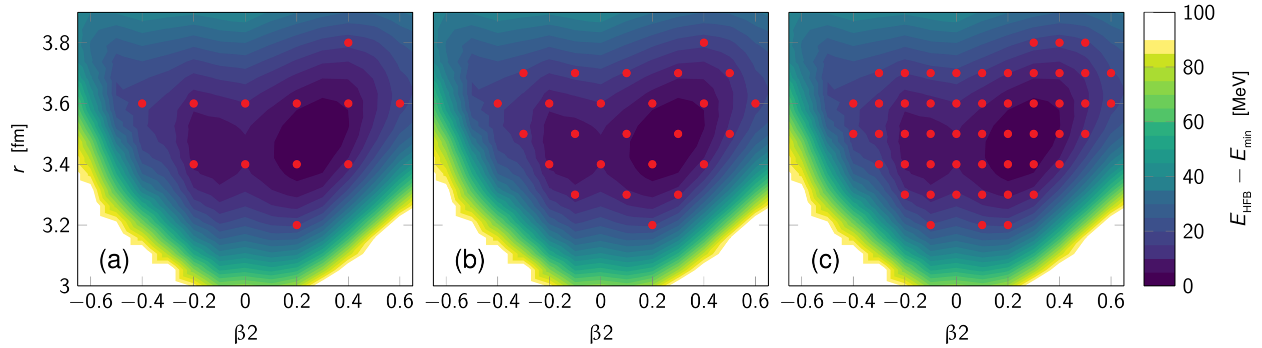
HFB vacua selection

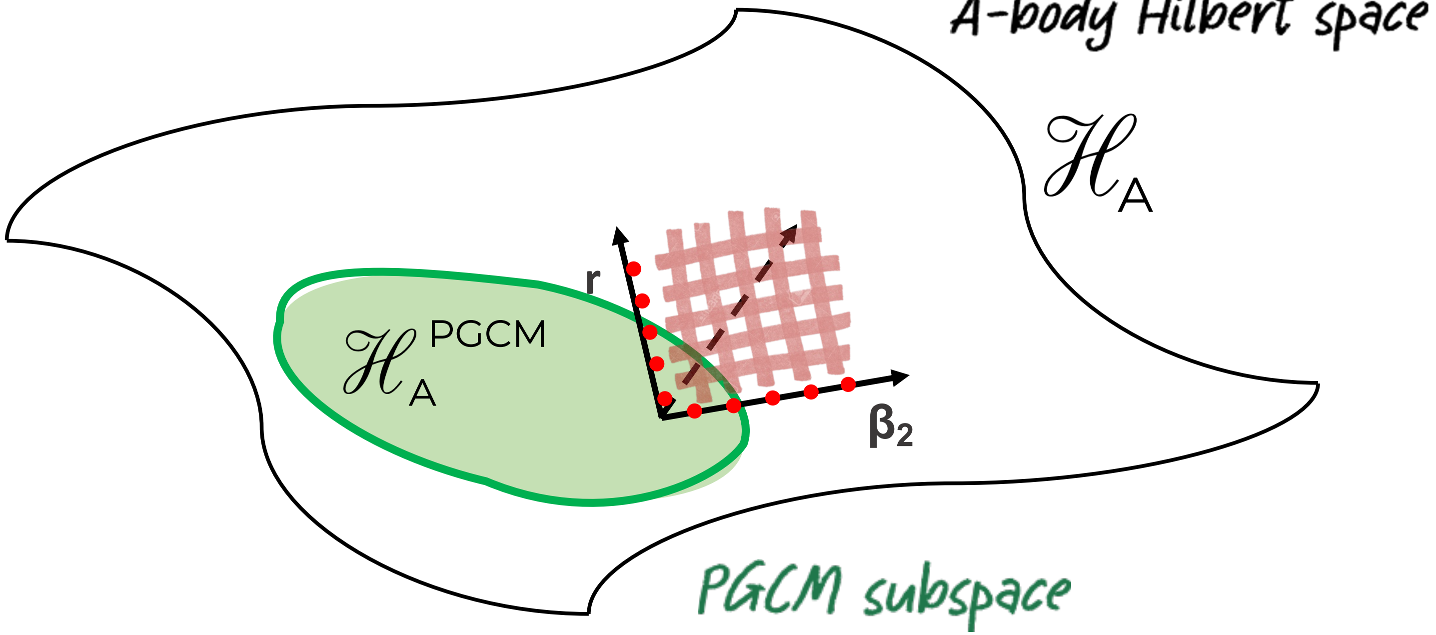
Must exhaust the PGCM subspace



HFB vacua selection

Mesh refinement

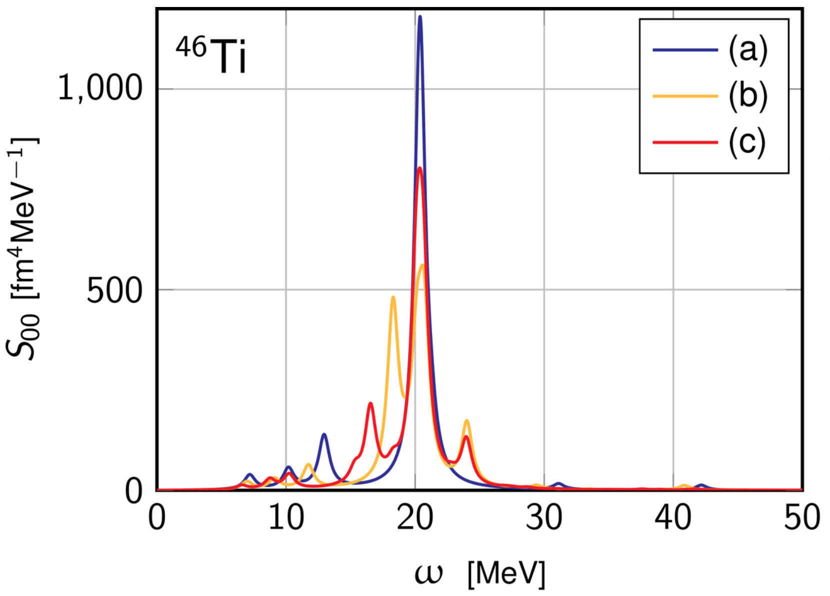


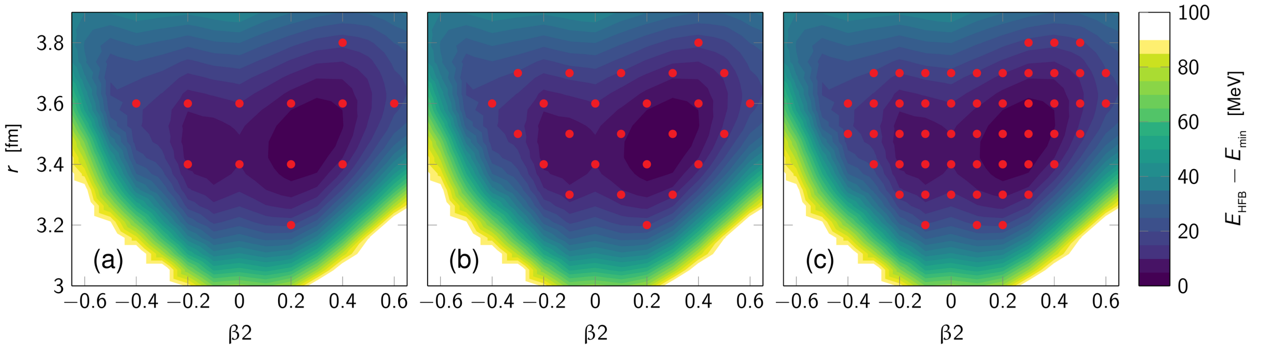


Generator coordinates ?

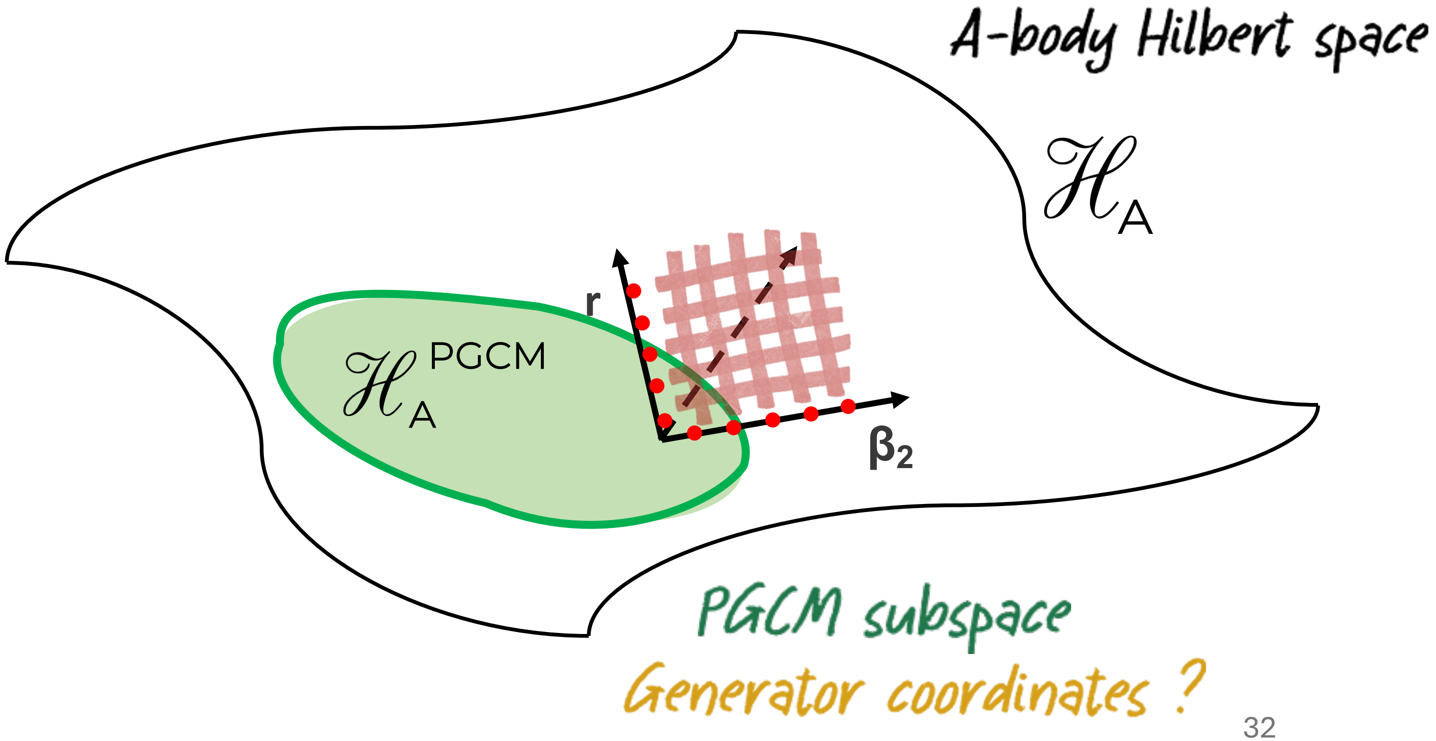
HFB vacua selection

Mesh refinement



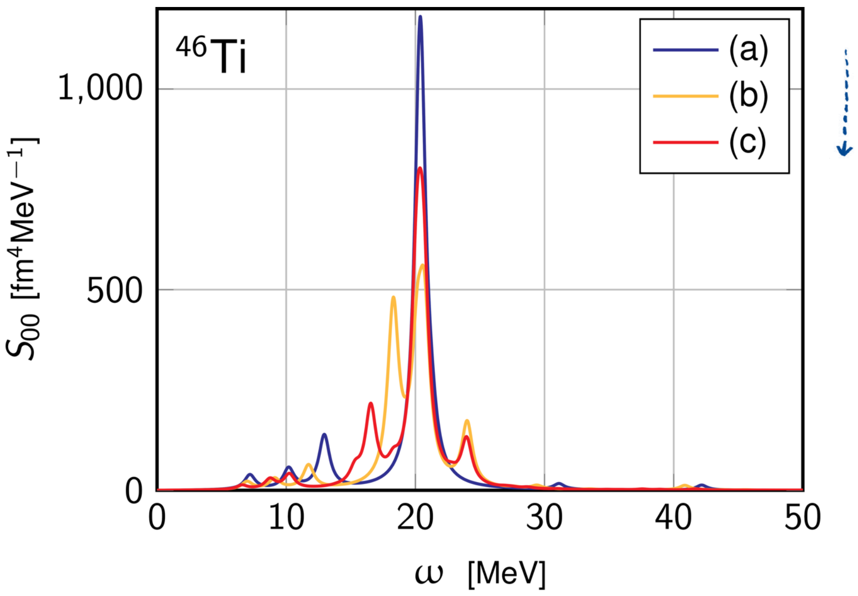


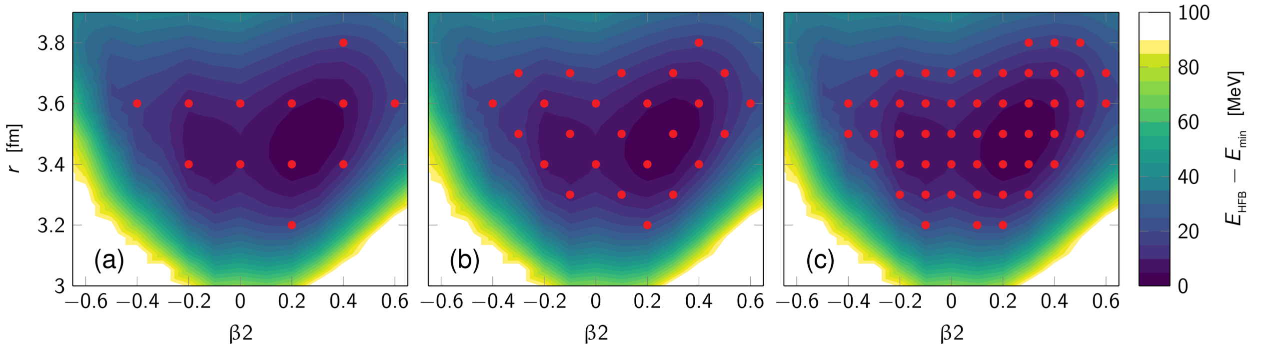
- Qualitative convergence ~



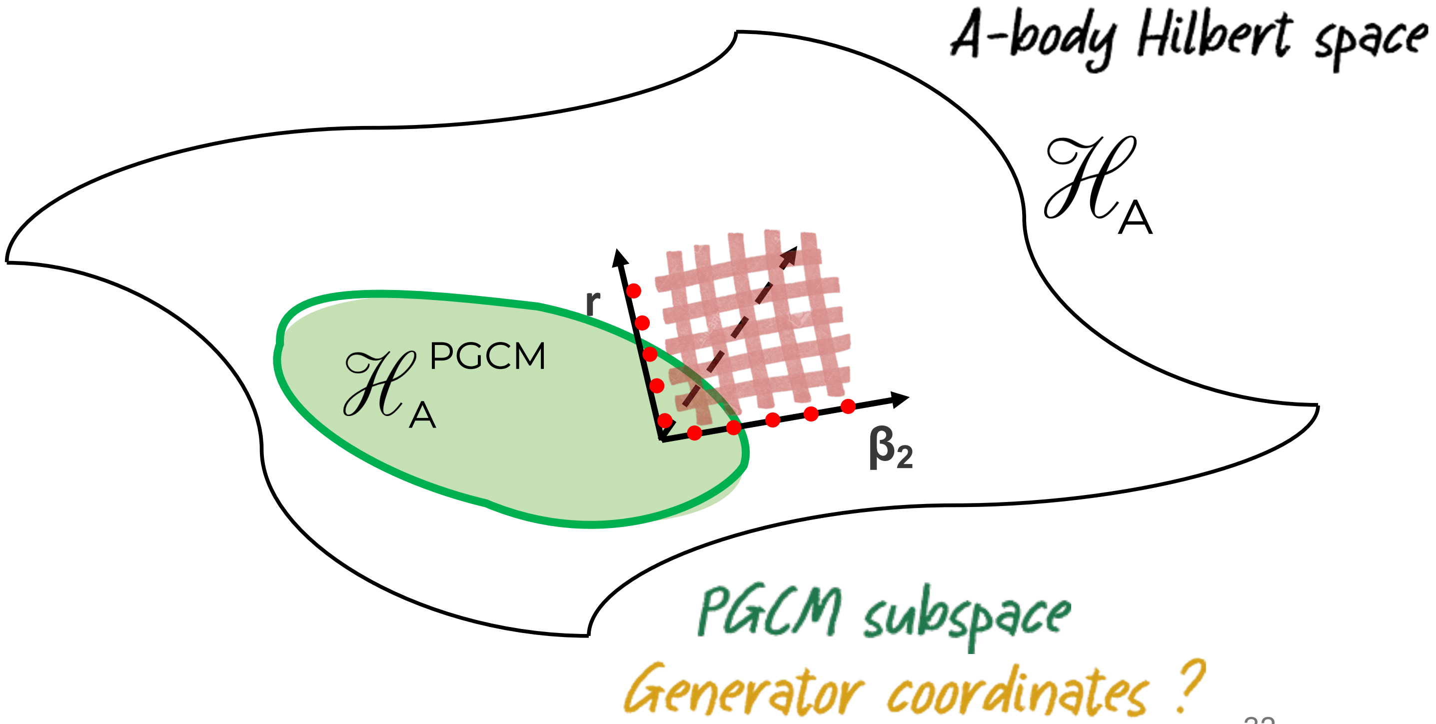
HFB vacua selection

Mesh refinement



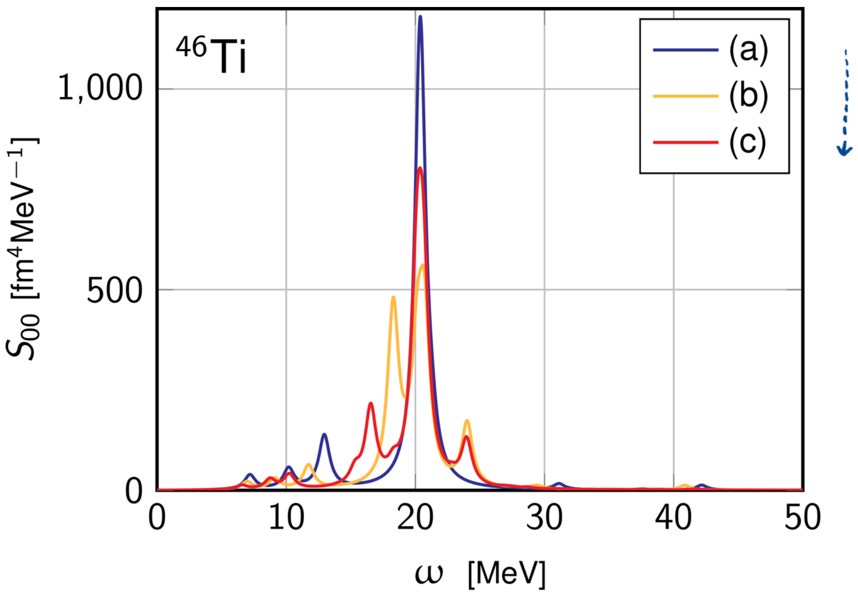


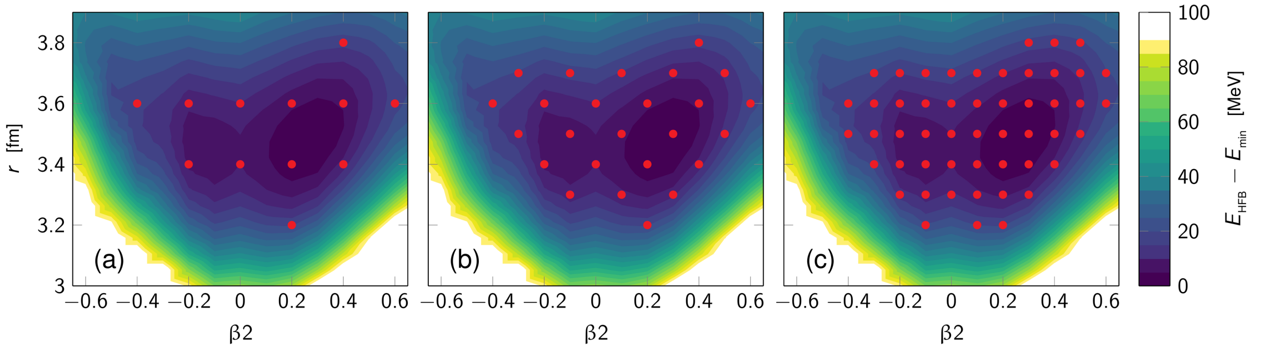
- Qualitative convergence ~
- Centroid relative error ~ 0,2 % ✓

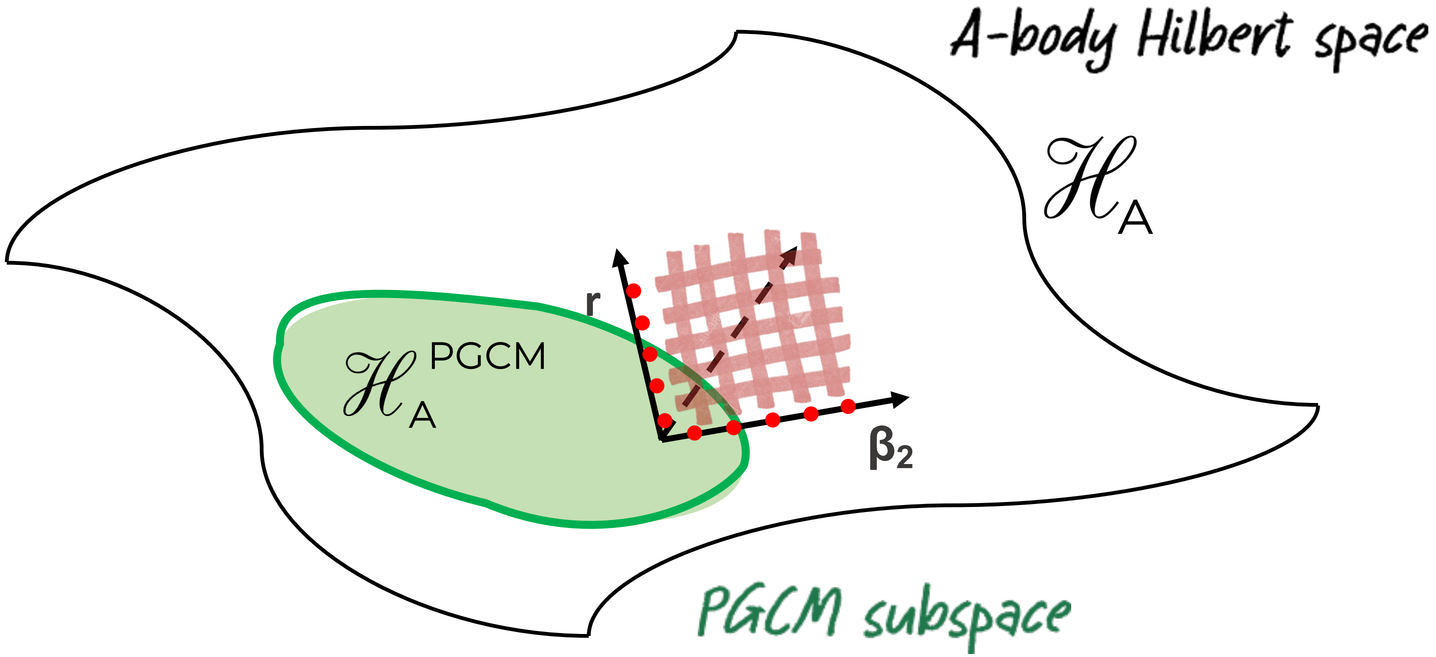


HFB vacua selection

Mesh refinement



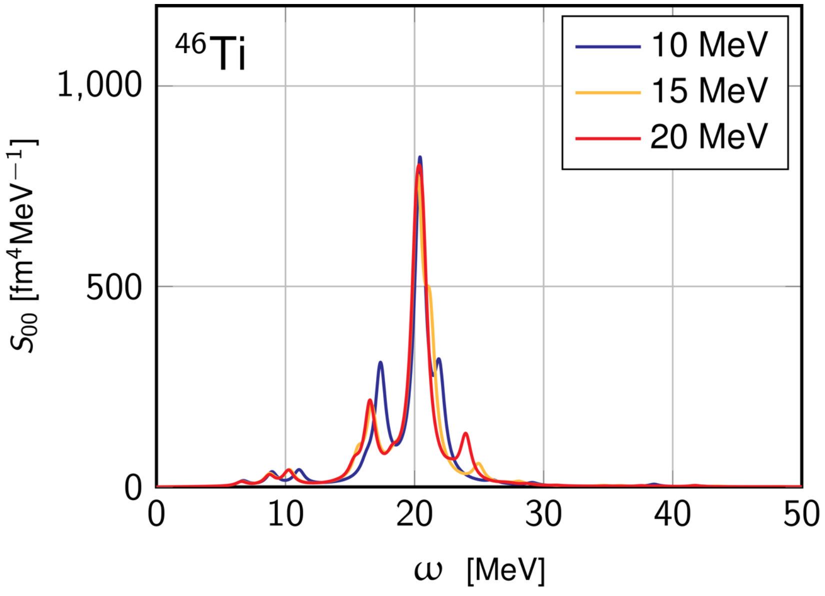


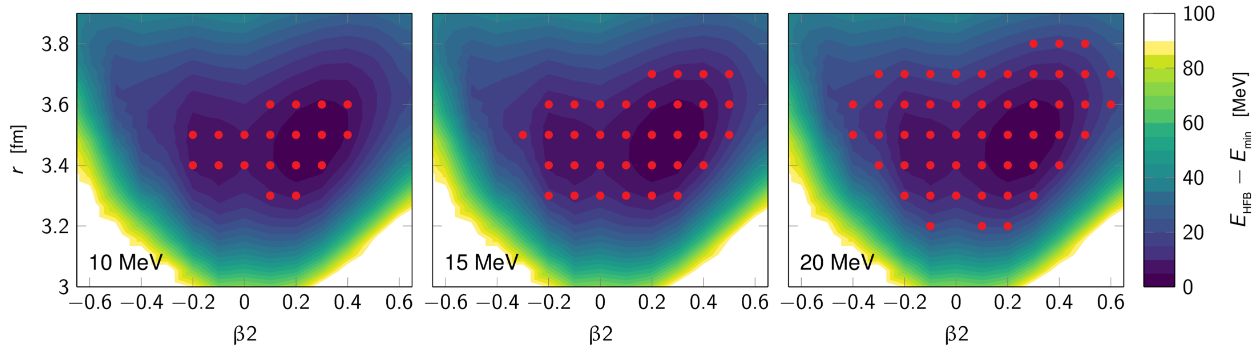


- Qualitative convergence ~
- Centroid relative error ~ 0,2 % ✓
- Dispersion relative error ~ 1,6 % ✓

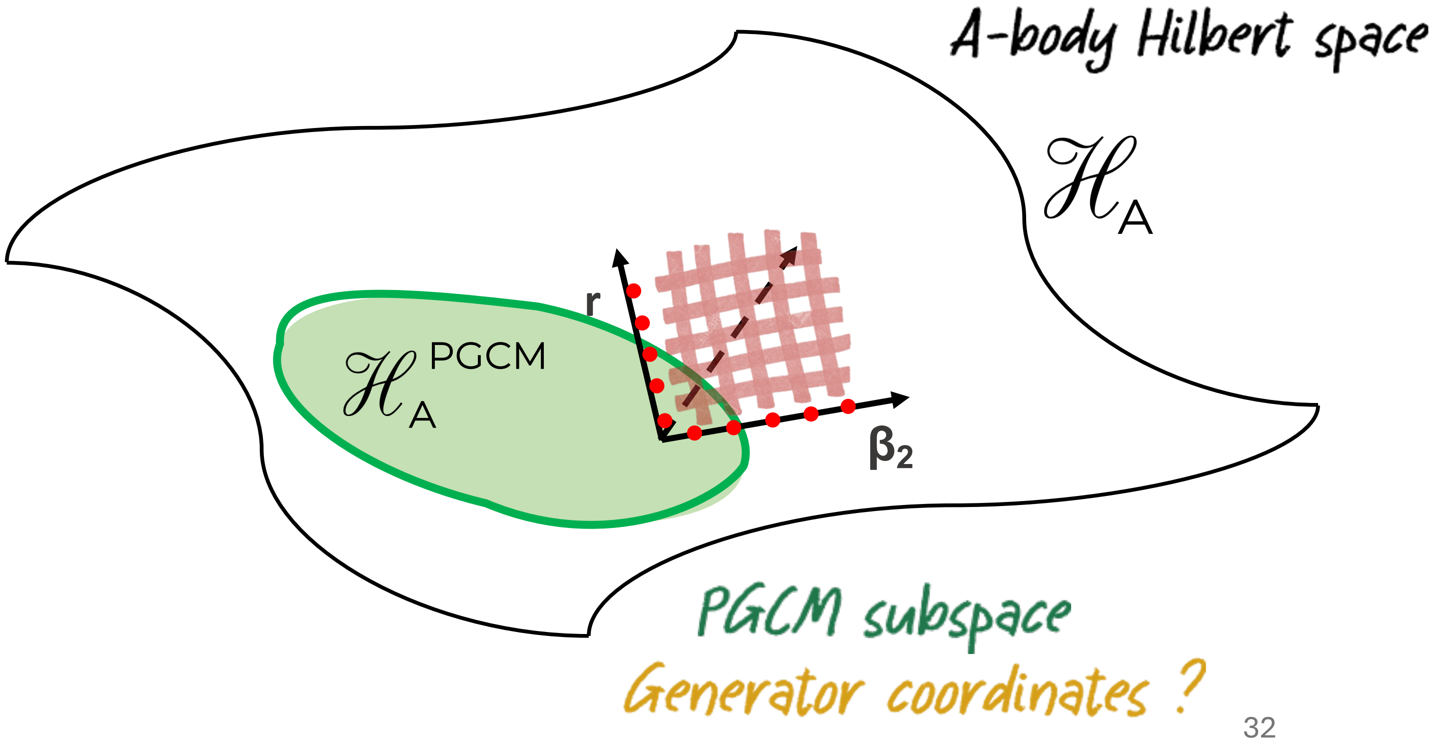
HFB vacua selection

Energy window



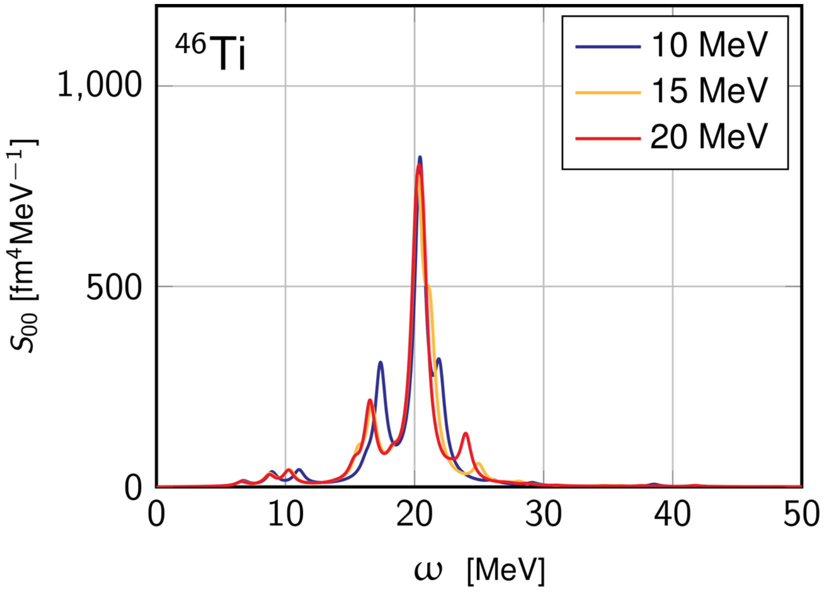


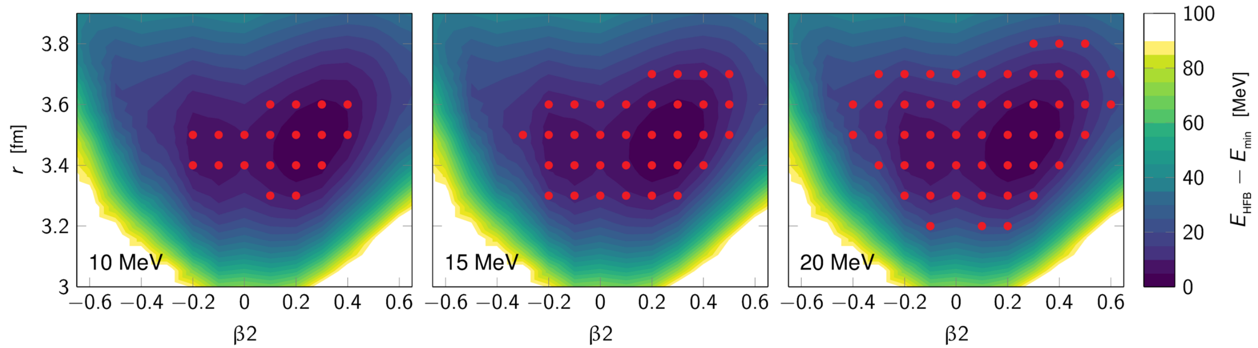
- Good overall convergence ✔

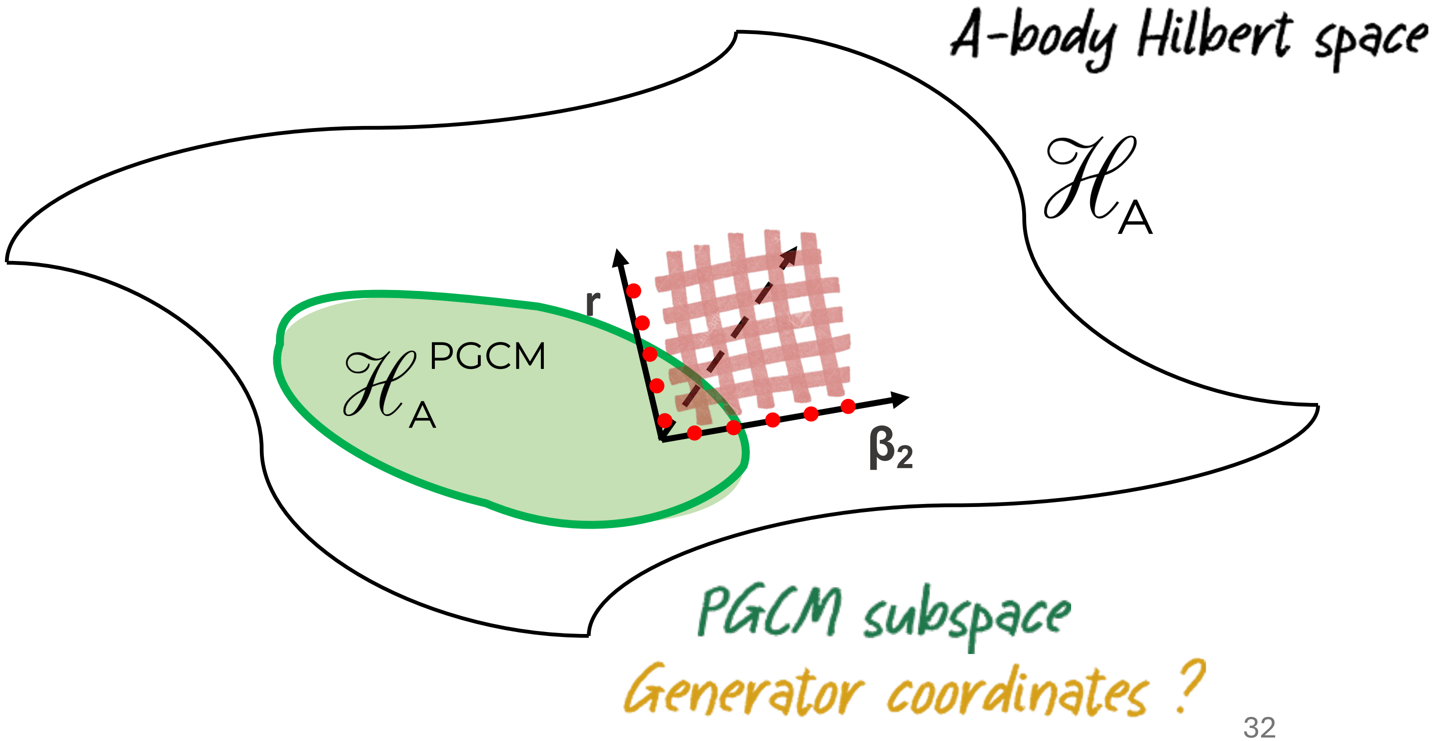


HFB vacua selection

Energy window



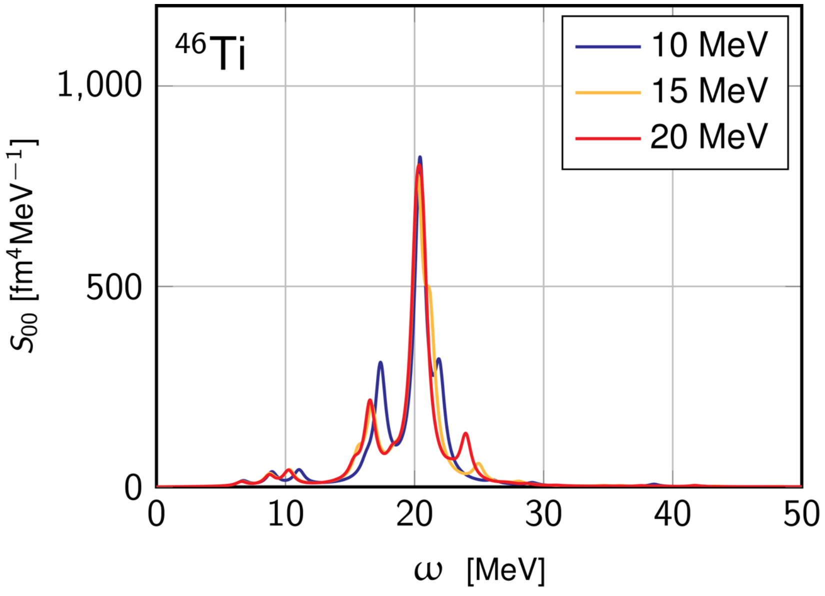


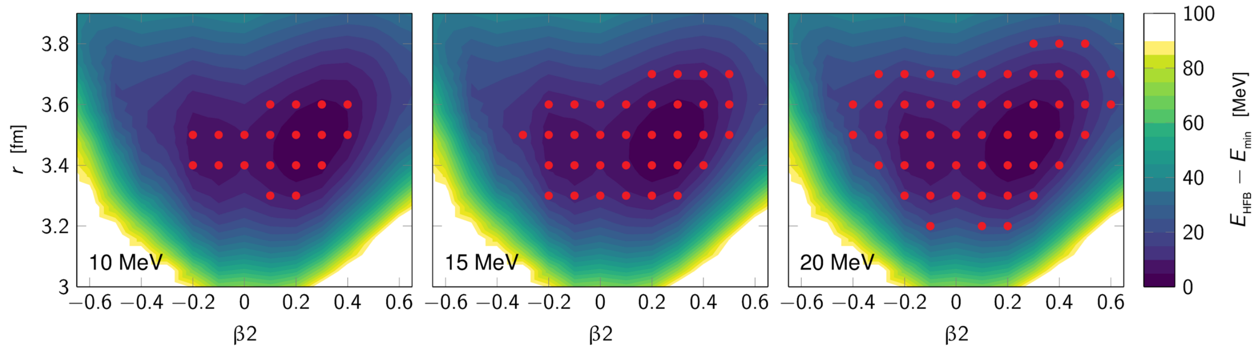


- Good overall convergence ✔
- Centroid relative error ~ 0,3 % ✔

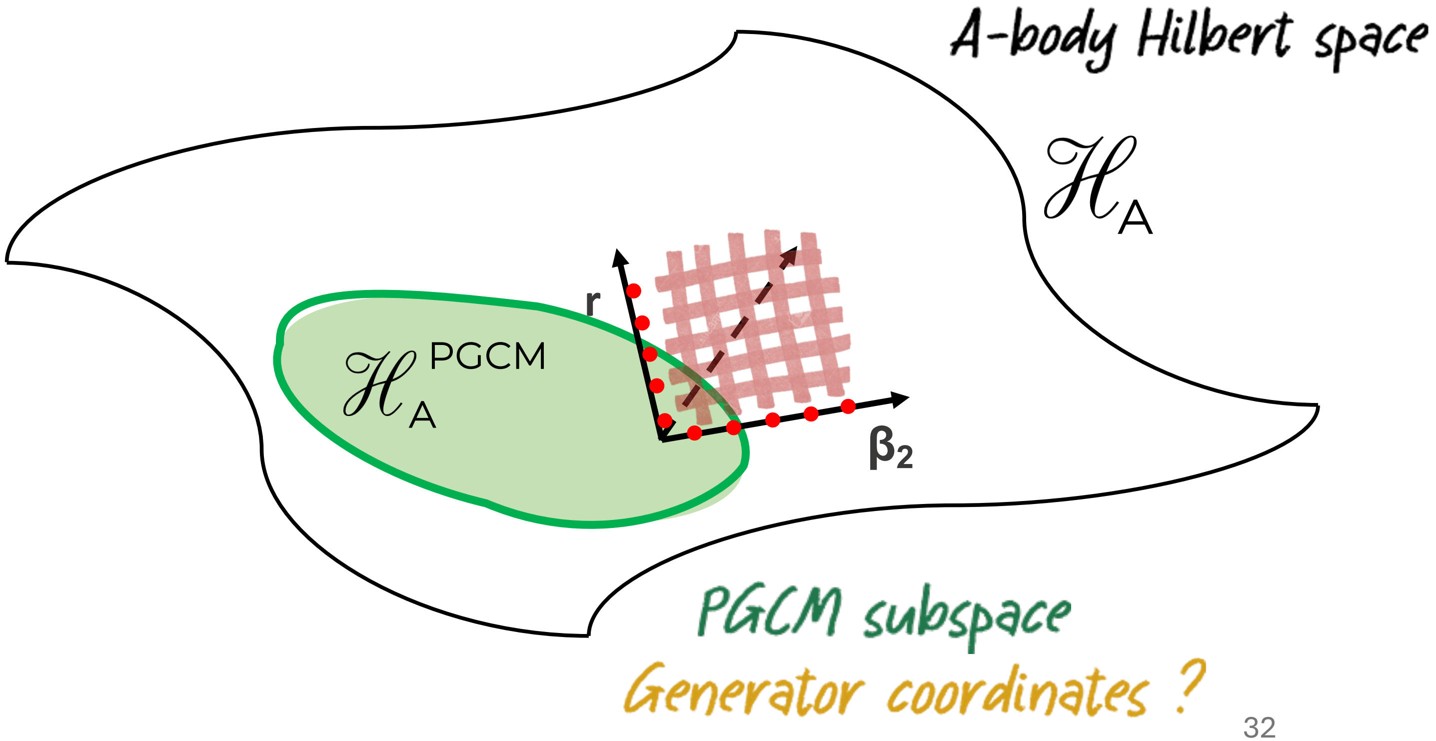
HFB vacua selection

Energy window



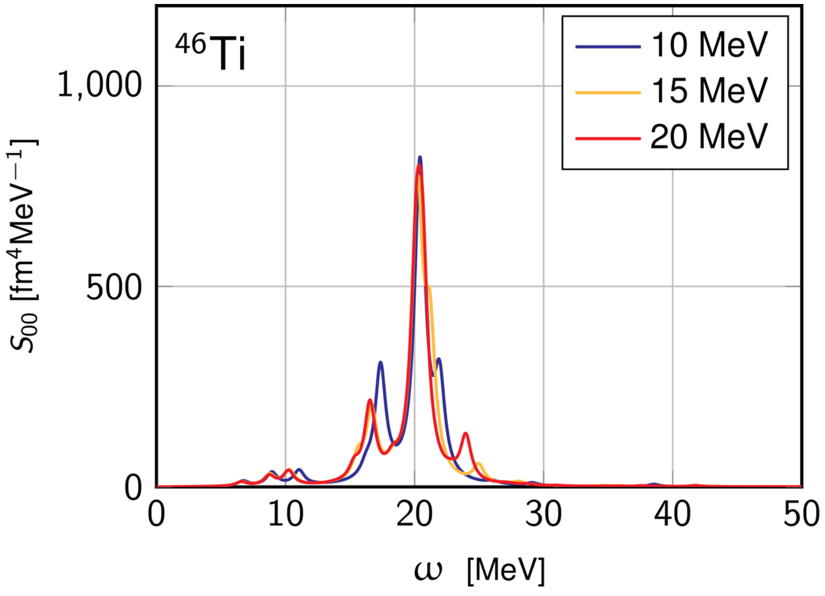


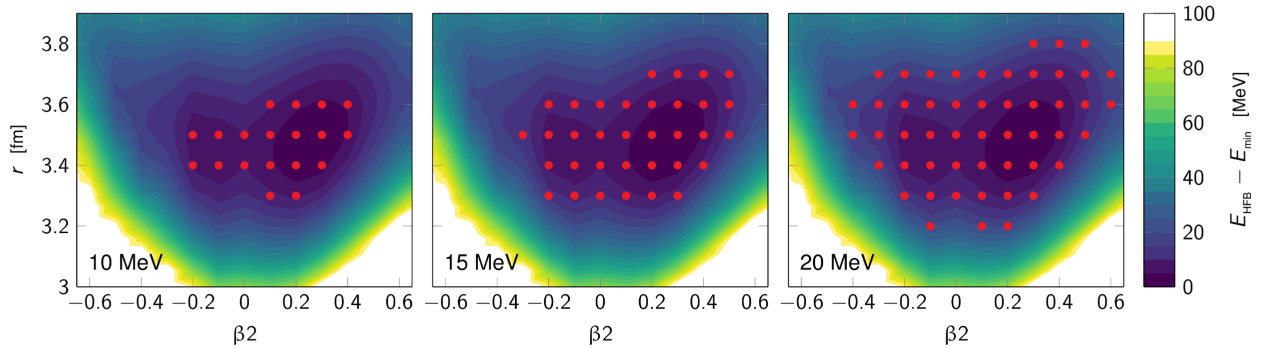
- Good overall convergence ✓
- Centroid relative error ~ 0,3 % ✓
- Dispersion relative error ~ 0,3 % ✓

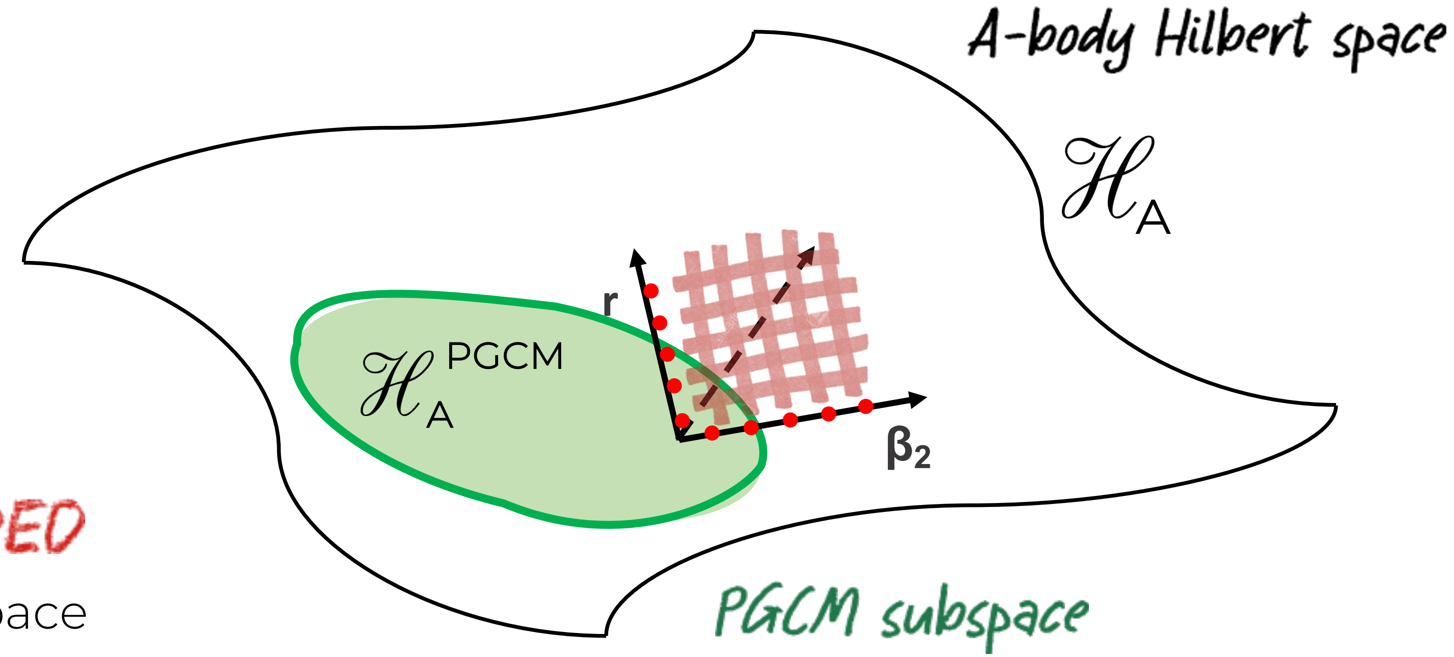


HFB vacua selection

Energy window







SYSTEMATIC CRITERION NEEDED

Unbiased realisation of the PGCM subspace

[Matsumoto, Tanimura, Hagino, 2023]