Collective excitations of even-even open-shell nuclei via PGCM and QRPA calculations

Nuclear ab initio spectroscopy workshop

Espace de Structure Nucléaire Théorique

May 21st, 2024

Andrea Porro
Technische Universität Darmstadt

WITH

Thomas Duguet CEA IRFU
Jean-Paul Ebran CEA DAM
Mikael Frosini CEA Cadarache
Robert Roth TUD
Vittorio Somà CEA IRFU

Based on

arXiv > nucl-th > arXiv:2402.02228

Nuclear Theory

[Submitted on 3 Feb 2024]

Ab initio description of monopole resonances in light- and medium-mass nuclei: I. Technical aspects and uncertainties of ab initio PGCM calculations

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

[arXiv:2402.15901, 2024]

arXiv > nucl-th > arXiv:2402.15901

Nuclear Theory

[Submitted on 24 Feb 2024]

Ab initio description of monopole resonances in light- and medium-mass nuclei: II. Ab initio PGCM calculations in ^{46}Ti, ^{28}Si and ^{24}Mg

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

[arXiv:2402.02228, 2024]

arXiv > nucl-th > arXiv:2404.14154

Nuclear Theory

[Submitted on 22 Apr 2024]

Ab initio description of monopole resonances in light- and medium-mass nuclei: III. Moments evaluation in ab initio PGCM calculations

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

[arXiv:2404.14154, 2024]

Fourth (and last) paper of the series coming soon

Outline

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1 Introduction

- Giant Resonances Physics
- The PGCM
- Link between PGCM and QRPA

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2 Systematic study

- Numerical details
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- Shape coexistence
- Deformation

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- Proof of principle
- Realistic calculations

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- Preliminary incompressibility results

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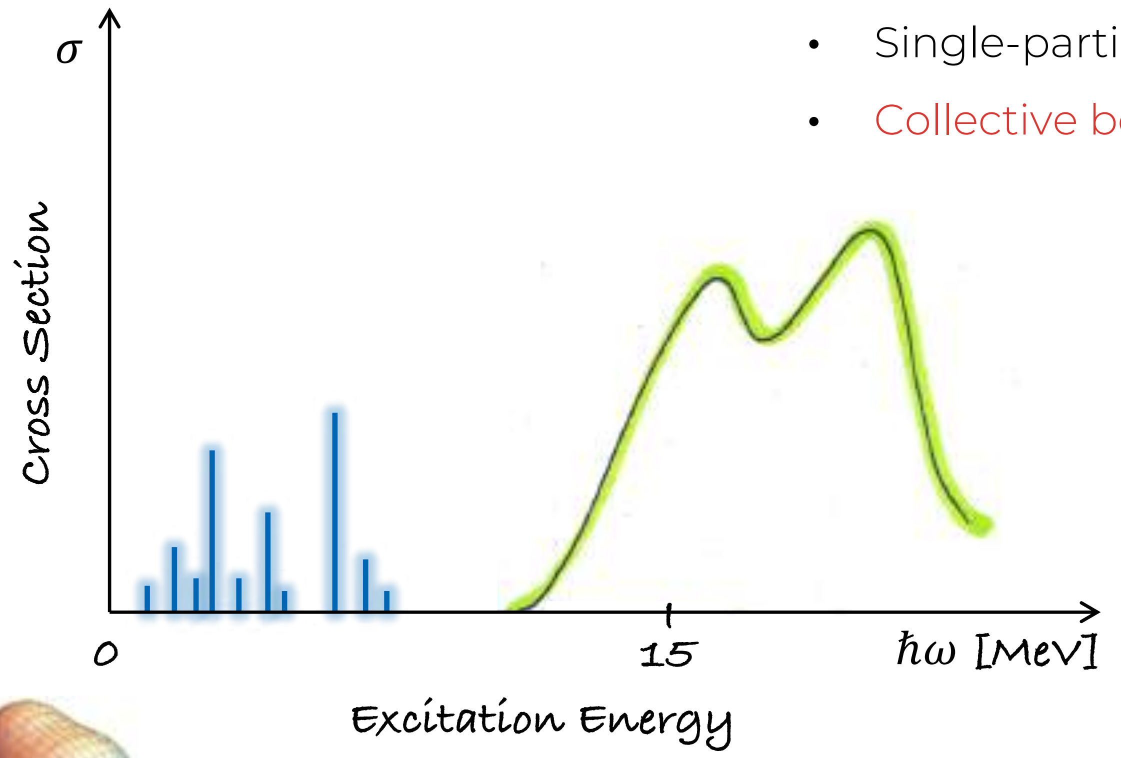
Giant Resonances

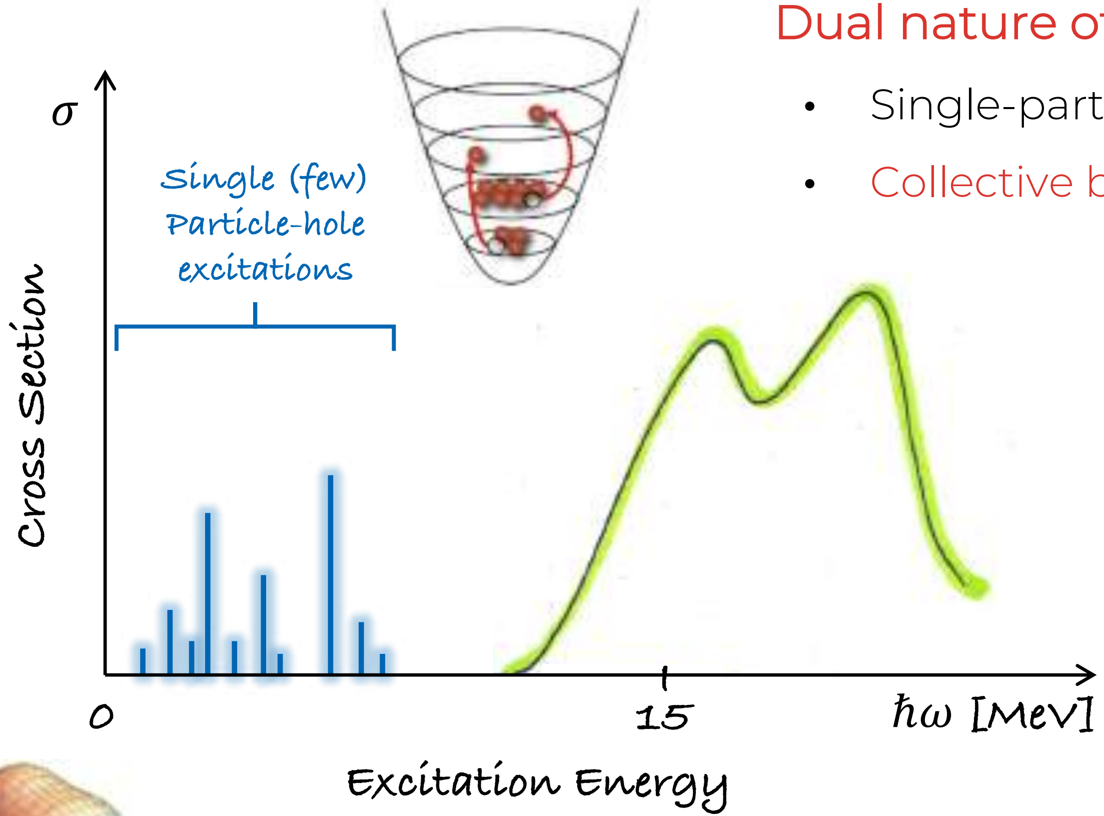


Dual nature of nucleus

- Single-particle features
- Collective behaviour

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

Giant Resonances



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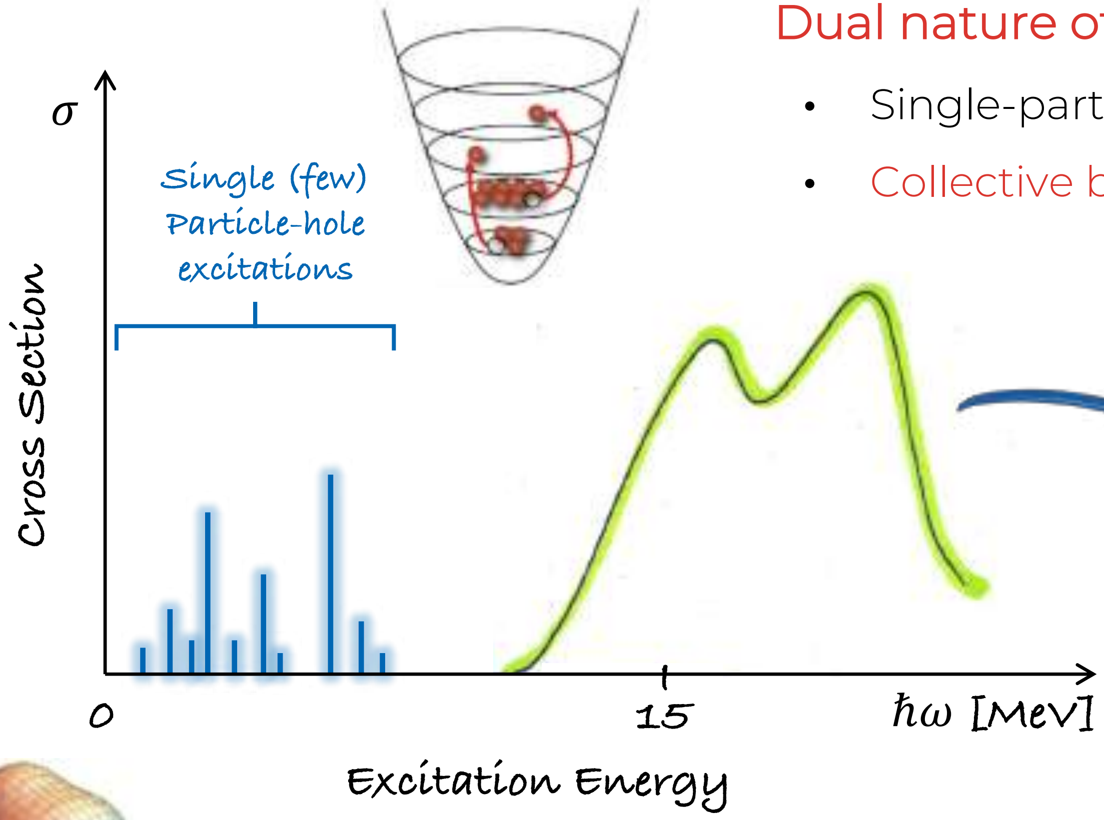

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Liquid drop picture
vibrations, oscillations

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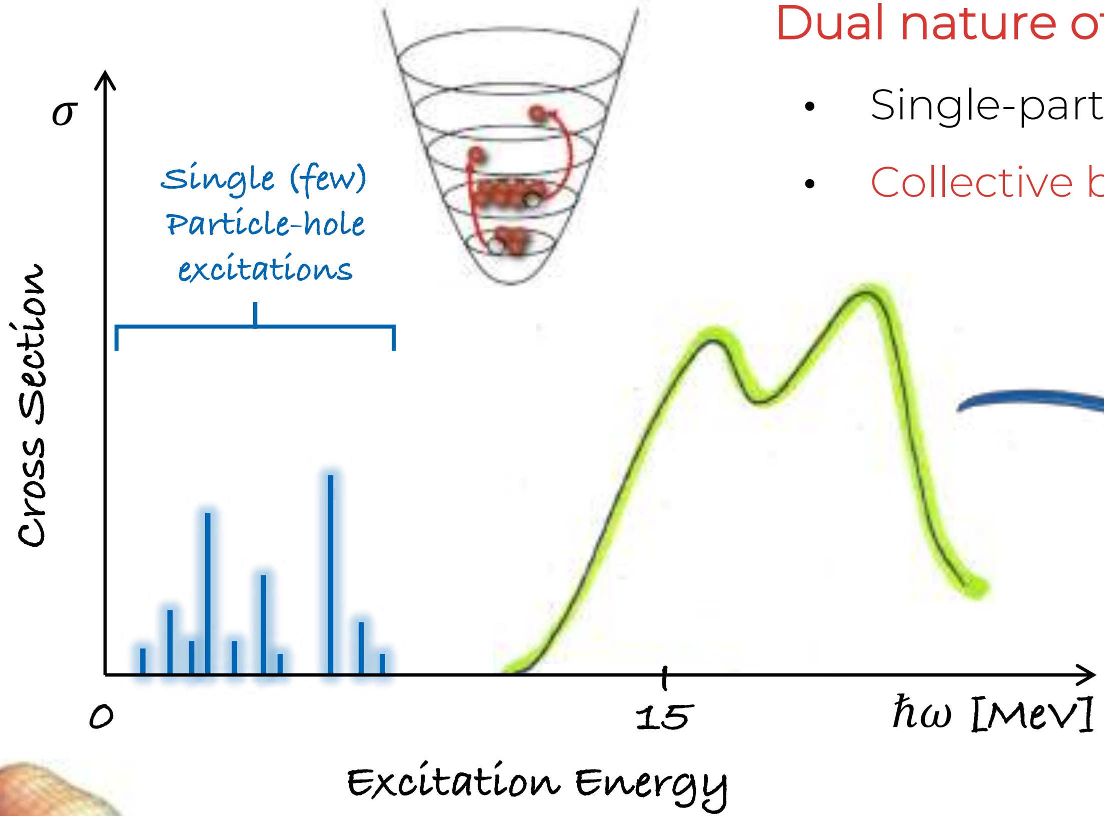

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Giant Resonances (GRs)

clearest manifestation of collective motion

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

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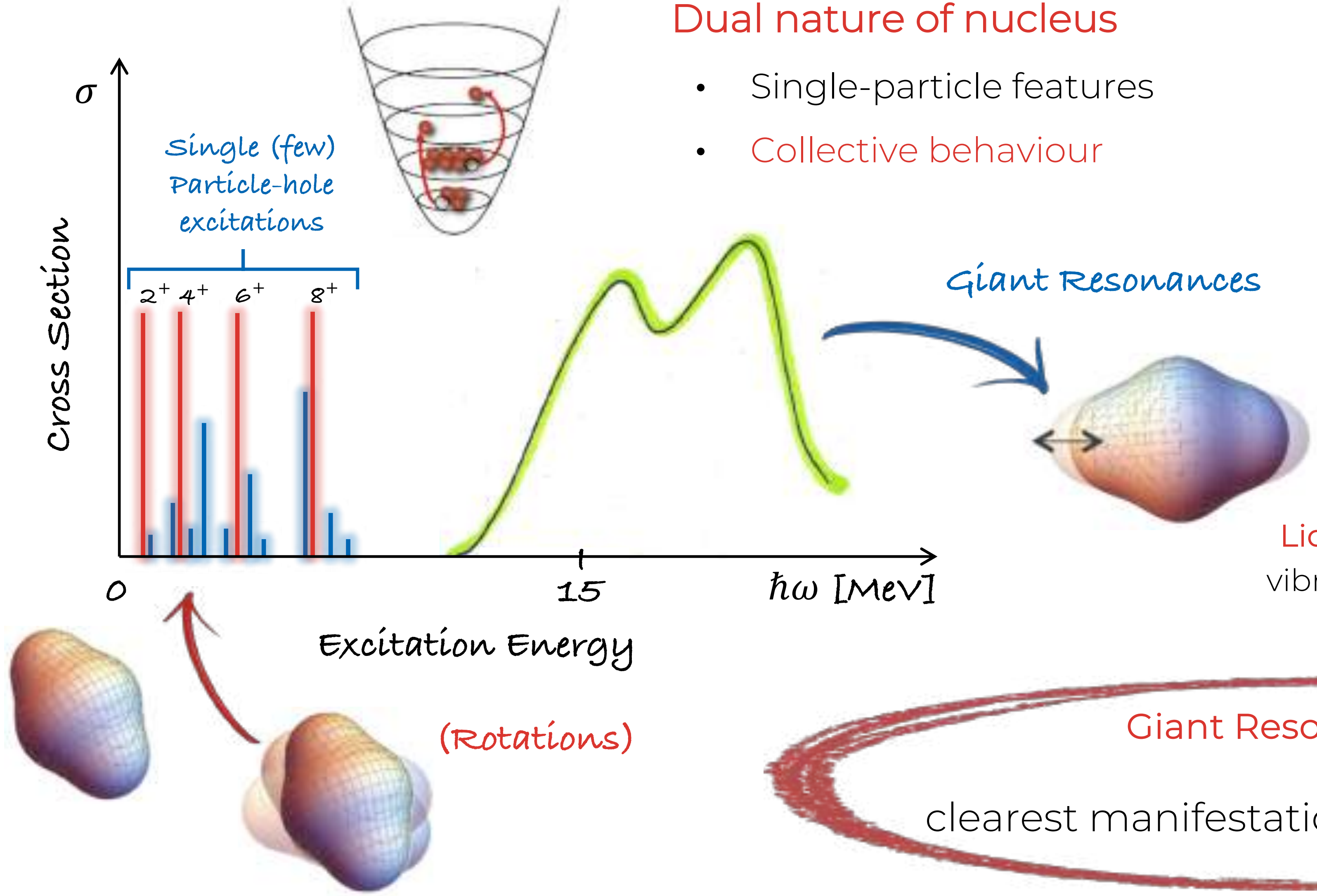

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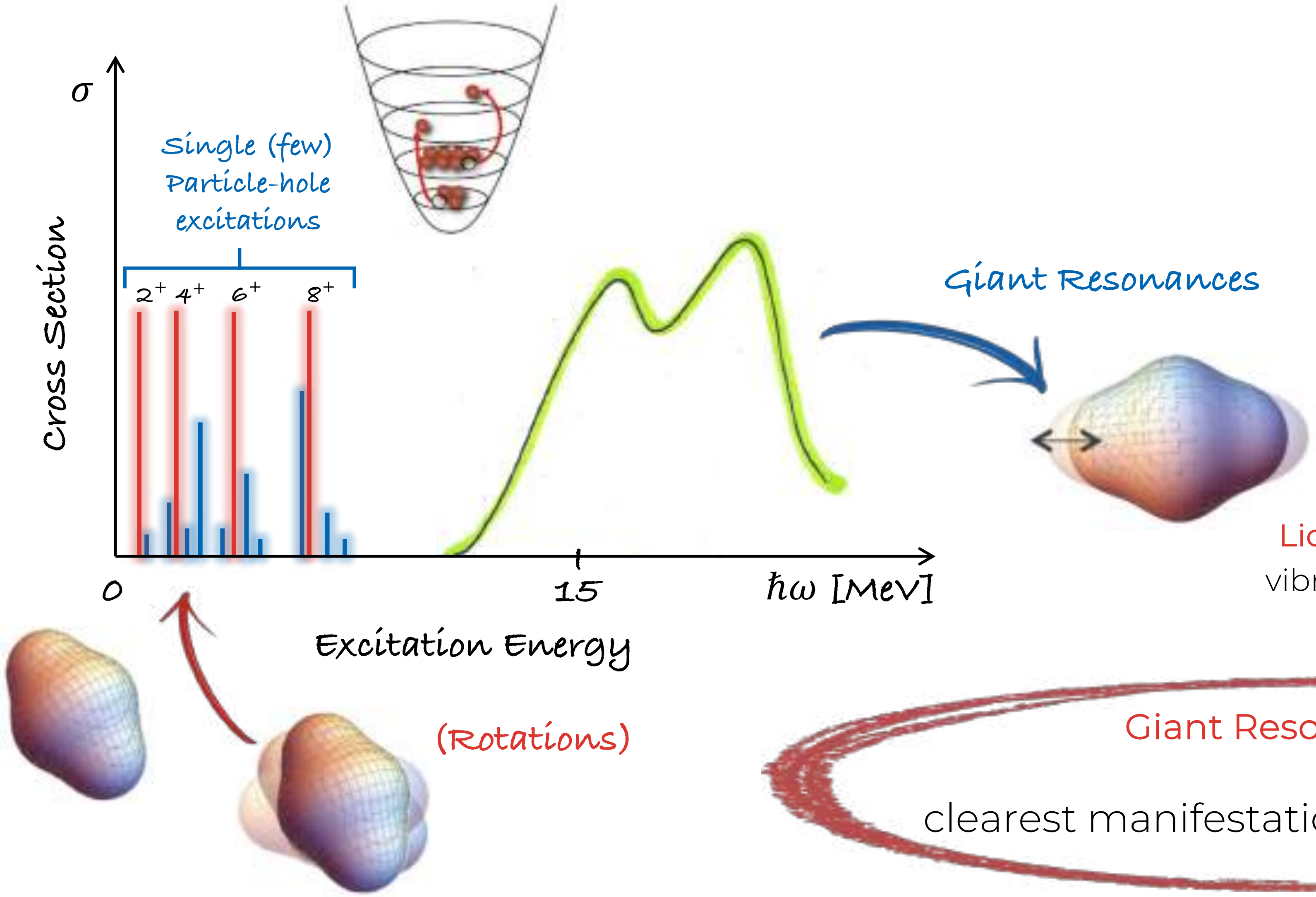

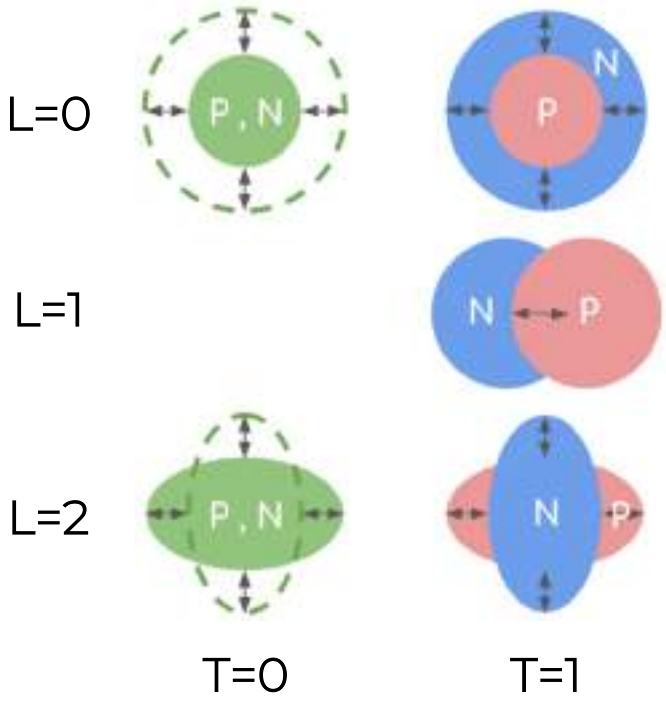

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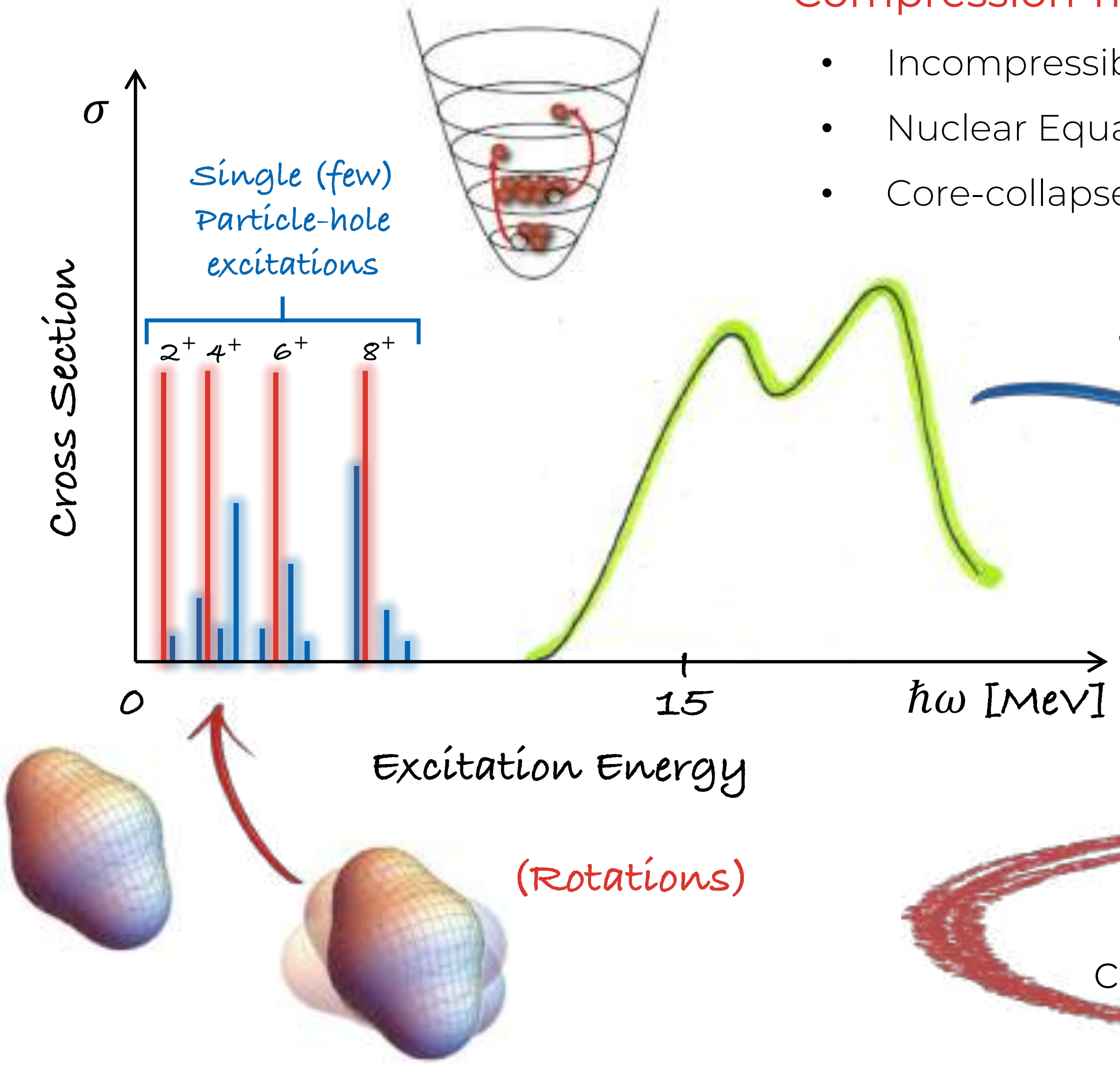
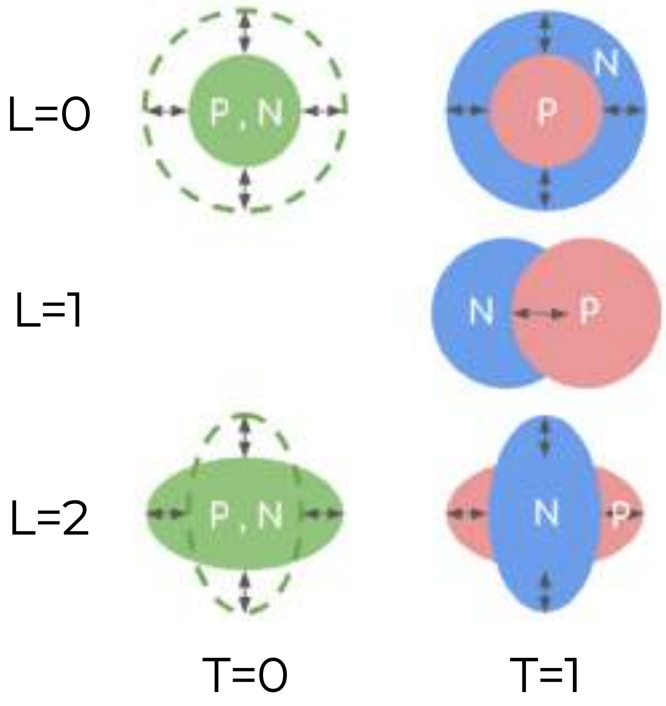


Compression-mode resonances

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



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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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Open-shell systems

Strong static correlations

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Open-shell systems

Symmetry-breaking reference states

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Open-shell systems

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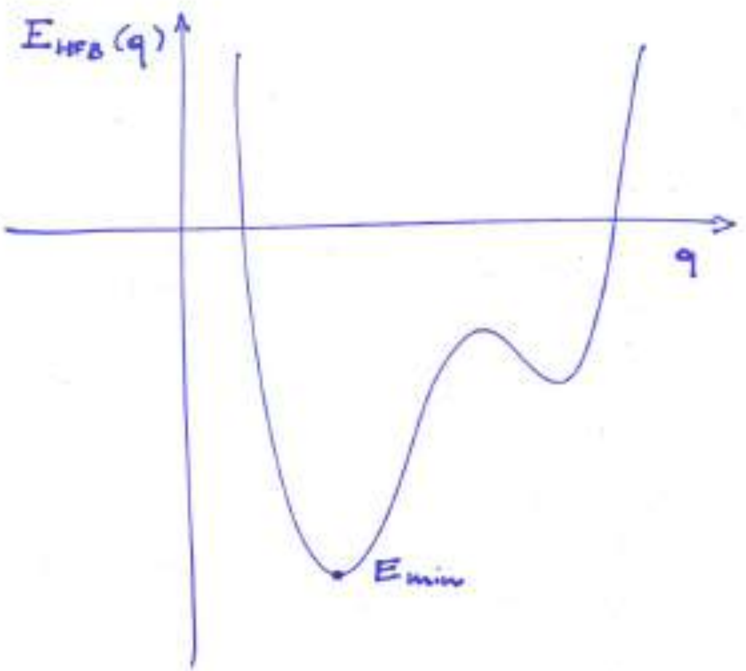
Strong static correlations

1 Constrained HFB solutions

$|\Phi(q)\rangle$



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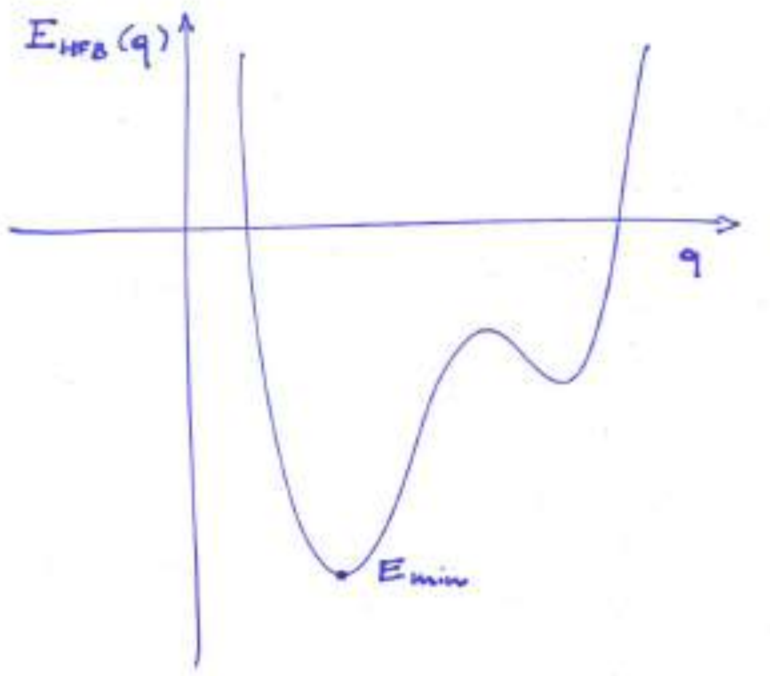
(q can be any coordinate)



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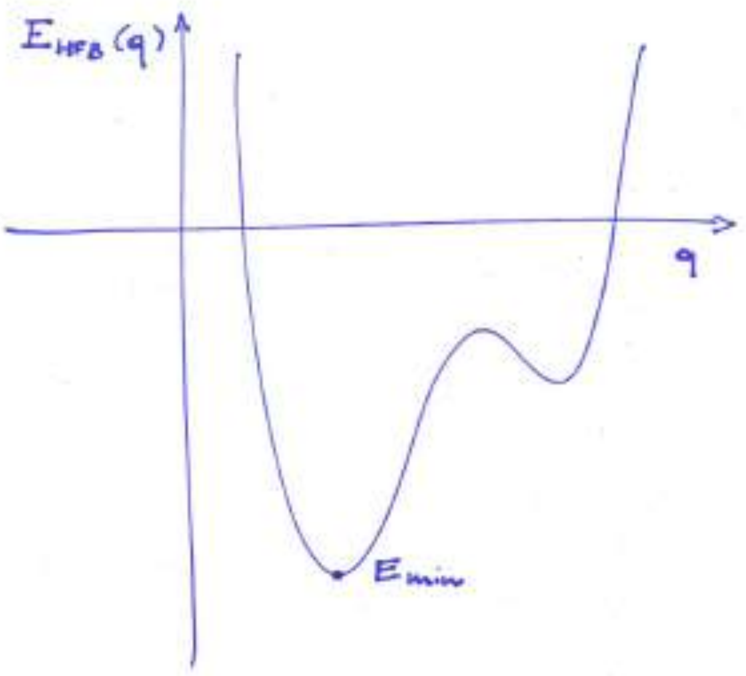

Open-shell systems

Symmetry-breaking reference states

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1 Constrained HFB solutions

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

Generator coordinates

(q can be any coordinate)

2 PGCM Ansatz

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

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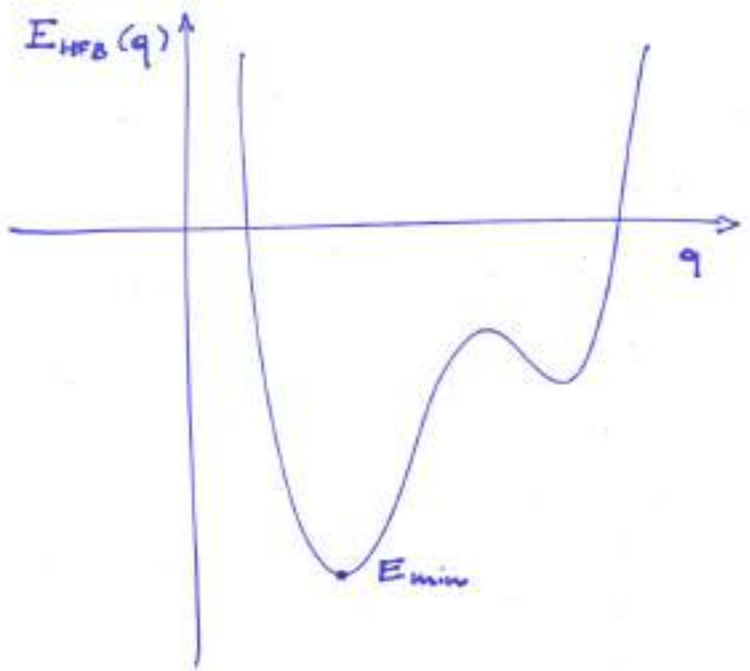

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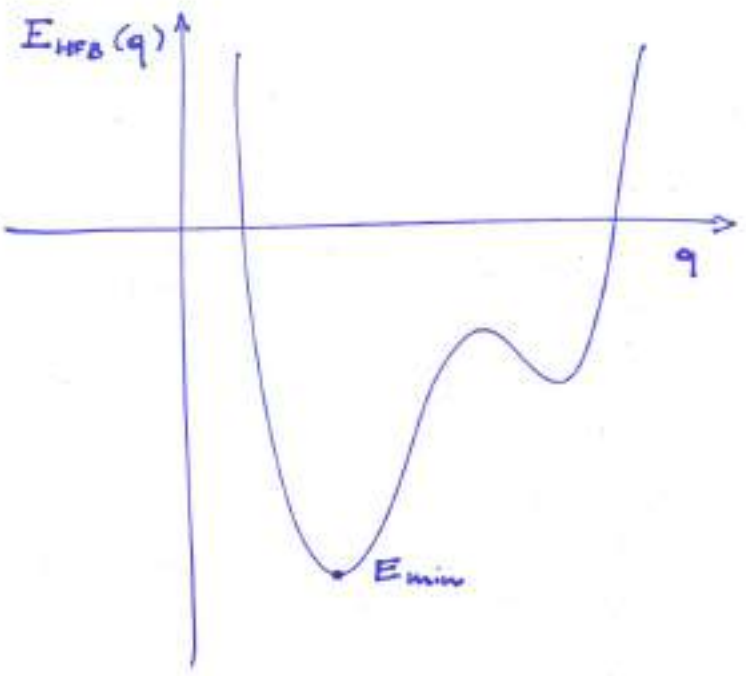

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3 HWG Equation

Variational method

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

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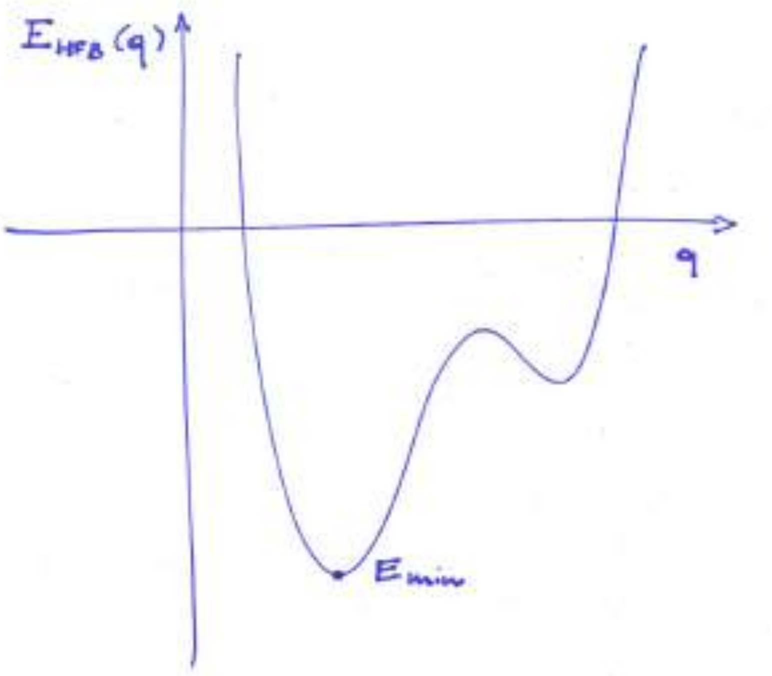

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Schrödinger-like equation

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

Kernels evaluation

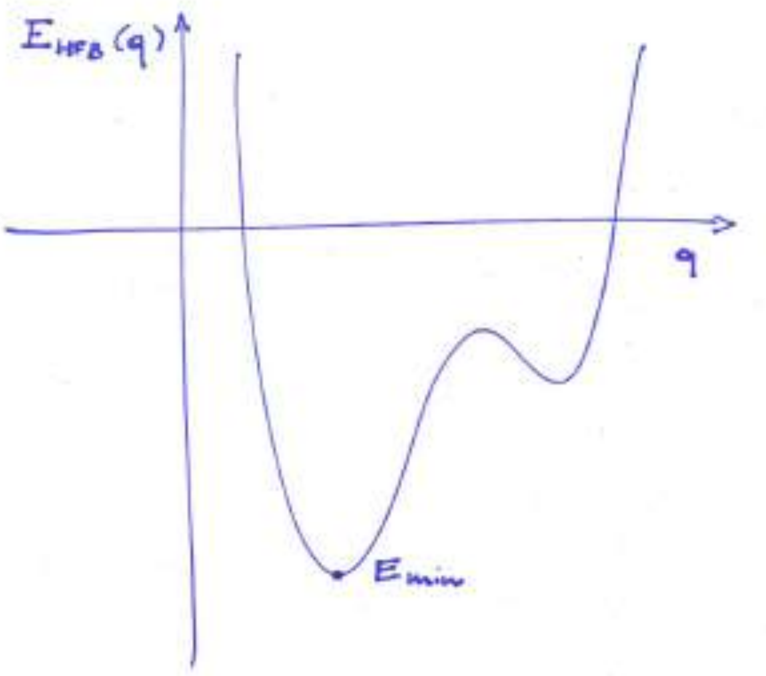
$$\mathcal{H}(p,q) \equiv \langle \Phi(p) | H | \Phi(q) \rangle$$
$$\mathcal{N}(p,q) \equiv \langle \Phi(p) | \Phi(q) \rangle$$

[Porro and Duguet, EPJA, 2022]

Projected Generator Coordinate Method

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

Diagonalization in a physically-informed
reduced Hilbert space



1 *Constrained HFB solutions*

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Generator coordinates
(q can be any coordinate)

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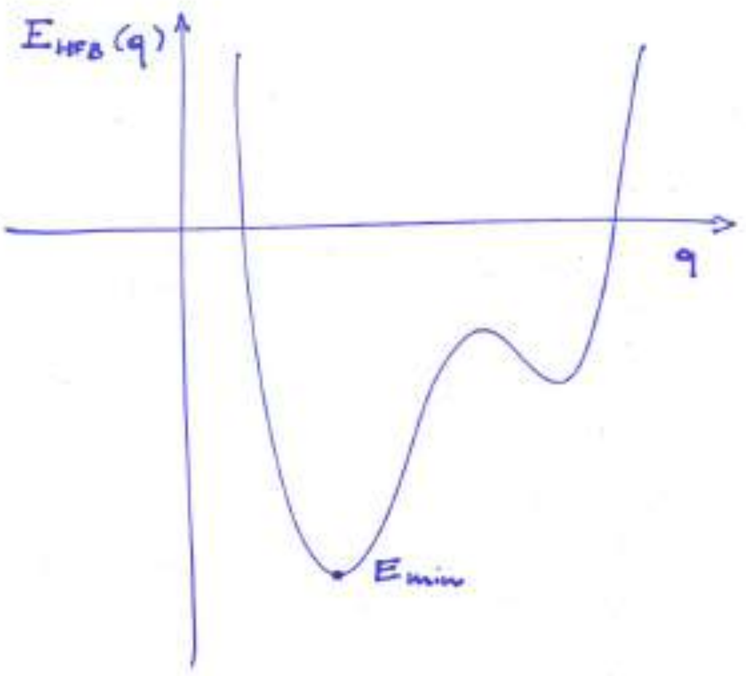

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GCM and (Q)RPA

Thouless theorem

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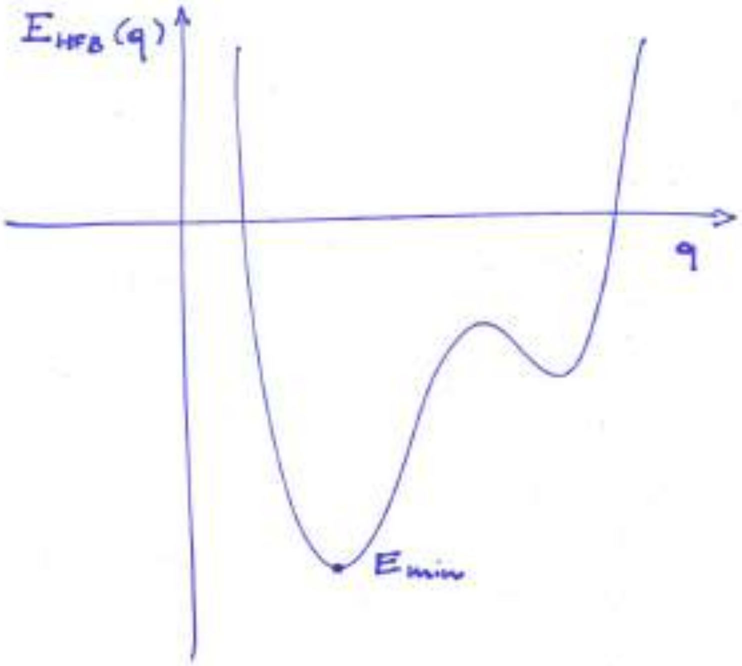

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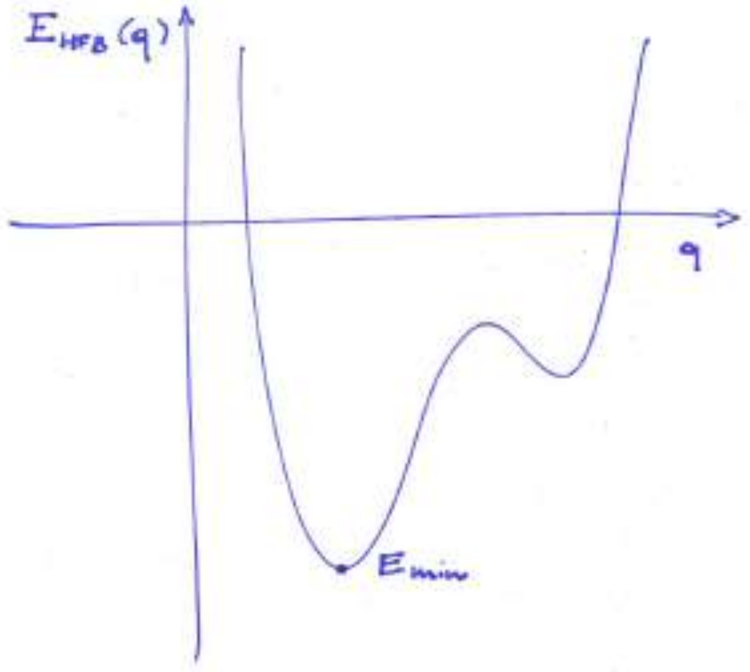

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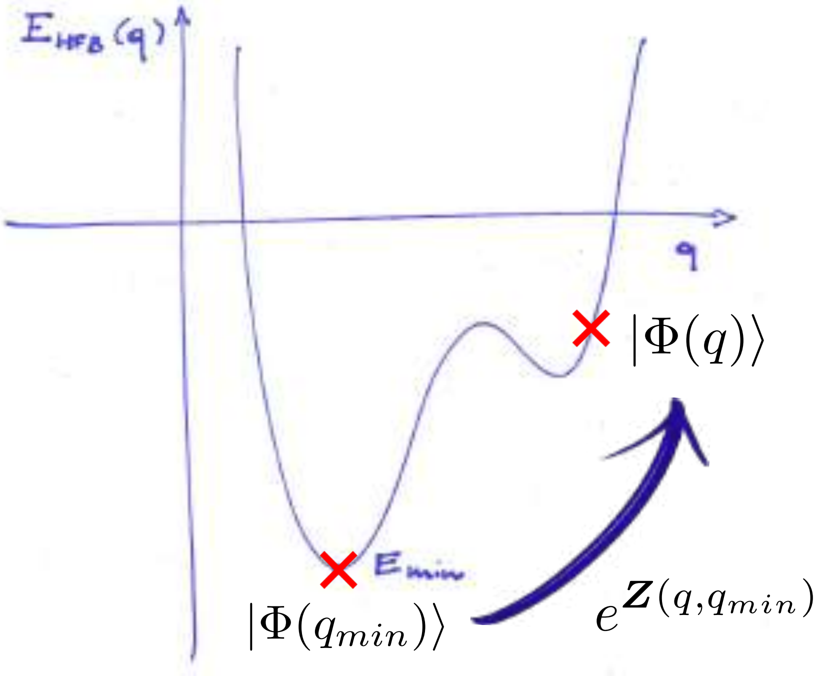

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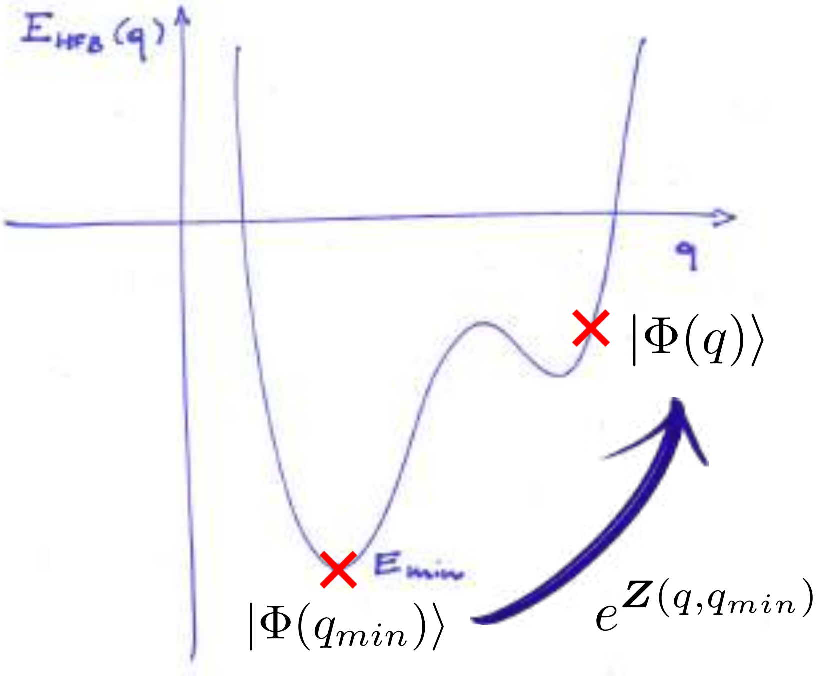

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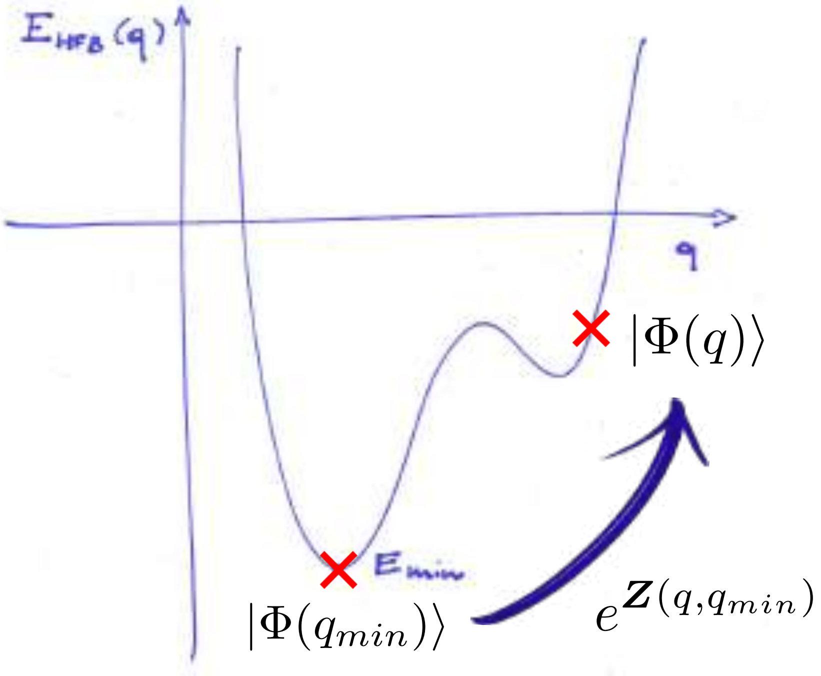

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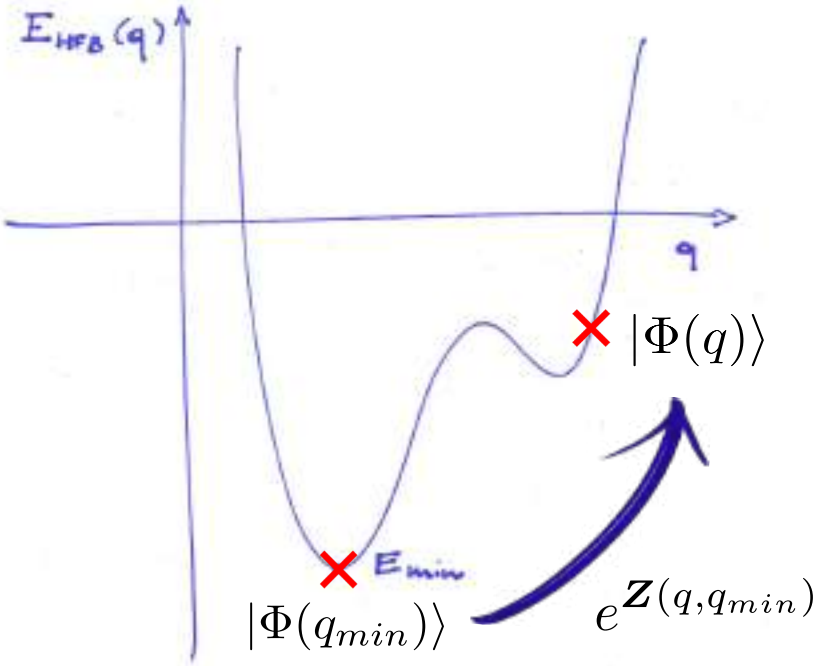

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Introduce the Quasi-Boson approximation (QBA)

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

GCM and (Q)RPA

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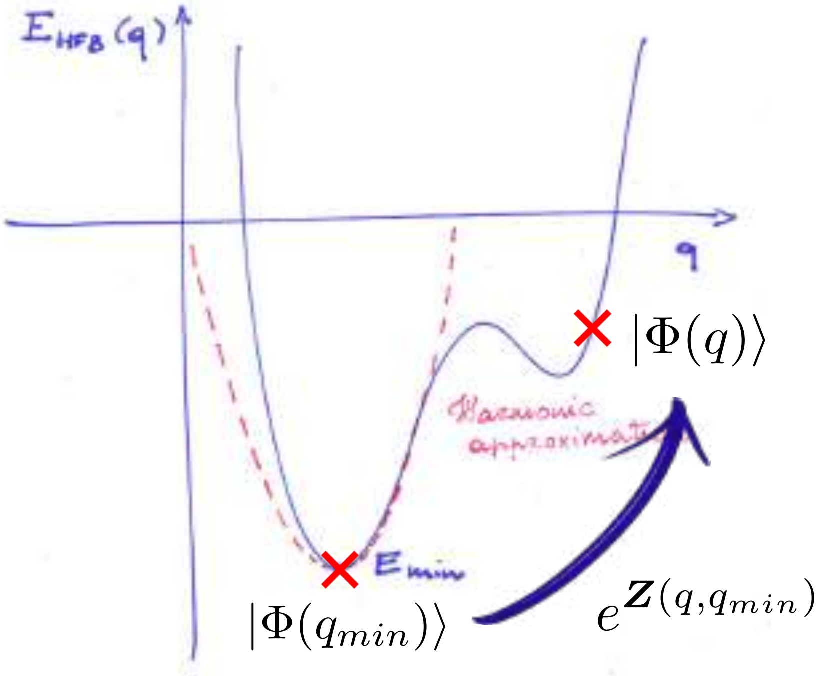

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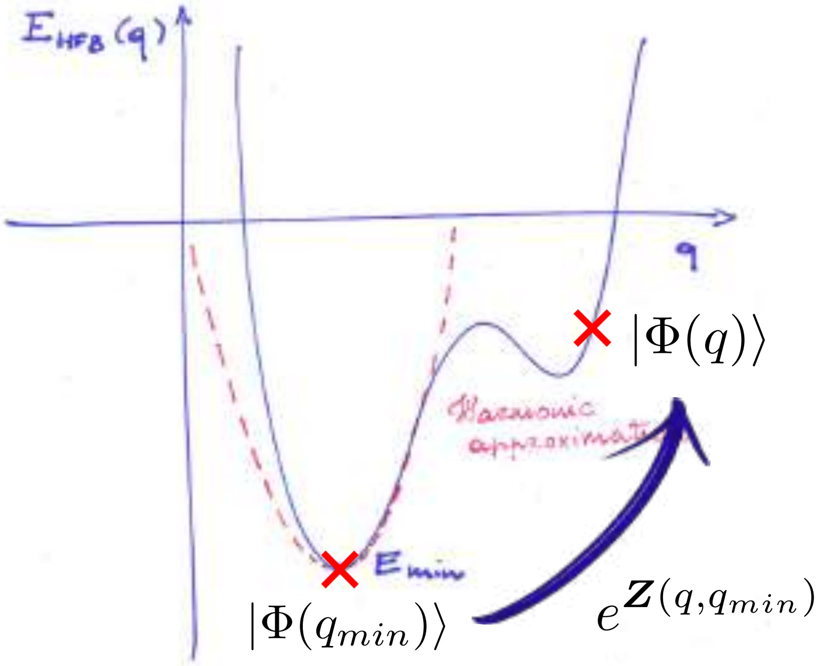

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No coordinates dependency !

All coordinates are explored (differently from GCM)

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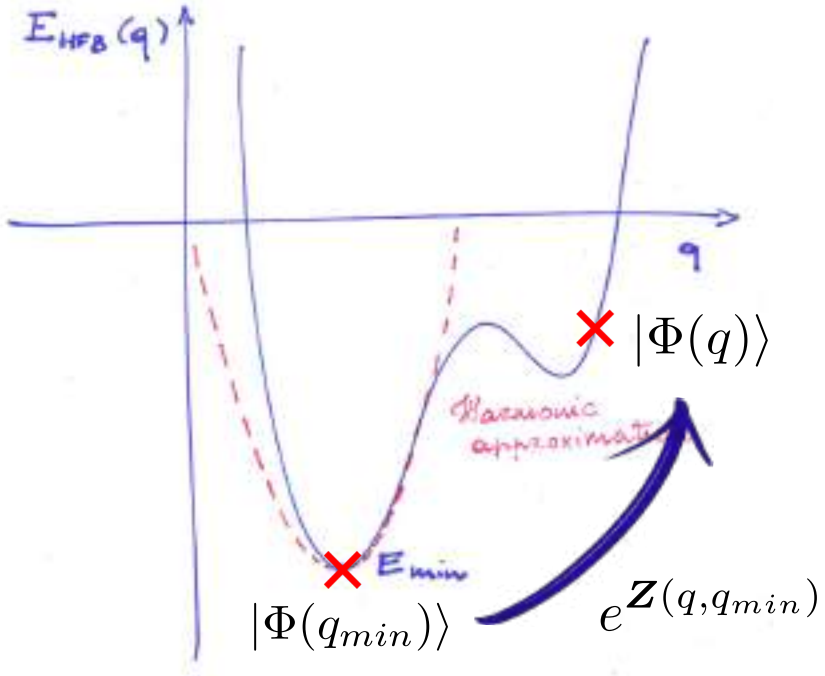

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Eventually rewrites as (Q)RPA equations

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

[Jancovici, Schiff, 1964]

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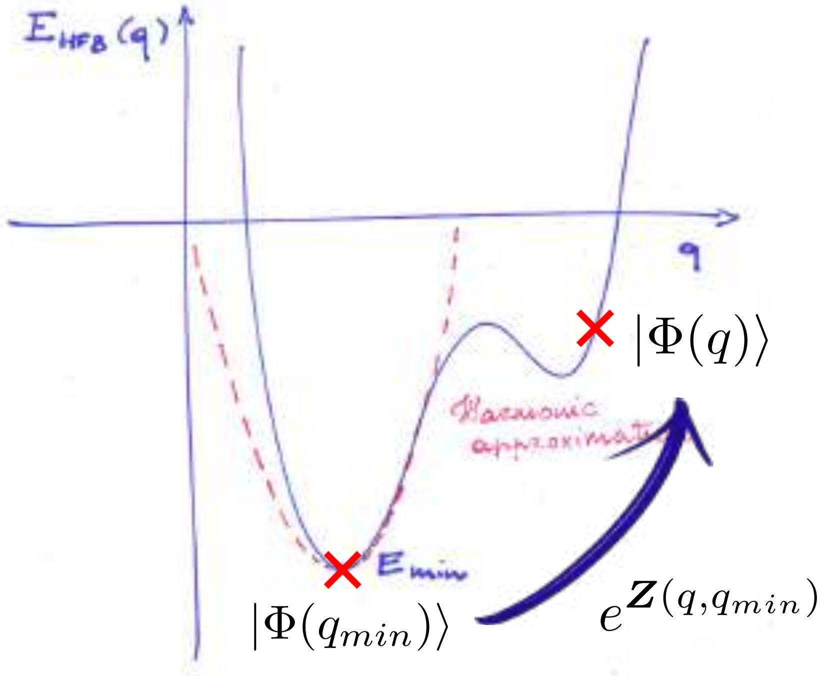

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Nuclei that are stiff against deformations

(anharmonic effects negligible)

[Jancovici, Schiff, 1964]

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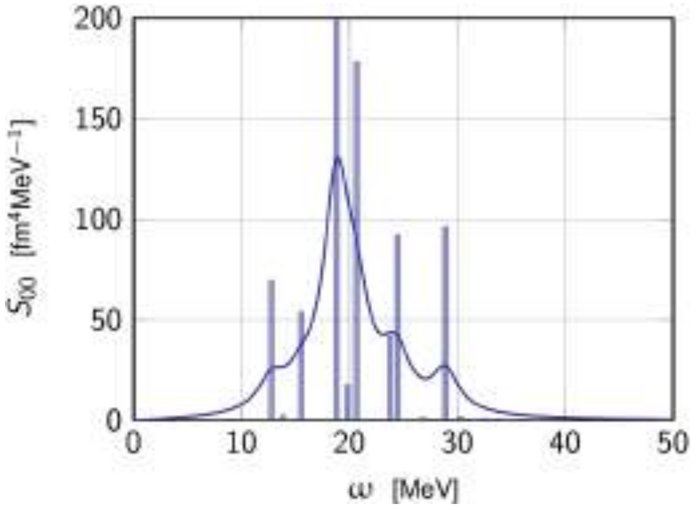
Setting

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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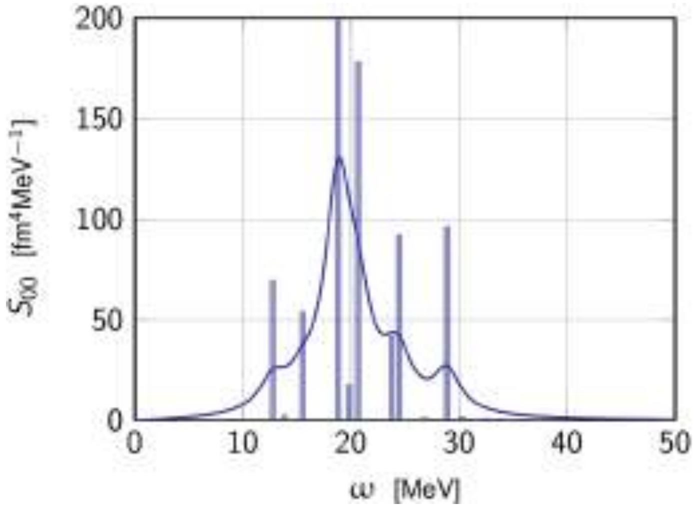
JM=00



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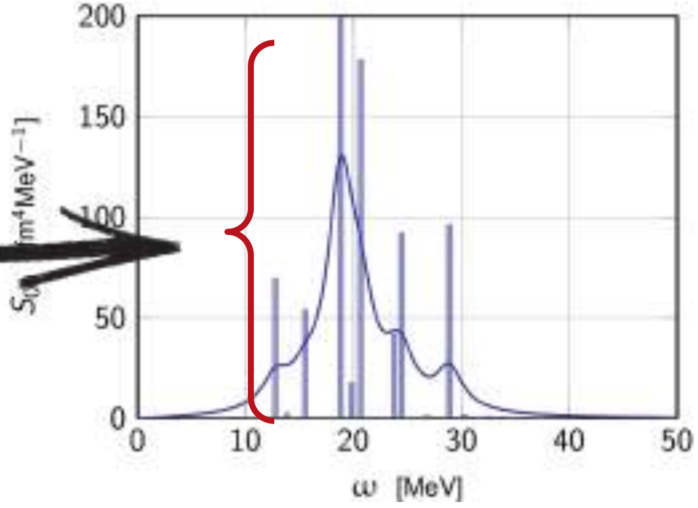

Setting

Studied quantity: monopole strength

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

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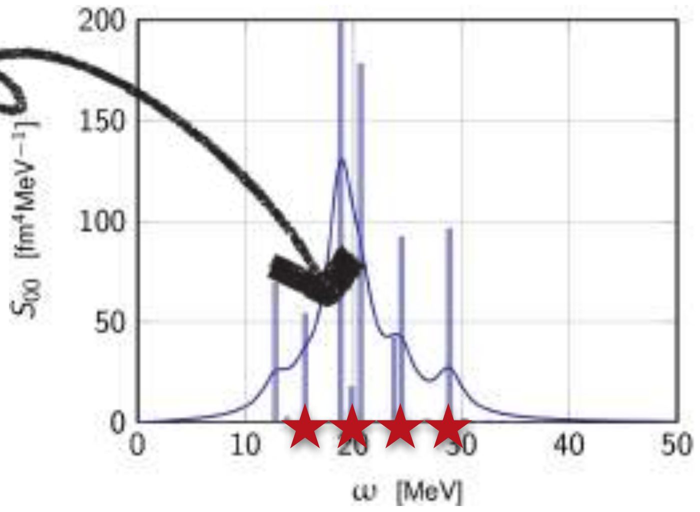

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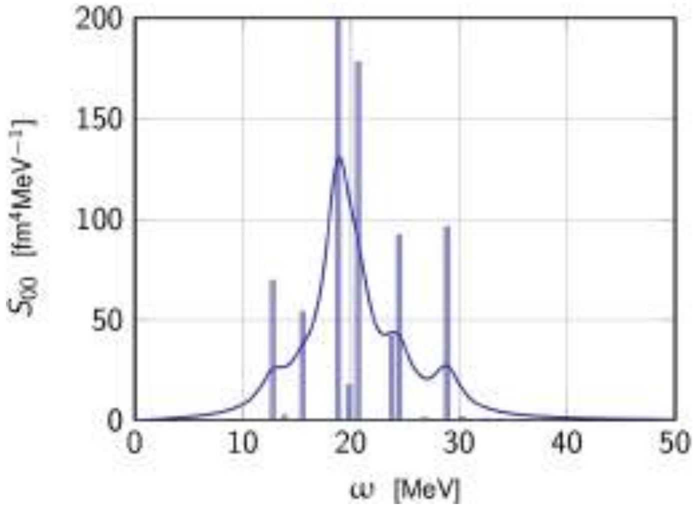

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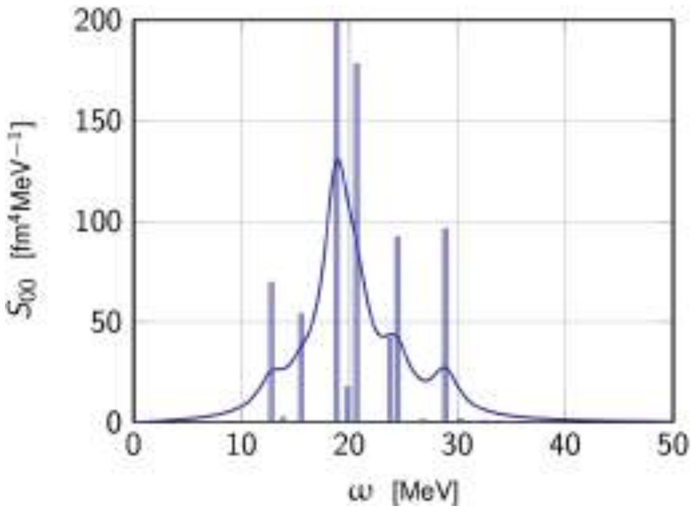

Related moments

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

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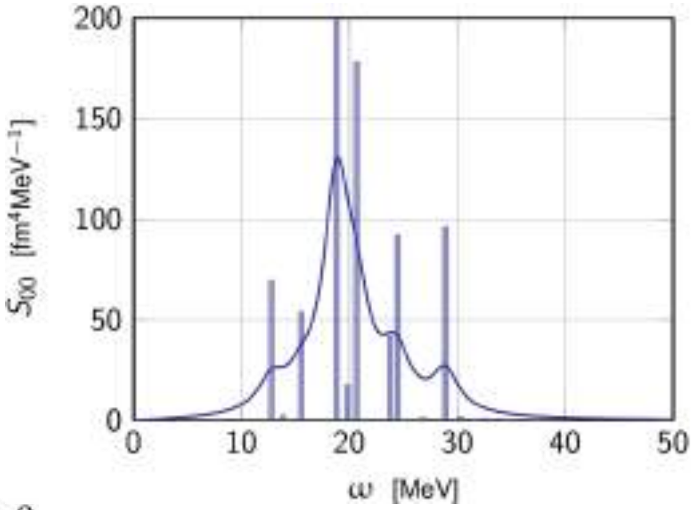

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Quantify the most relevant features of the strength

$$\bar{E}_1 = \frac{m_1}{m_0} \qquad \sigma^2 = \frac{m_2}{m_0} - \left(\frac{m_1}{m_0}\right)^2 \geq 0$$

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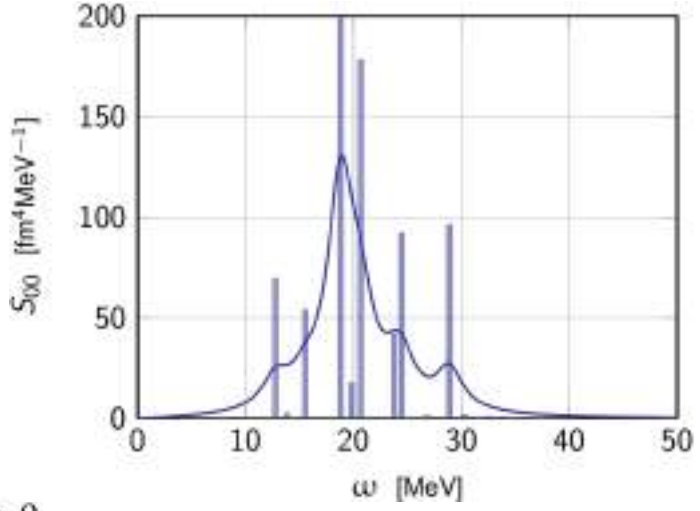

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Ab-initio PGCM and QRPA consistent numerical settings (systematic study in ^{46}Ti)

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

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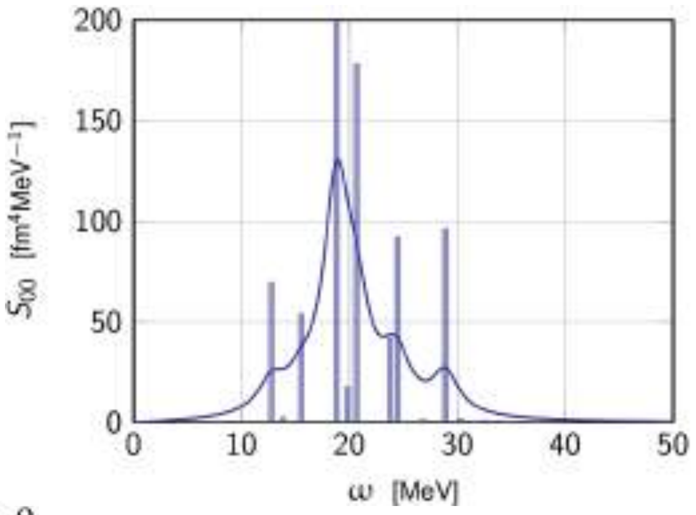

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Ab-initio PGCM and QRPA consistent numerical settings (systematic study in ^{46}Ti)

- 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 $\boldsymbol{\beta_2}$
- 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

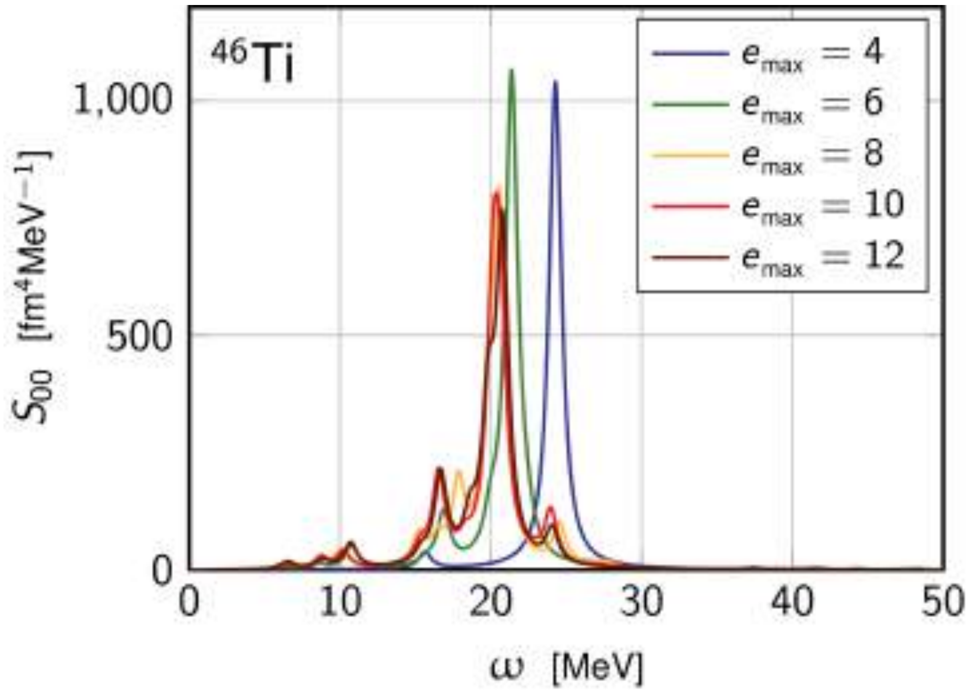
Finite Basis Size

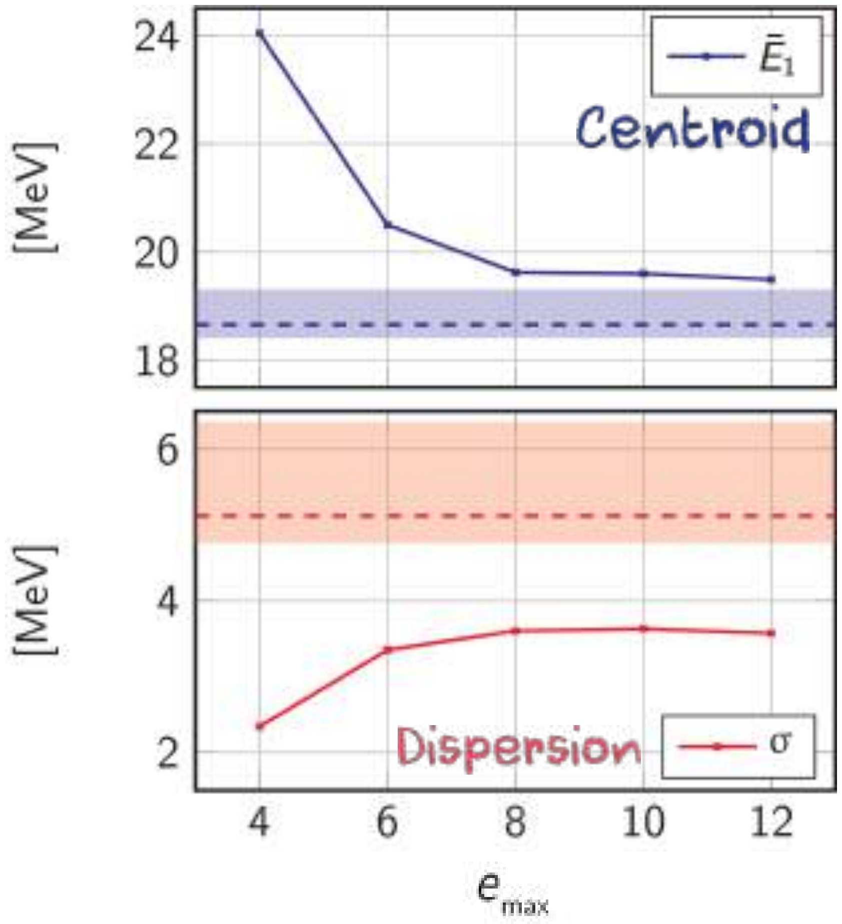
- Good **overall convergence**
- Centroid relative error ~ 0,6 %
- Dispersion relative error ~ 1,7 %
- $\mathbf{e_{3max}}$ not studied (14 safe for GS)

Hamiltonian parameters

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

Finite Basis Size





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[Myiagi et al., PRC, 2022]

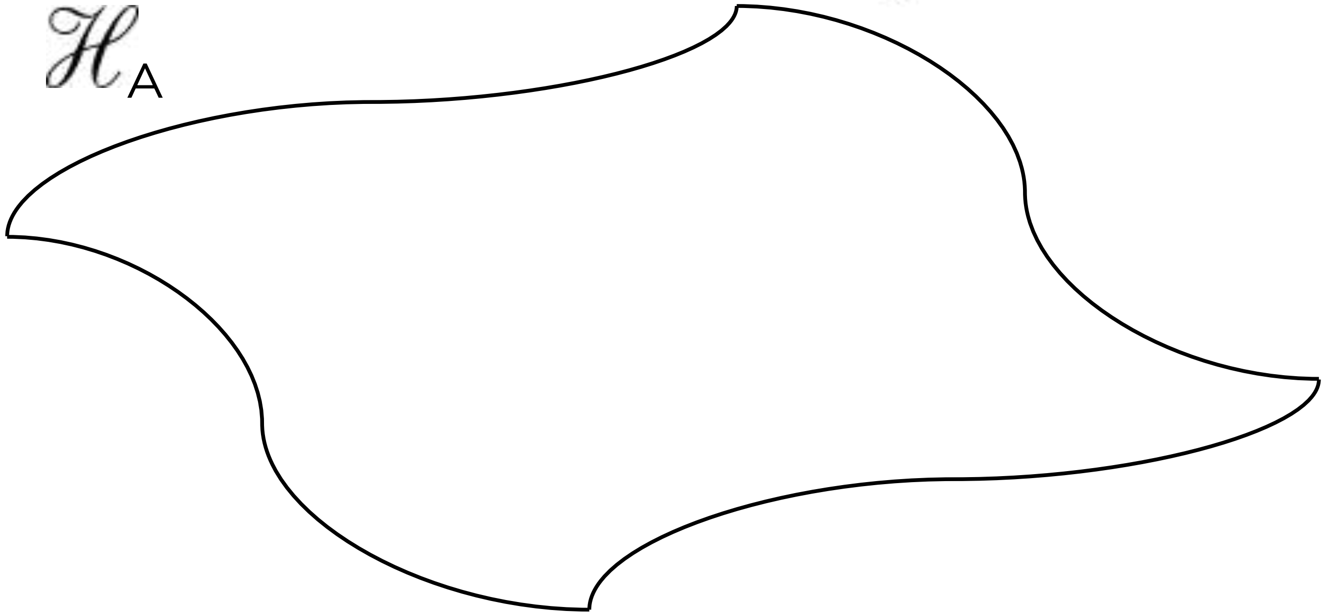
Many-body truncation

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

Exact solution

A-body Hilbert space

$\mathcal{H}_A$



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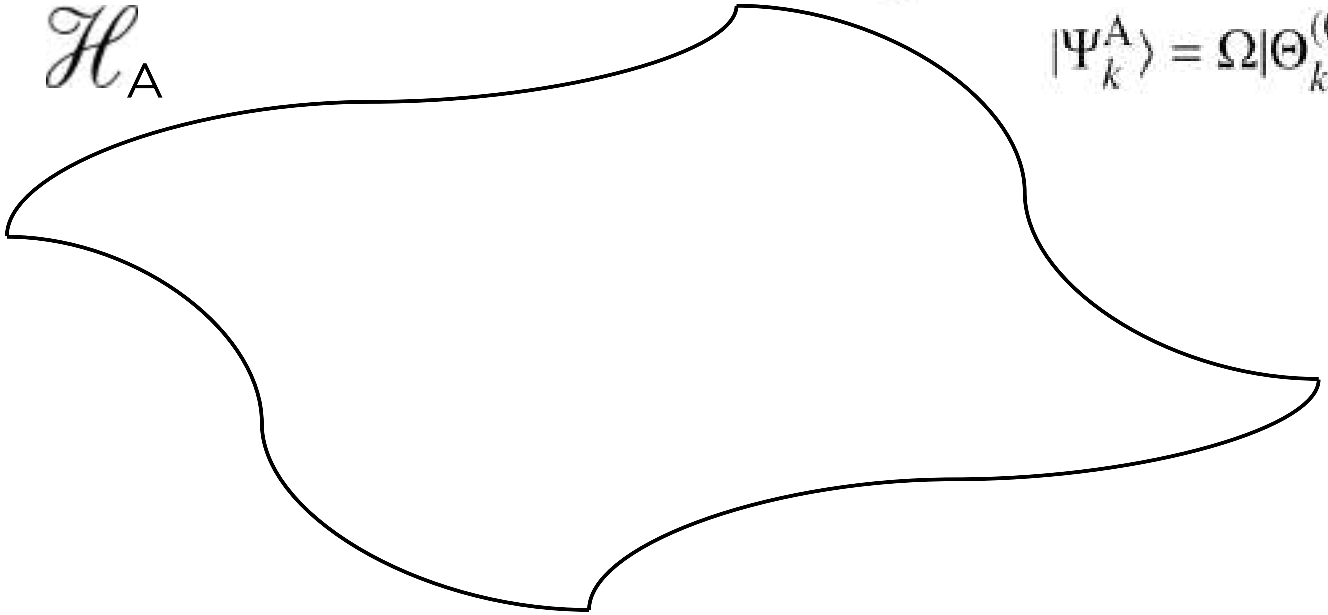

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PGCM : multi-reference unperturbed state

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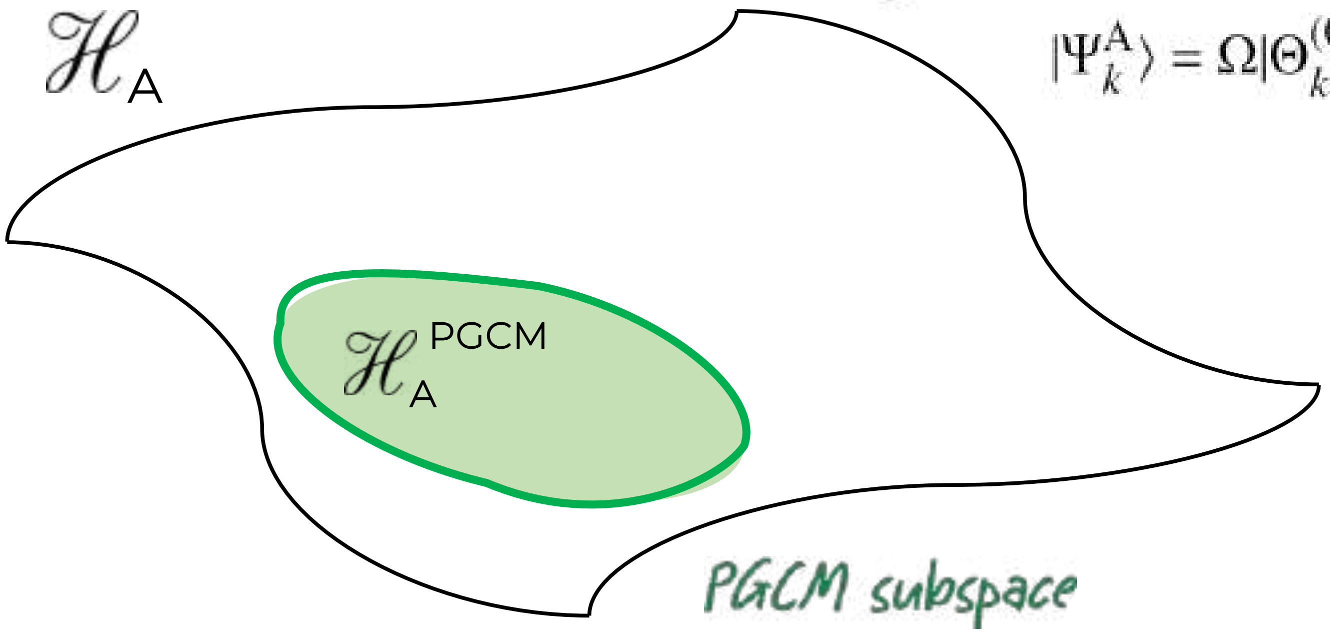

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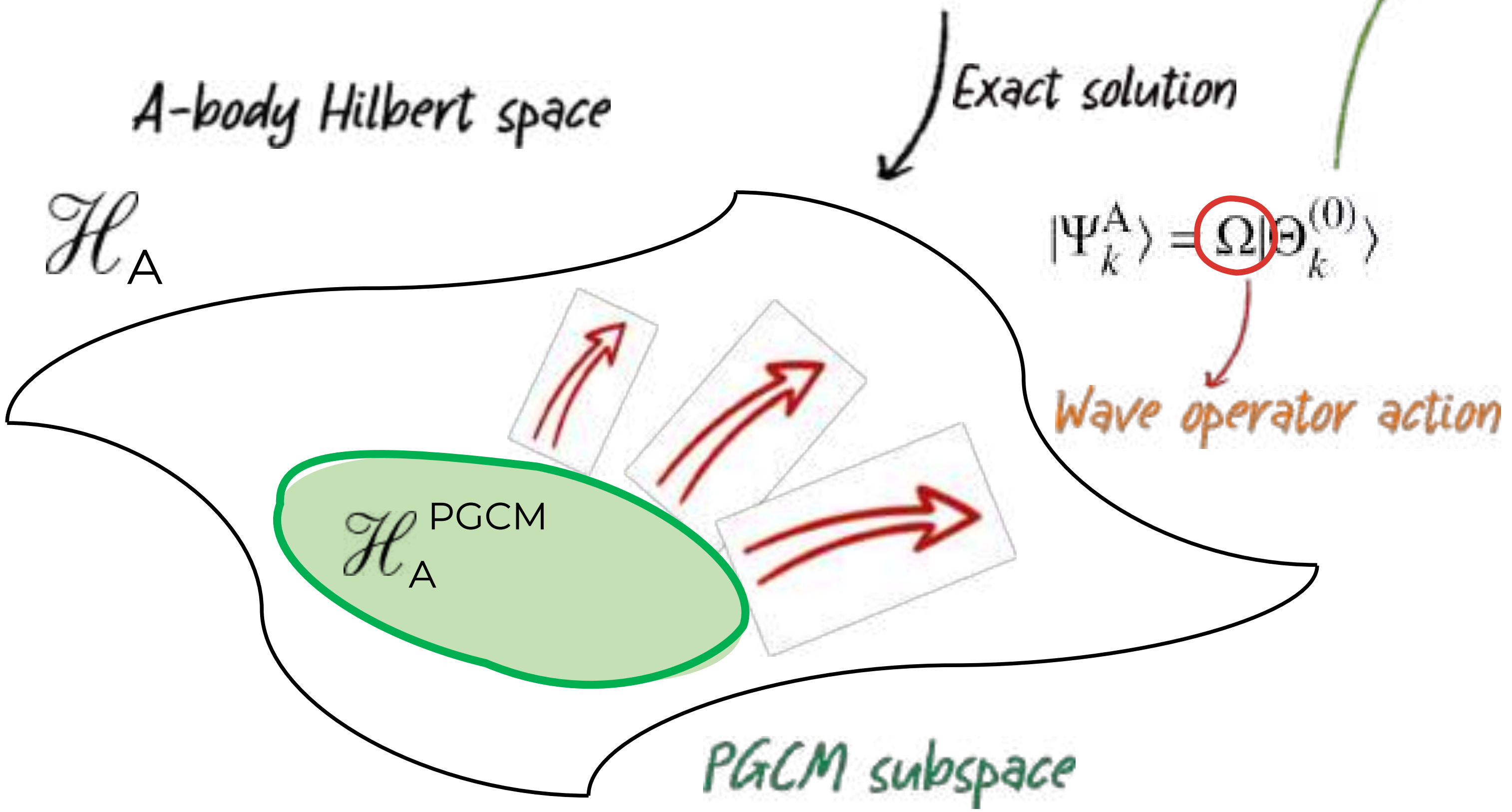

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PGCM : multi-reference unperturbed state

PGCM-PT : ab initio expansion method[1]

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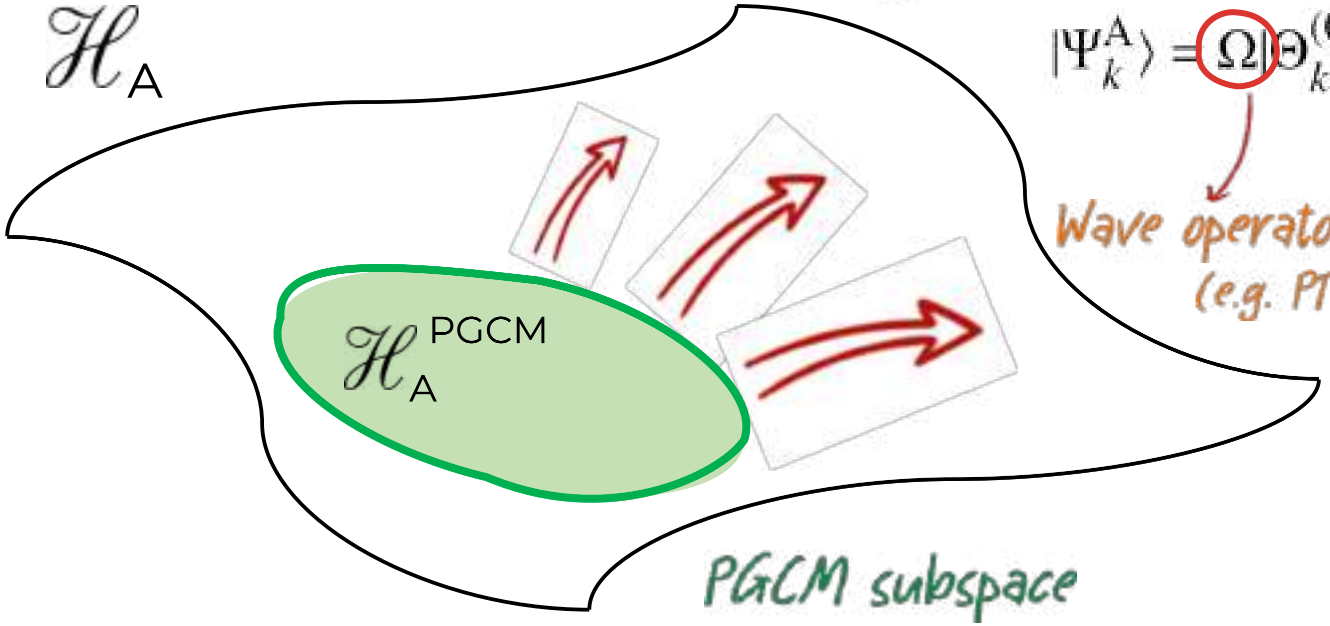

$$|\Psi_k^{\mathrm{A}}\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

Wave operator action
(e.g. PT)

PGCM subspace

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

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

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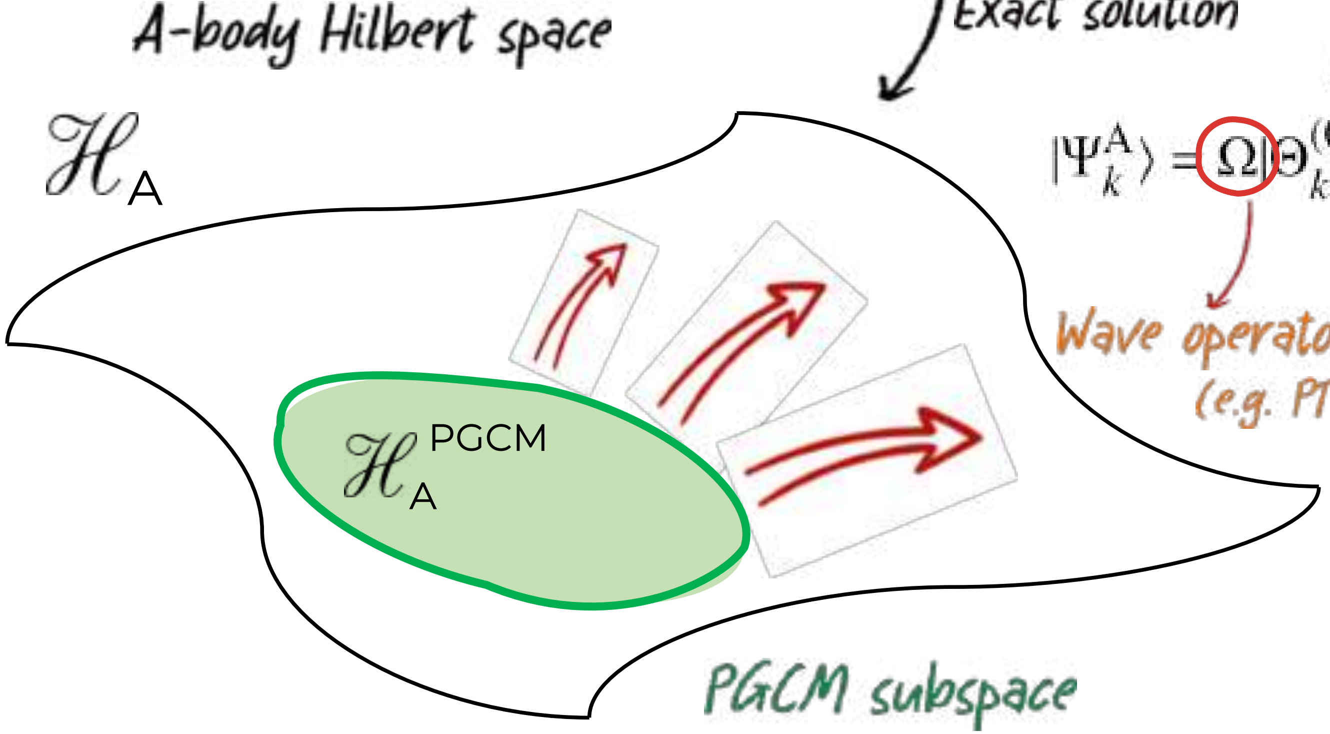

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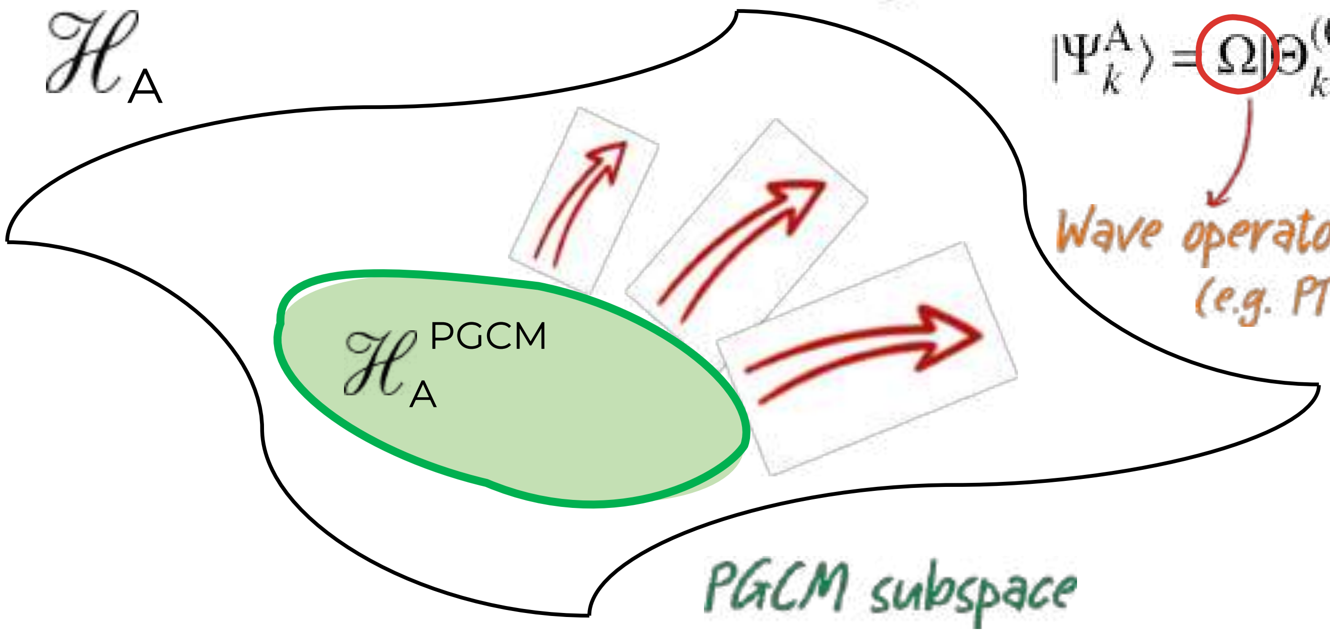

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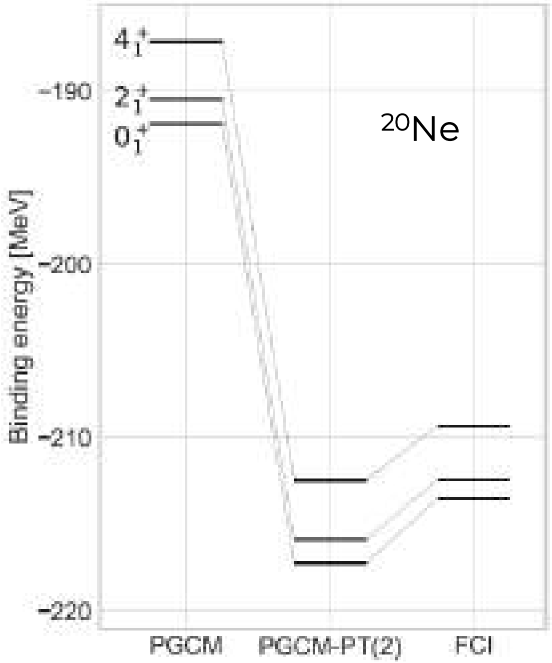

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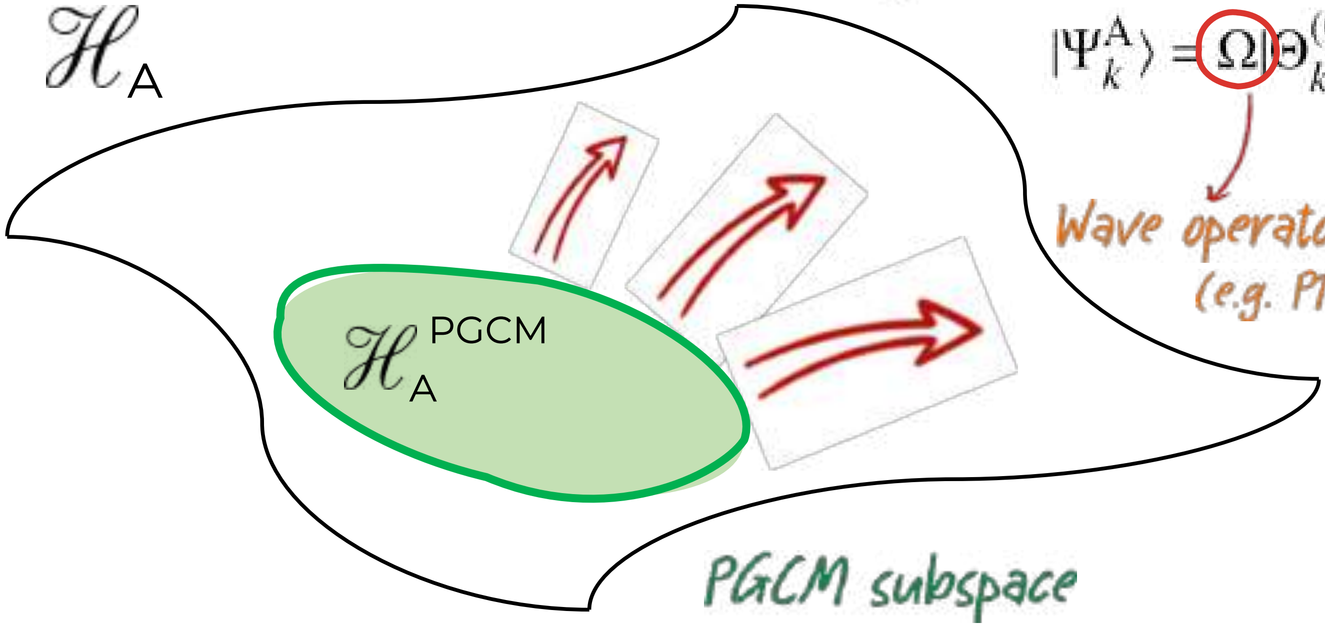

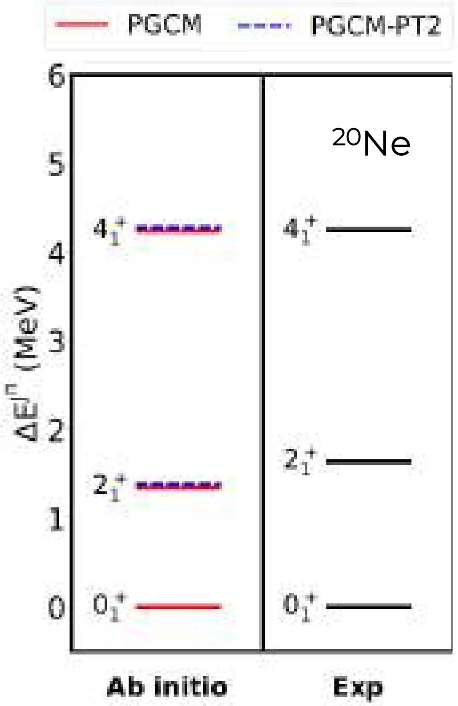

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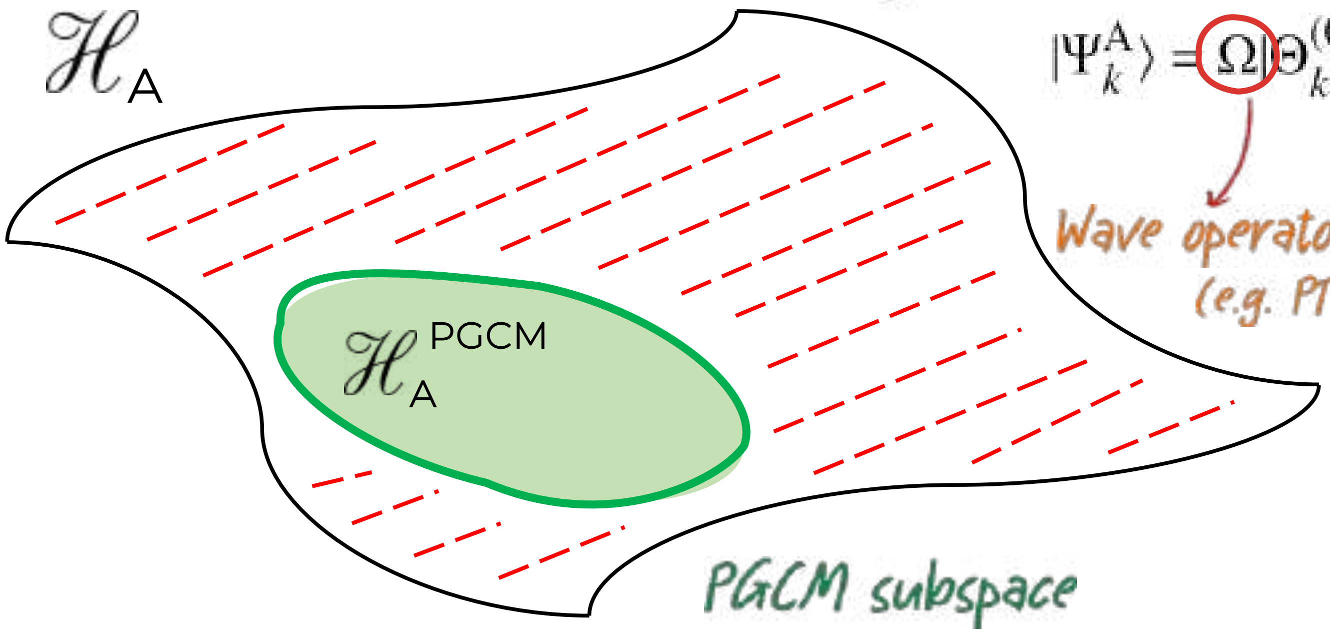

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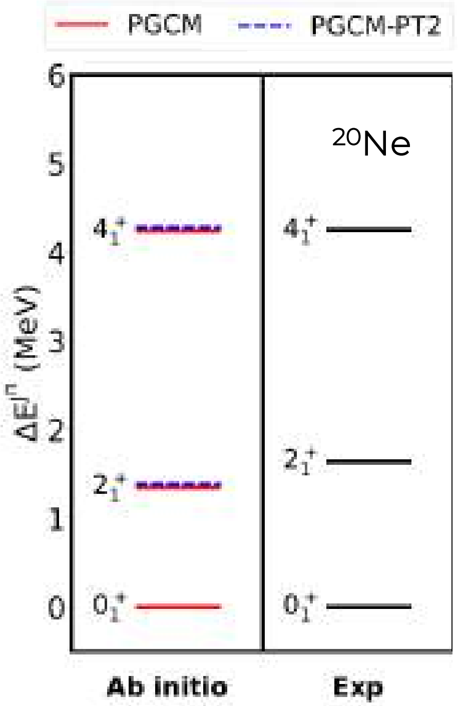
Wave operator action
(e.g. PT)

Dynamical correlations mostly cancel out

PGCM reliable for low-lying collective spectroscopy



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Outline

1 Introduction
- Giant Resonances Physics
- The PGCM
- Link between PGCM and QRPA

2 Systematic study
- Numerical details
- Uncertainty estimate

Results 3

Selected applications
- Shape coexistence
- Deformation

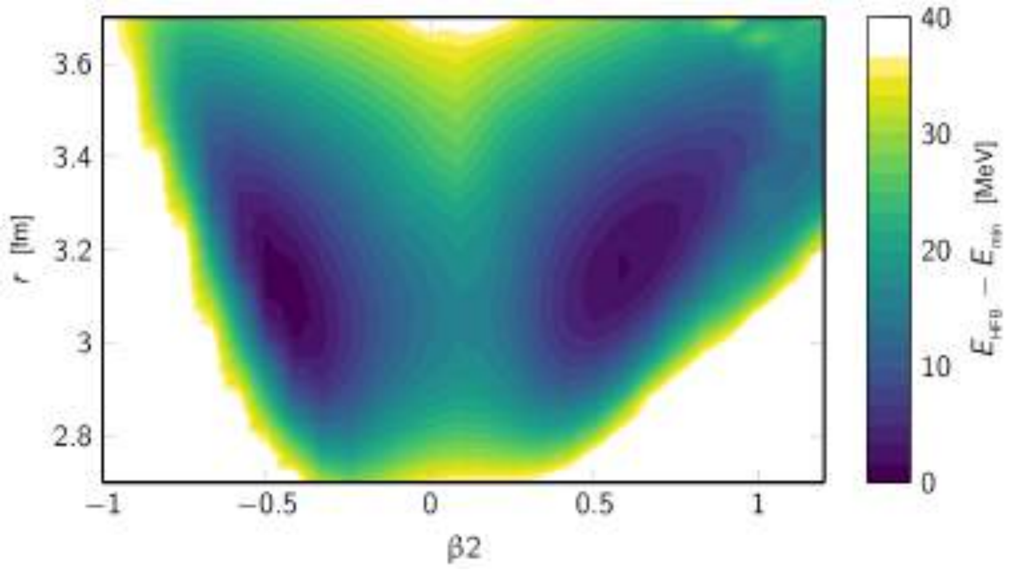
Multi-phonon states
- Proof of principle
- Realistic calculations

From finite nuclei to Astrophysics
- Preliminary incompressibility results

Conclusions and perspectives

Shape coexistence effects in ^{28}Si

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



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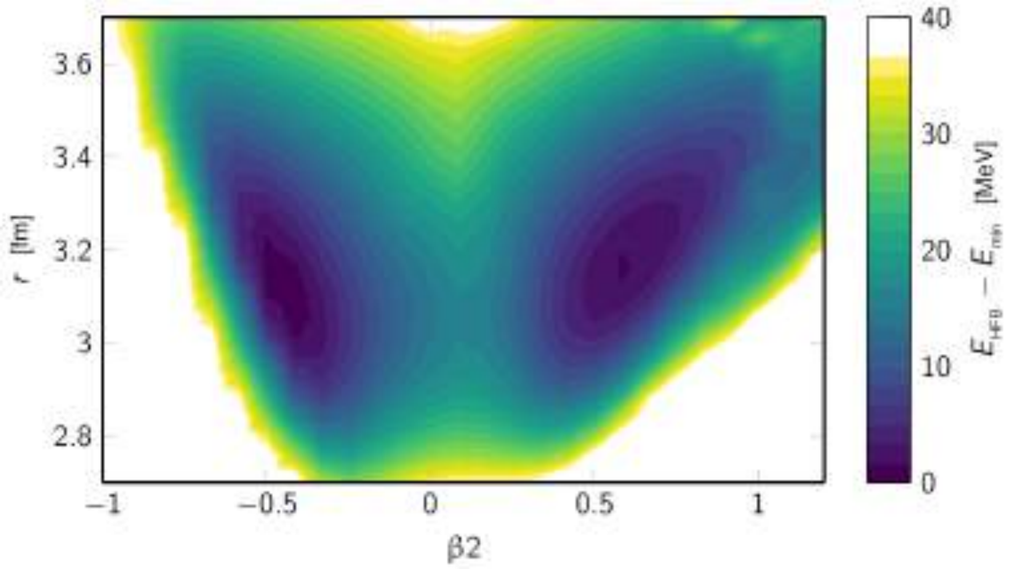

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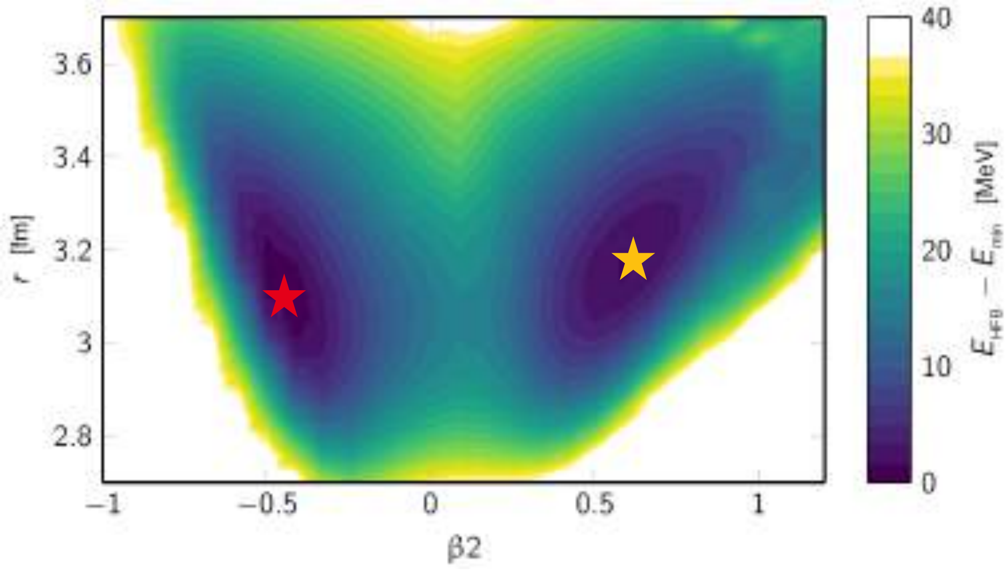

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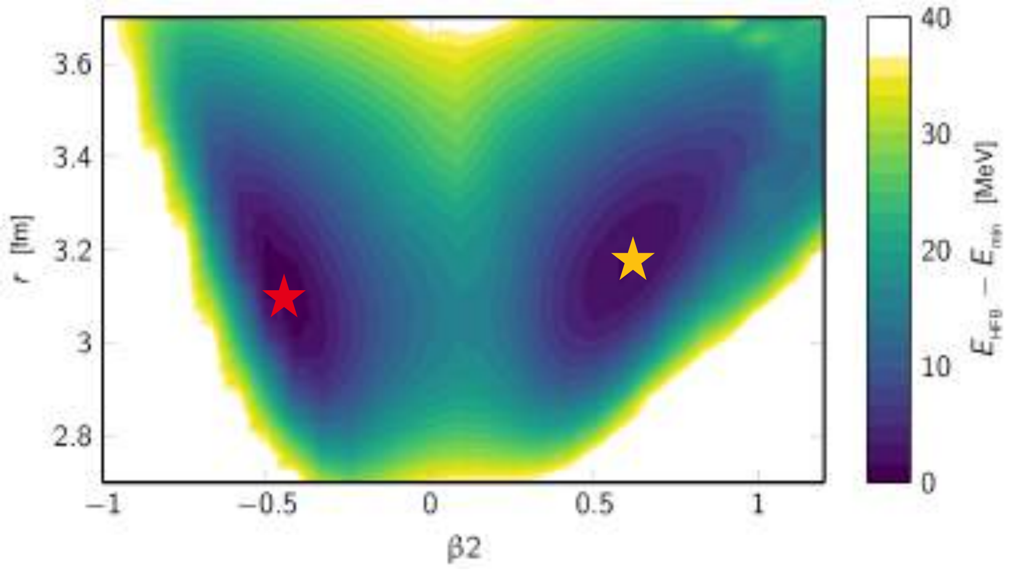

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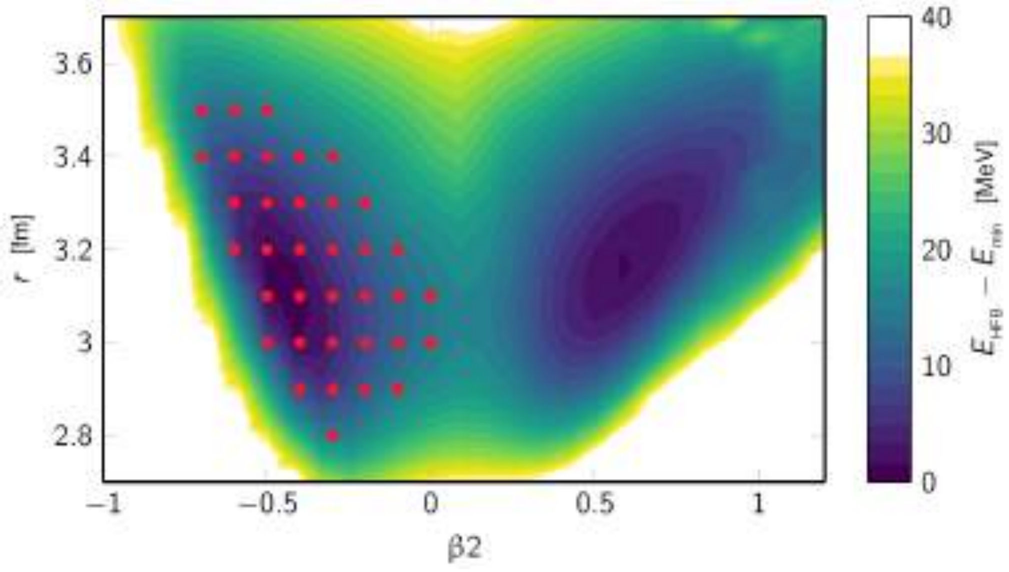

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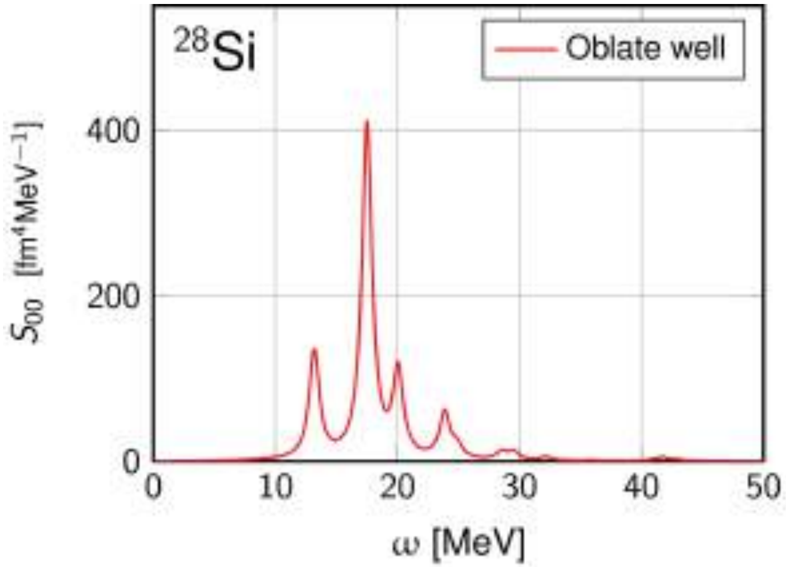

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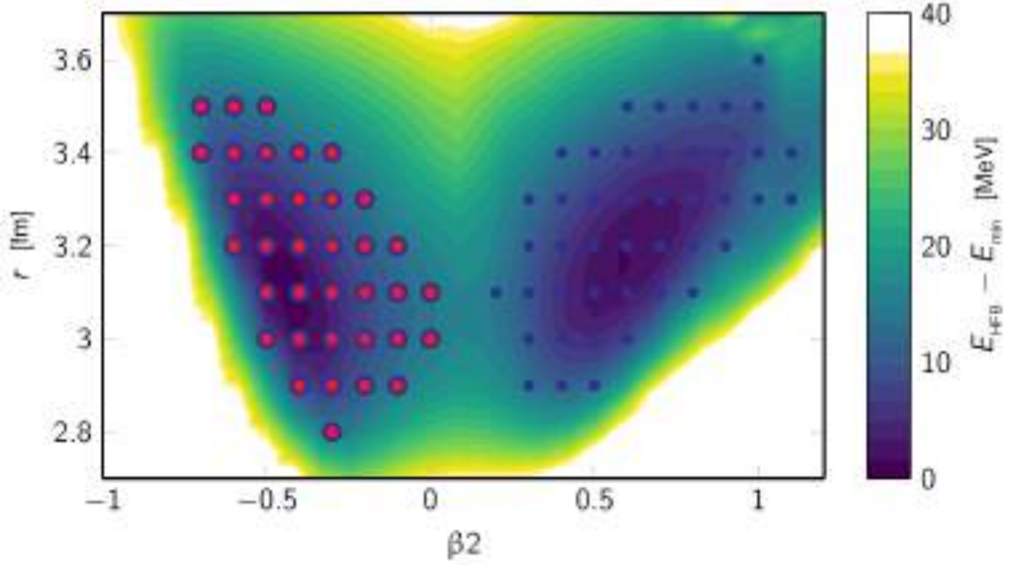

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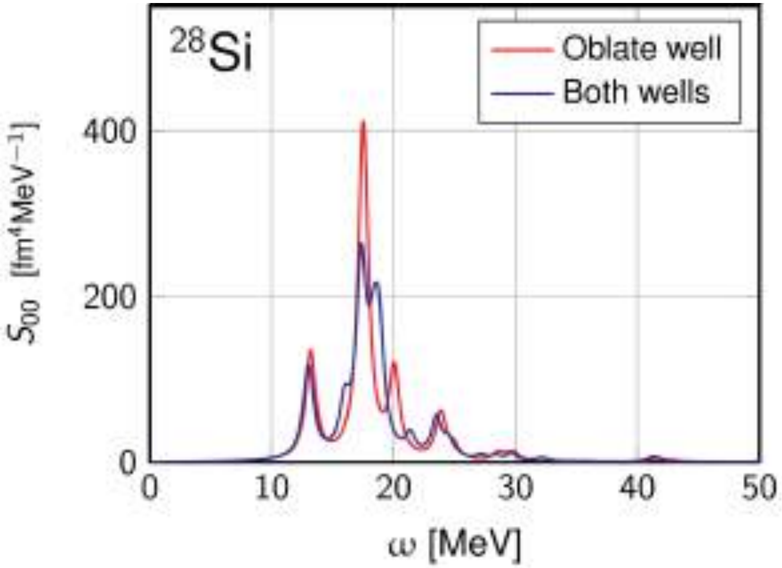

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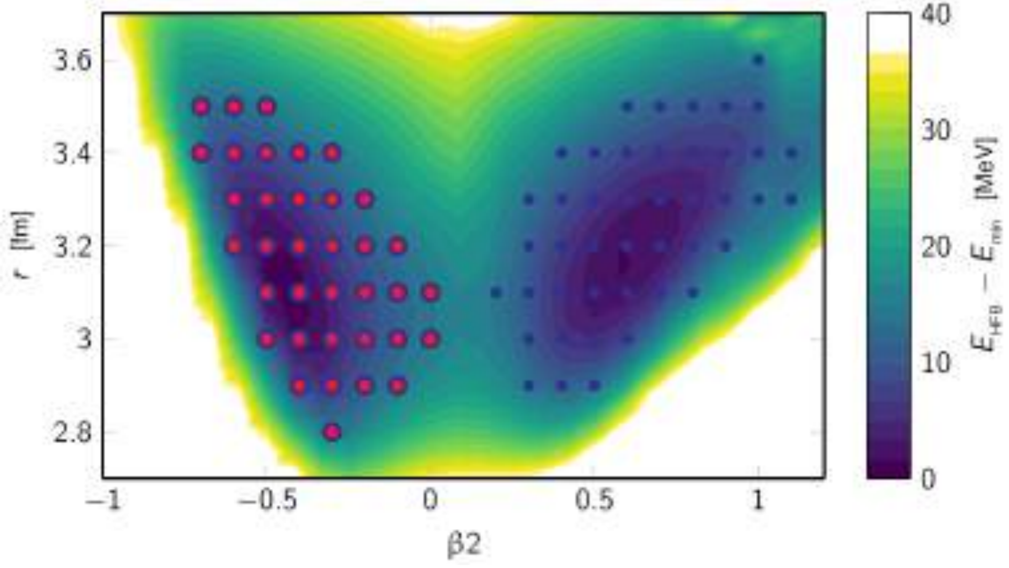

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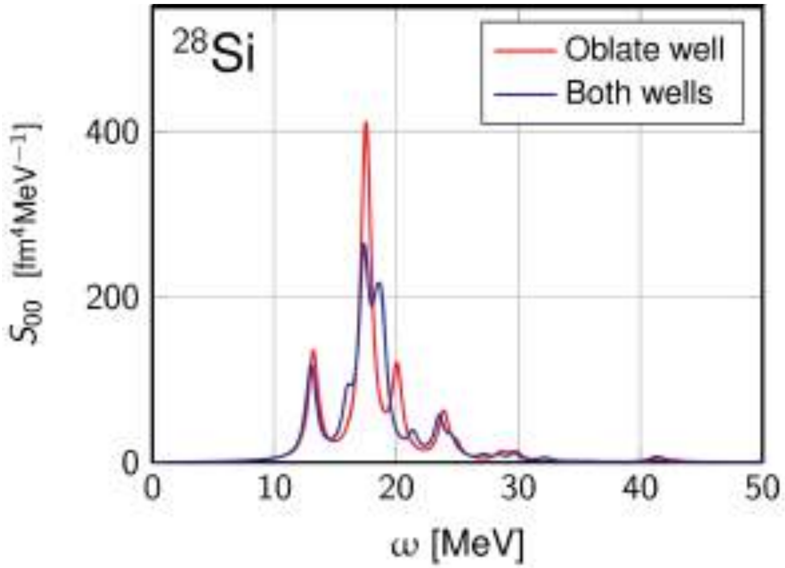

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Nuclei with stronger signature ?

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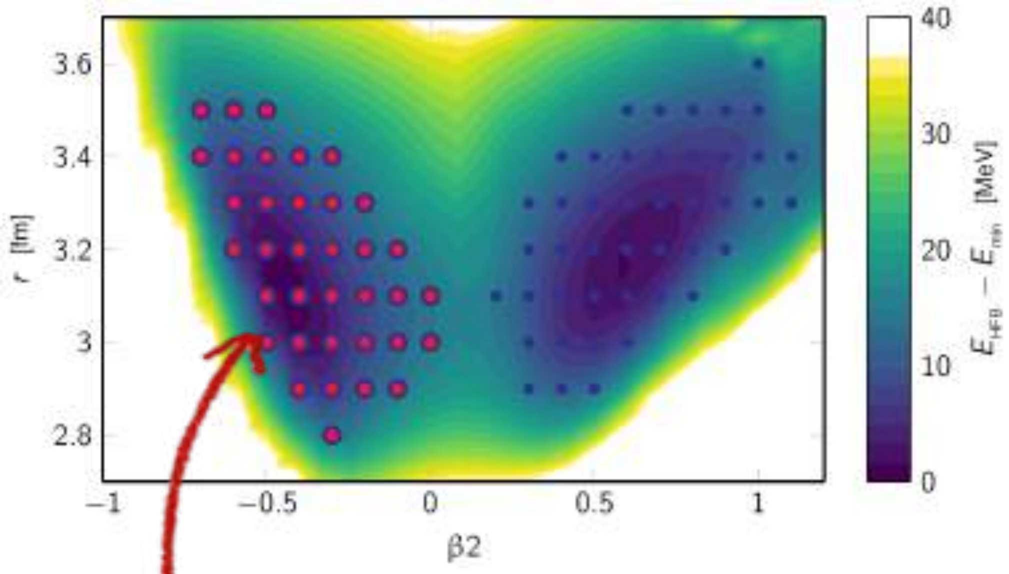

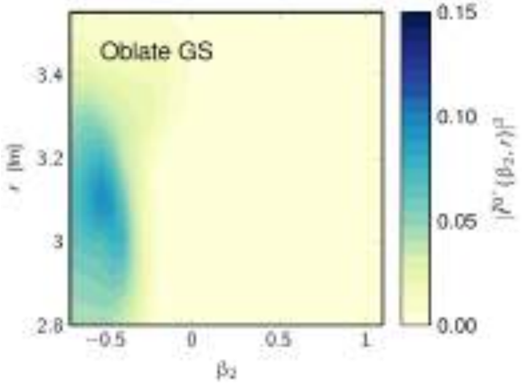

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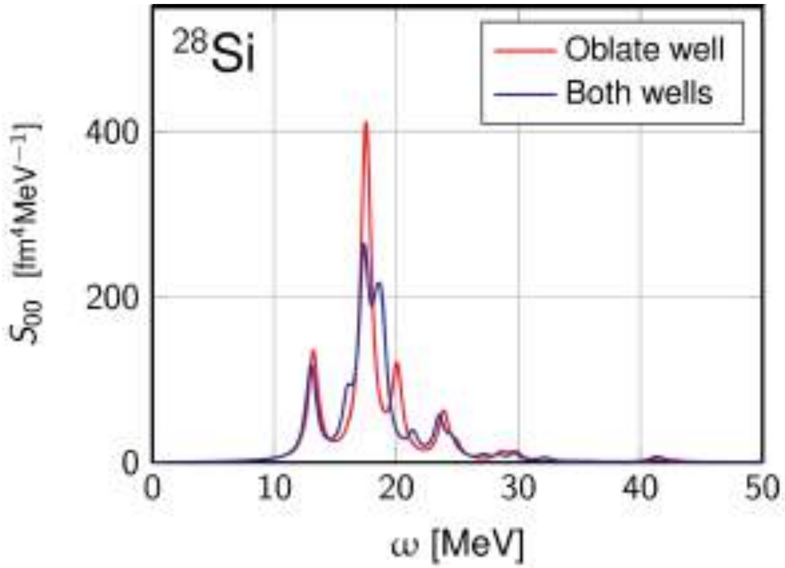

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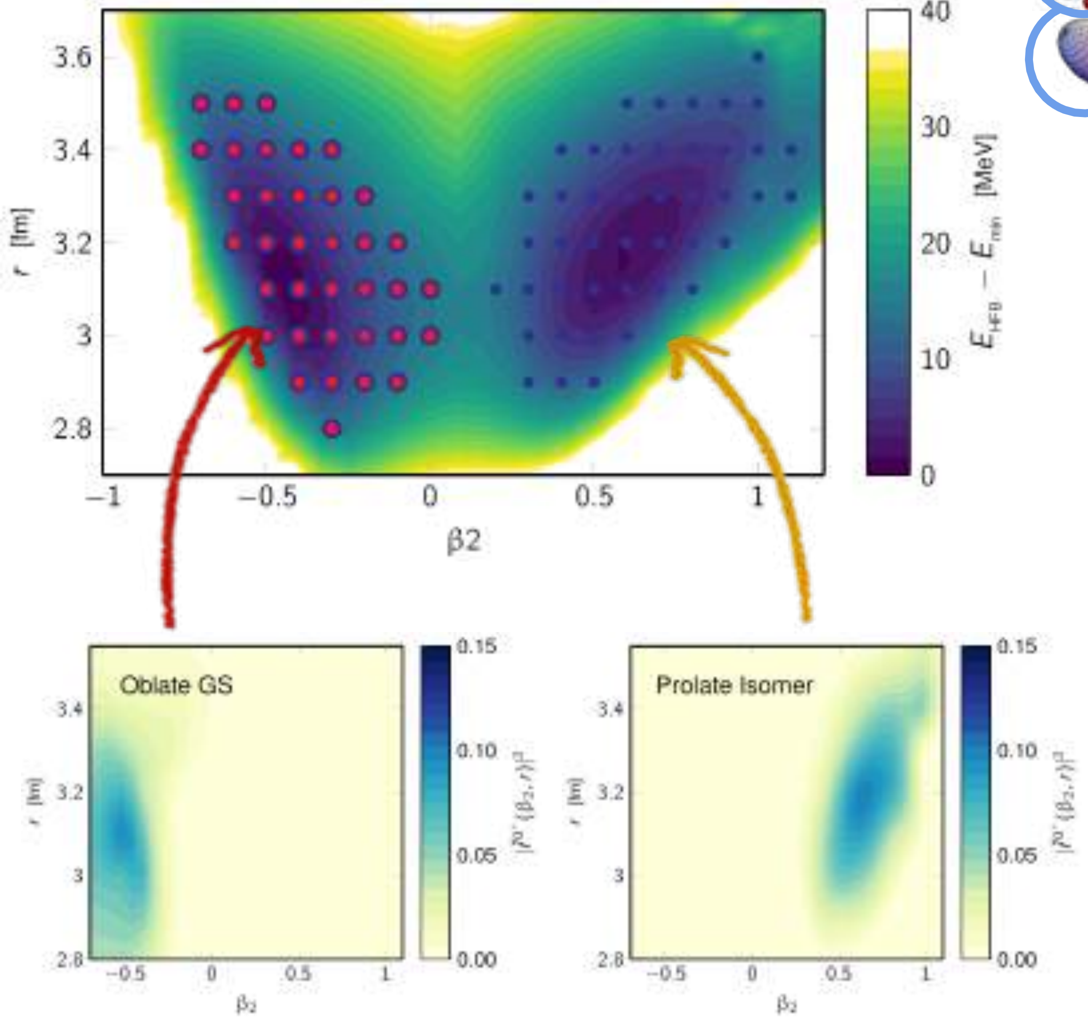

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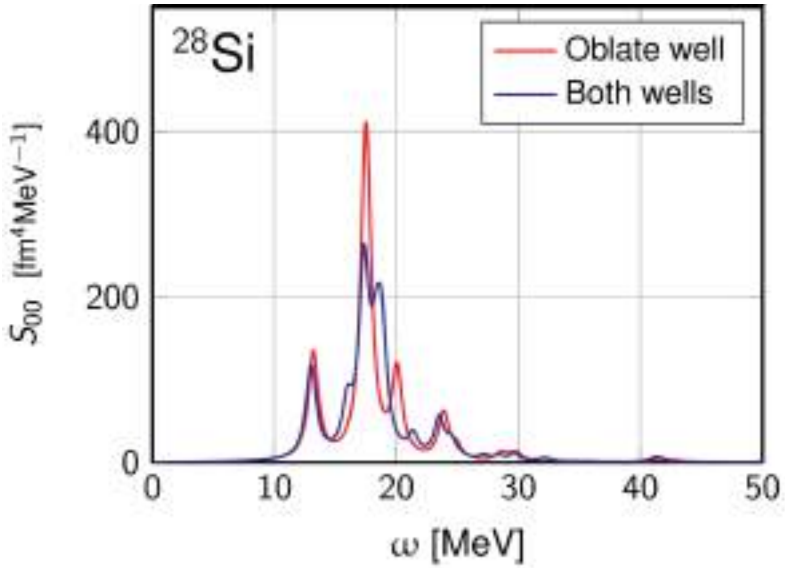

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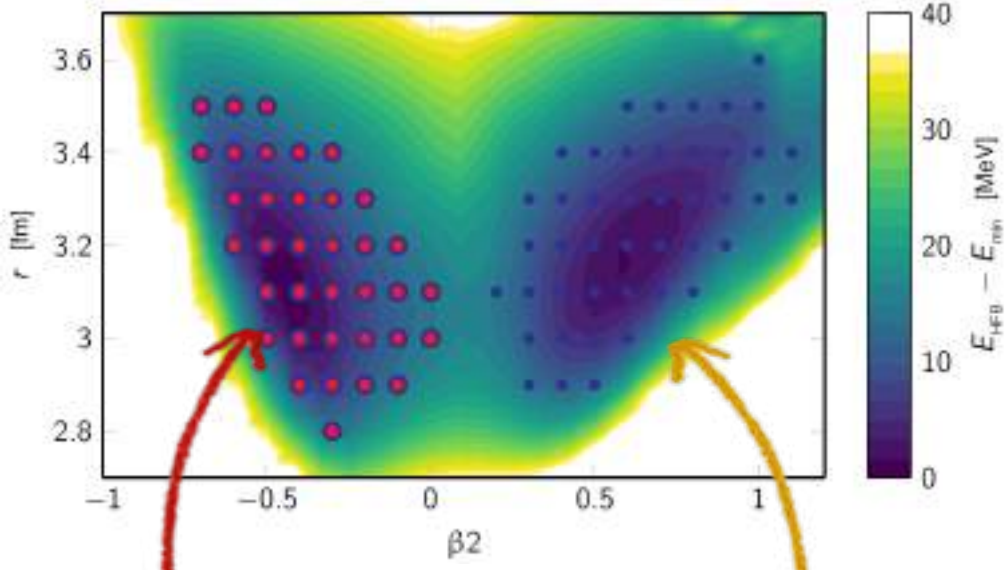

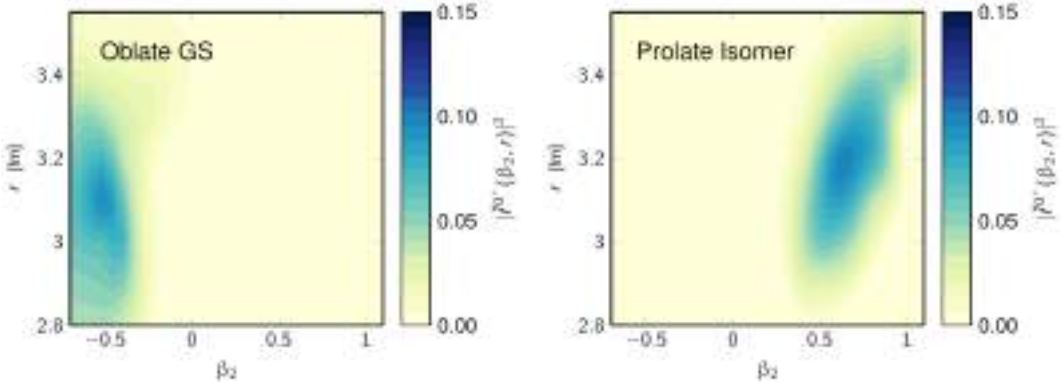

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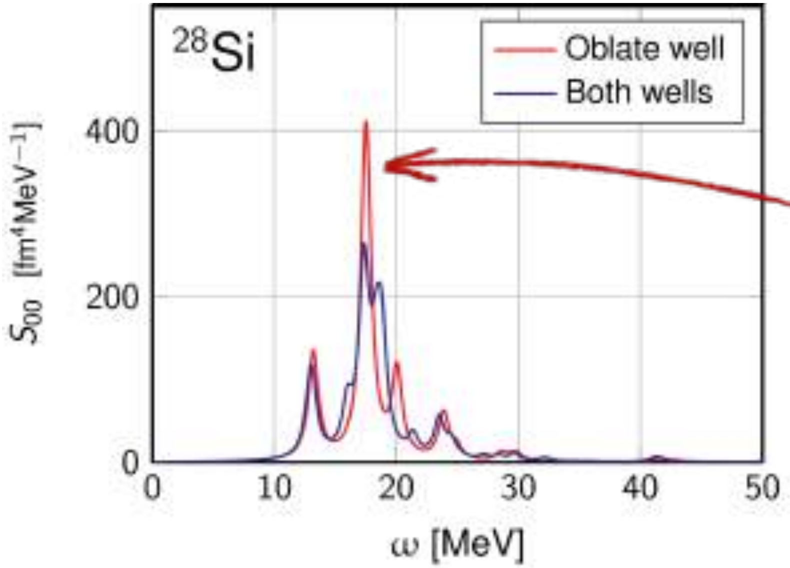
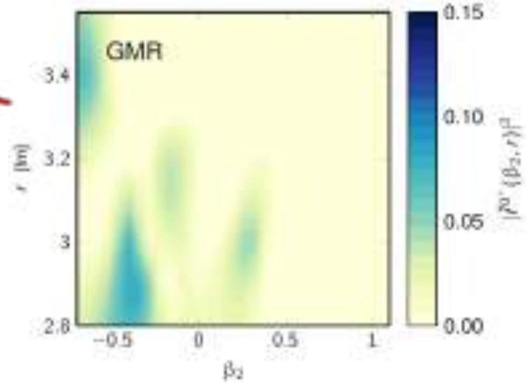


Radial vibration on oblate GS



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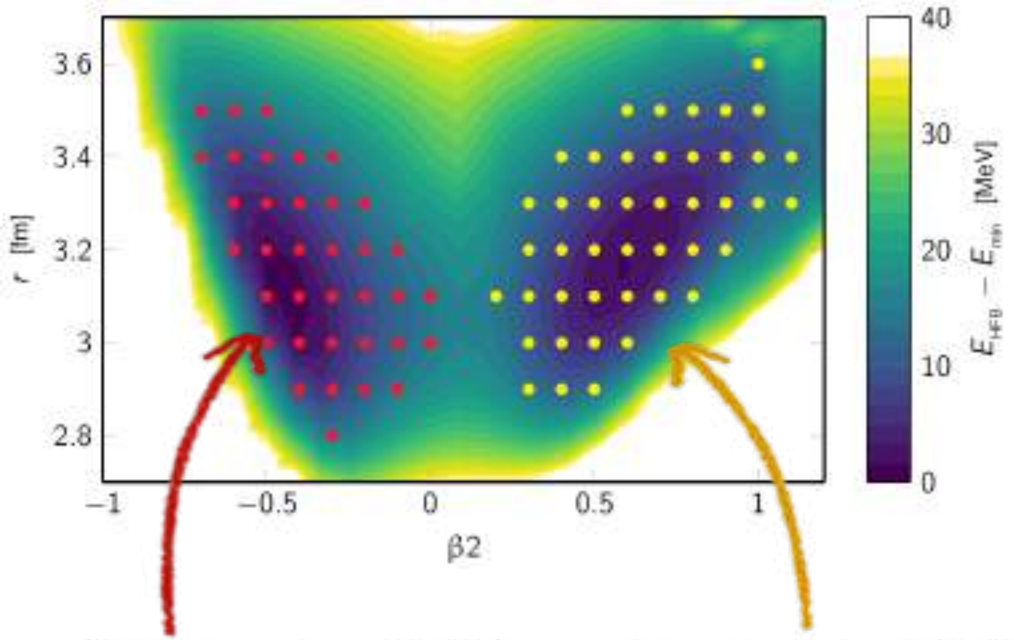
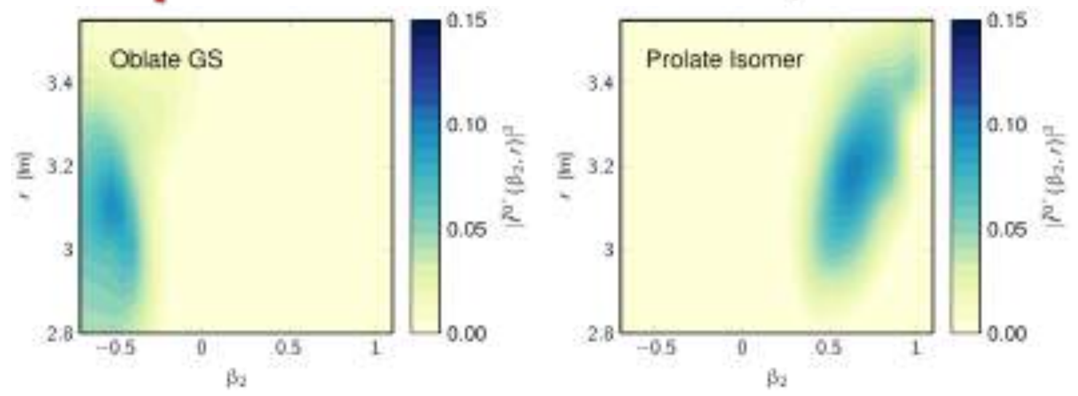
Shape coexistence effects in ^{28}Si

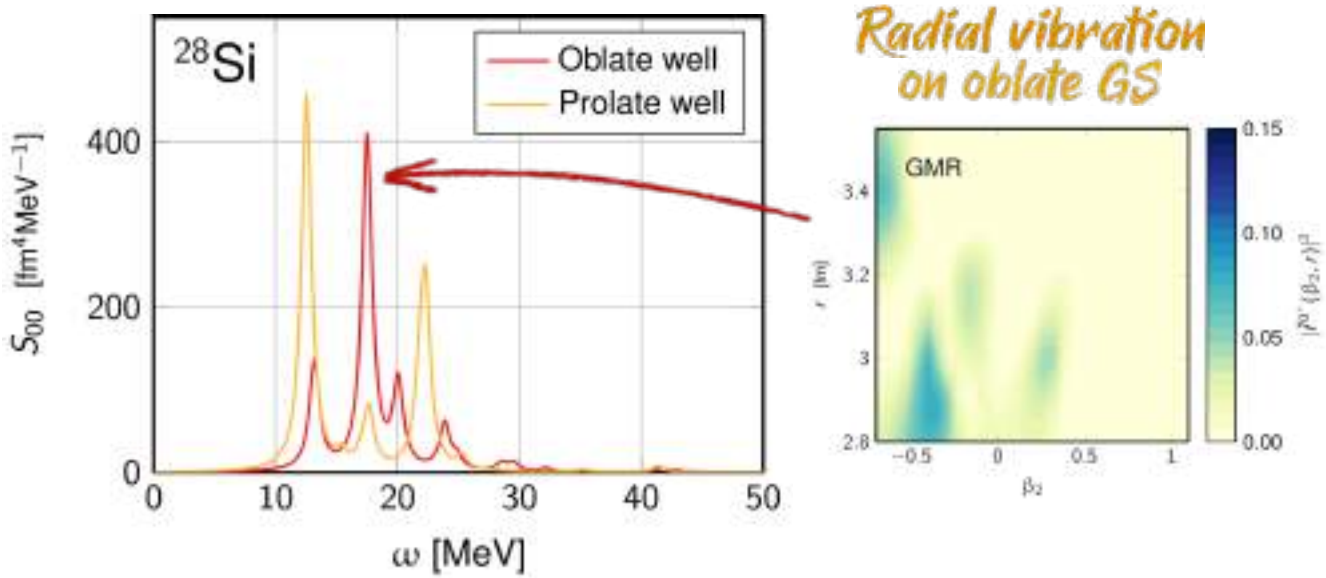
Total Energy Surface $E_{HFB}(\beta_2,r)$





Shape coexistence [Jenkins et al., 2012]

Deformation



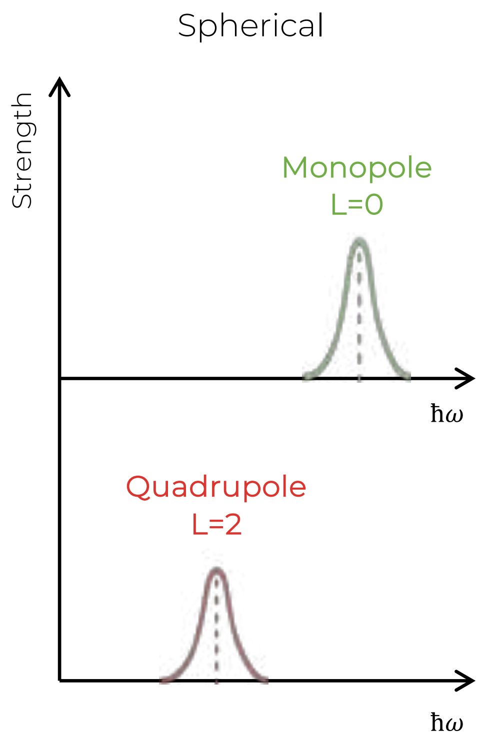
- Oblate GS and prolate-shape isomer
- Proper study of shape coexistence in PGCM
  - Shape coexistence but weak mixing

Nuclei with stronger signature ?

Deformation effects

Deformation effects

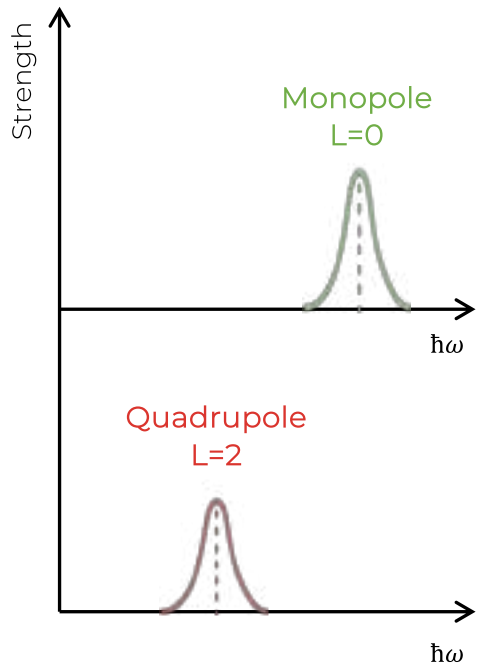
Spherical
(no deformation)



Deformation effects

Spherical
(no deformation)

Spherical

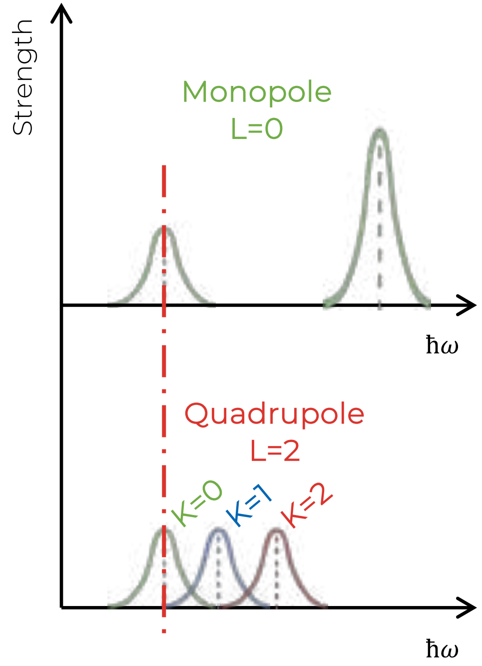


Spheroidal
(deformed)

Prolate
(cigar type)

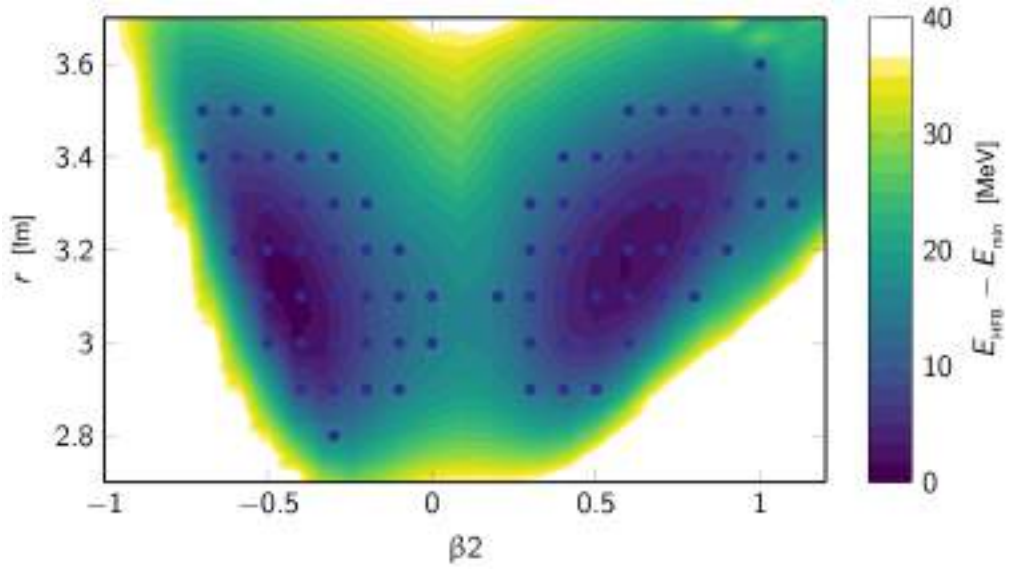
Oblate
(pancake type)

Deformed



Deformation effects in prolate ^{28}Si

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



Deformation effects in prolate ^{28}Si

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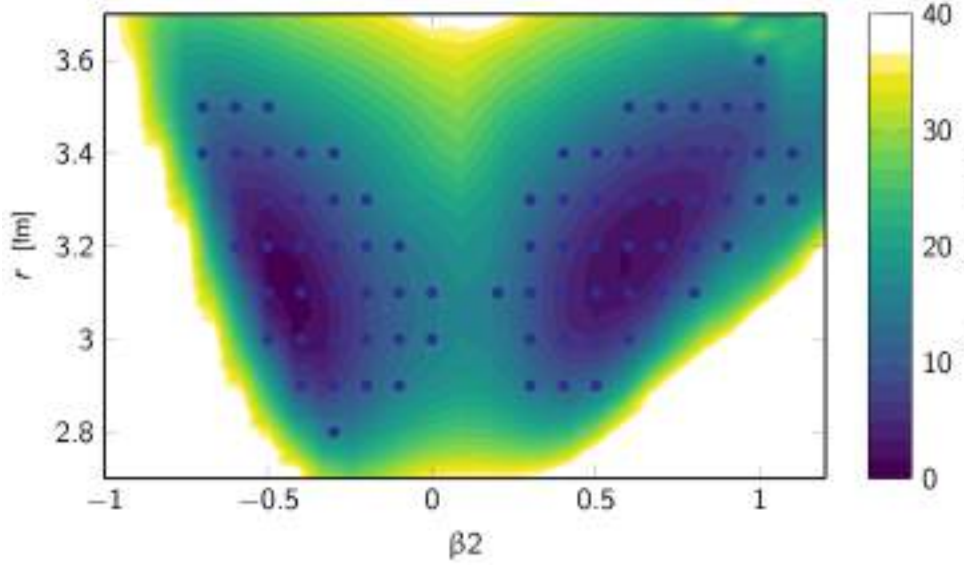
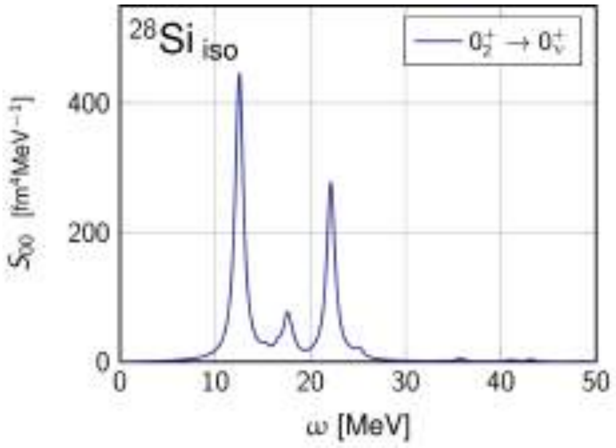
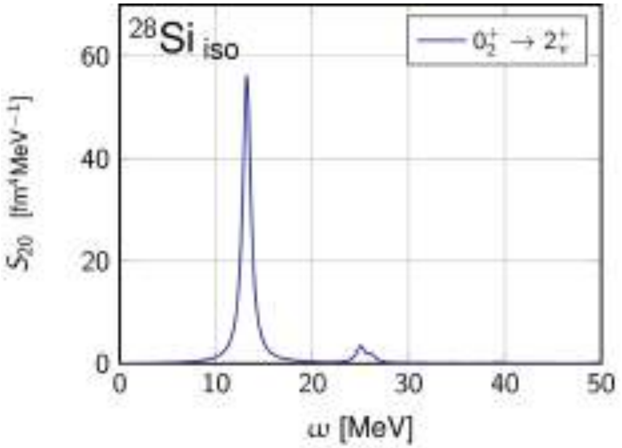


Monopole Strength



K=0 Quadrupole Strength



- Focus on the prolate-shape isomer
- Coupling to GQR generates splitting
  - x High peak = shifted “spherical” breathing mode
  - x Low peak = induced by coupling to GQR (K=0)
- Two-peak GMR on the prolate shape isomer

Deformation effects in prolate ^{28}Si

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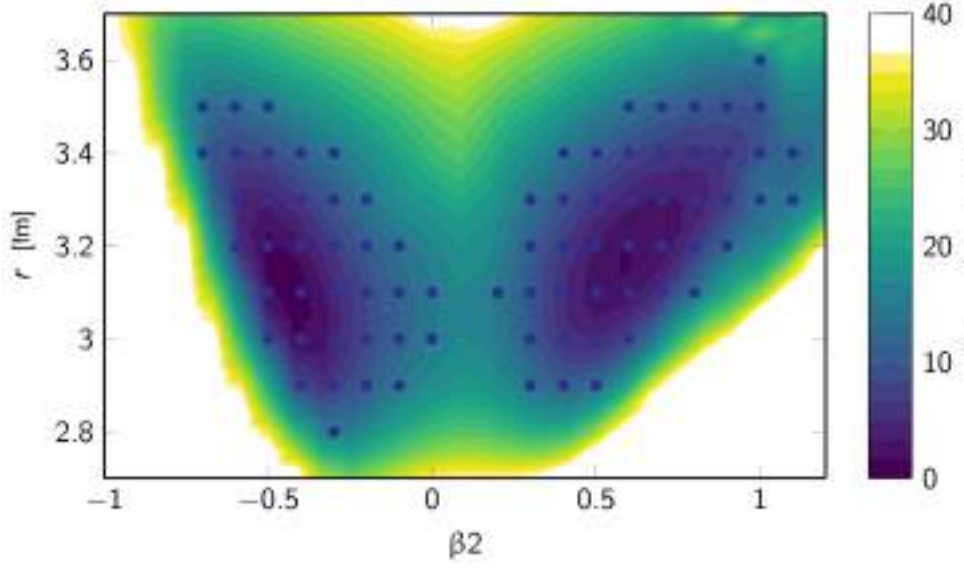

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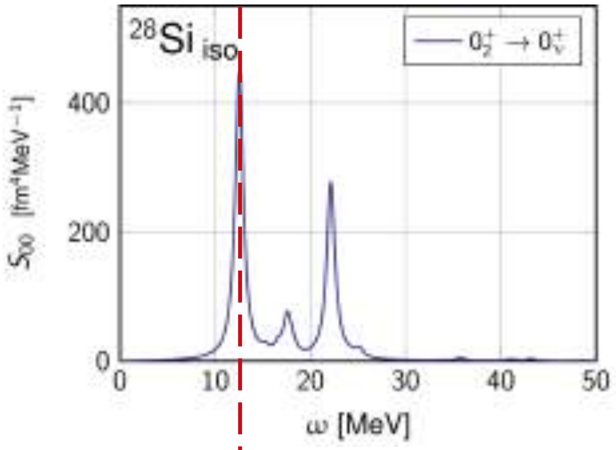

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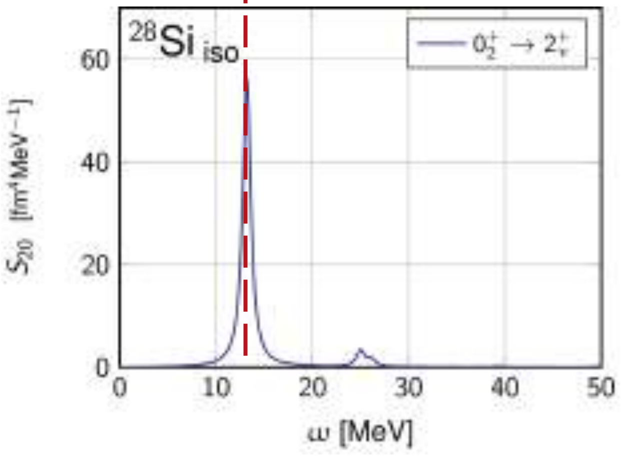

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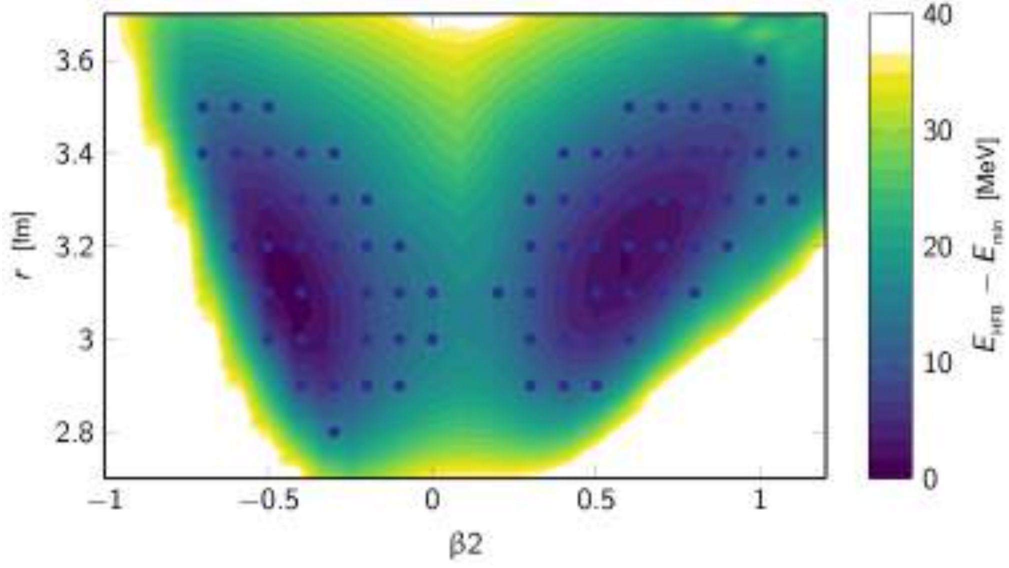

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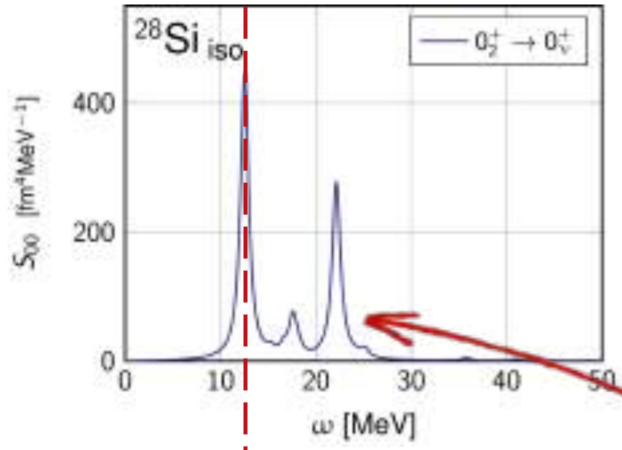

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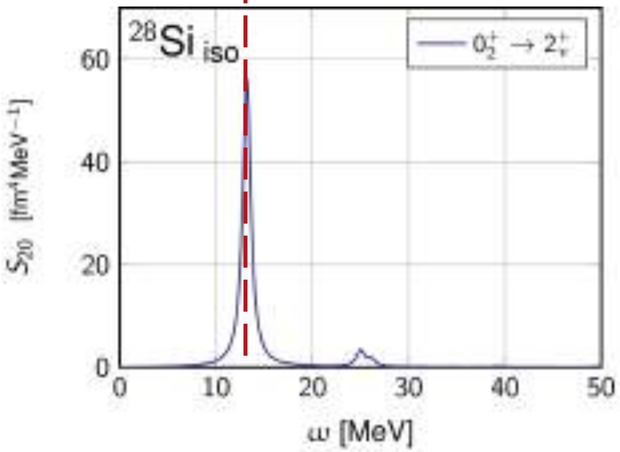

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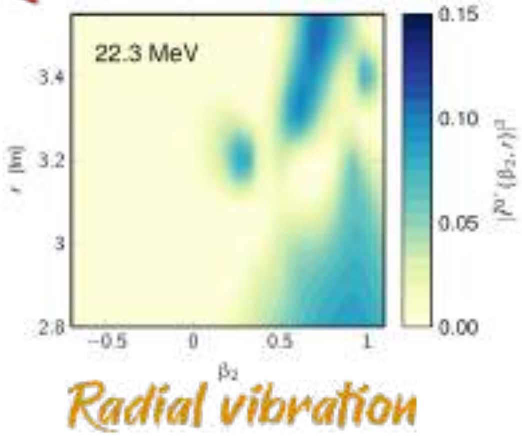

Deformation effects in prolate ^{28}Si

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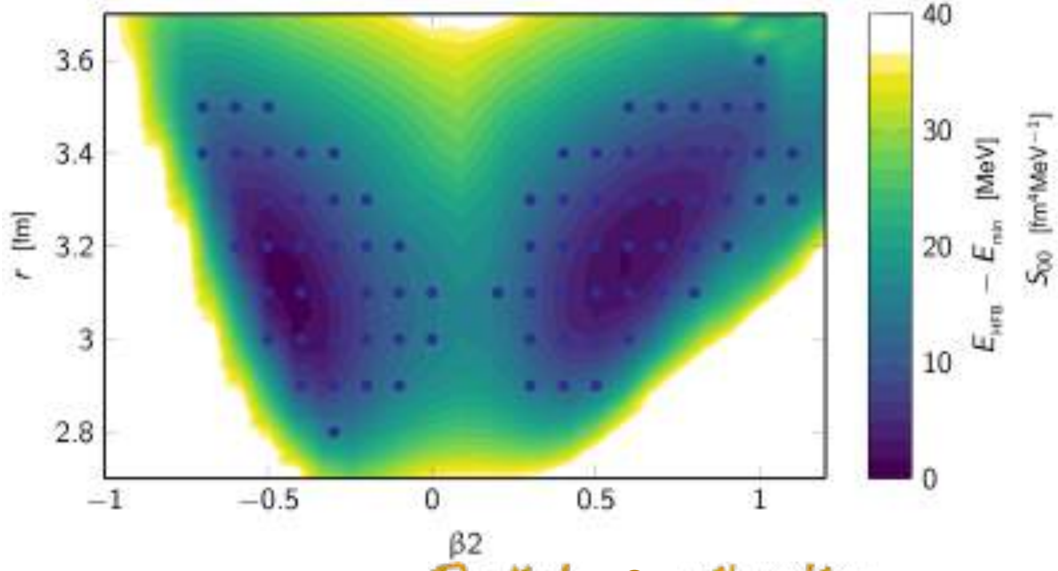
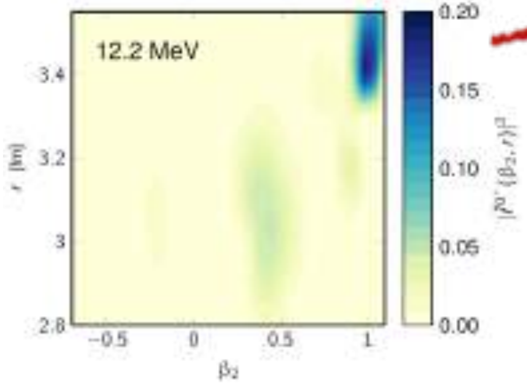
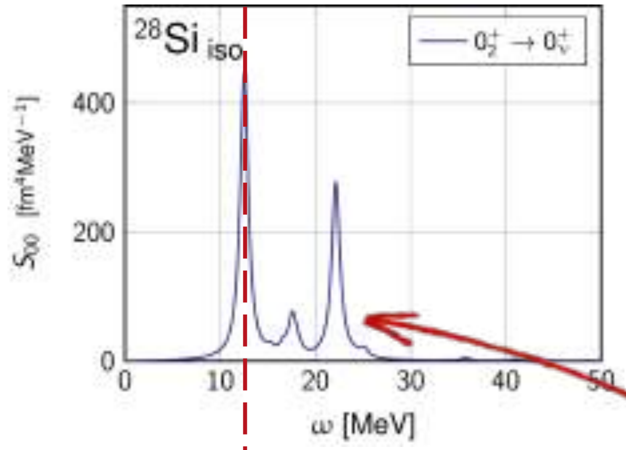


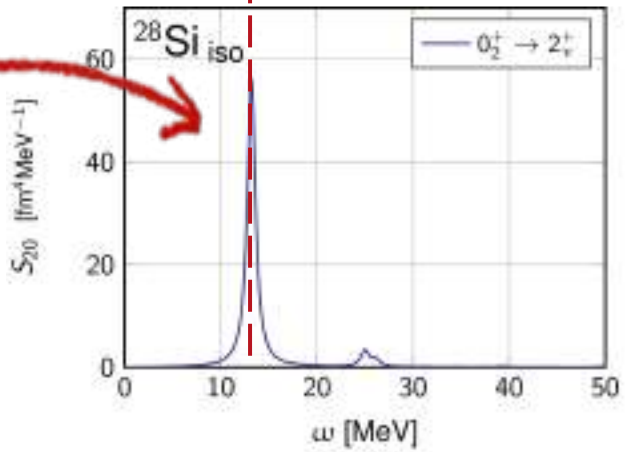
Radial + β_2 vibration



Monopole Strength



K=0 Quadrupole Strength



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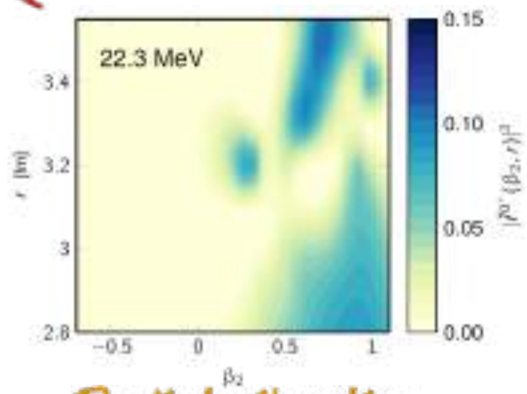
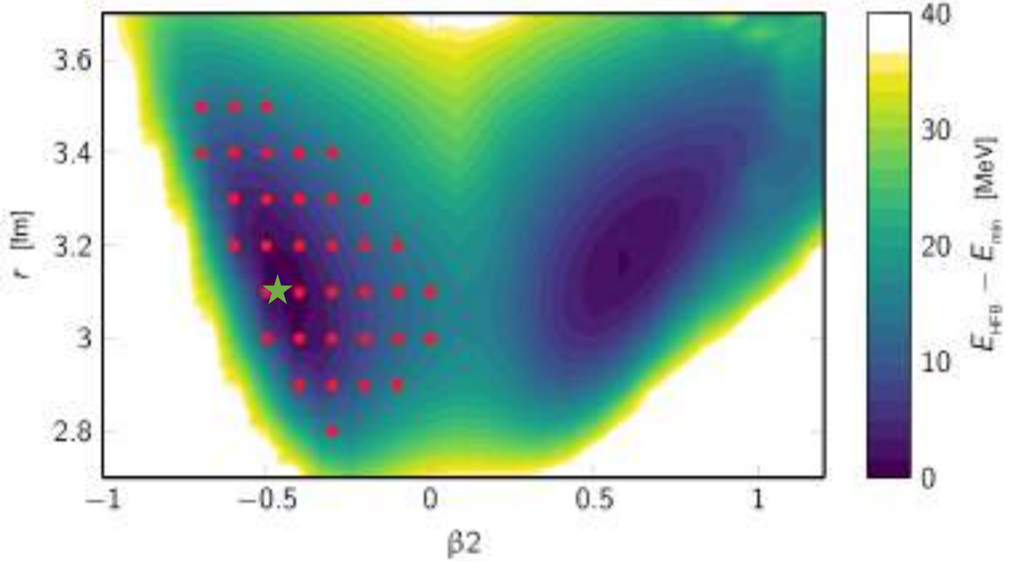


Radial vibration

Anharmonic effects

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



Anharmonic effects

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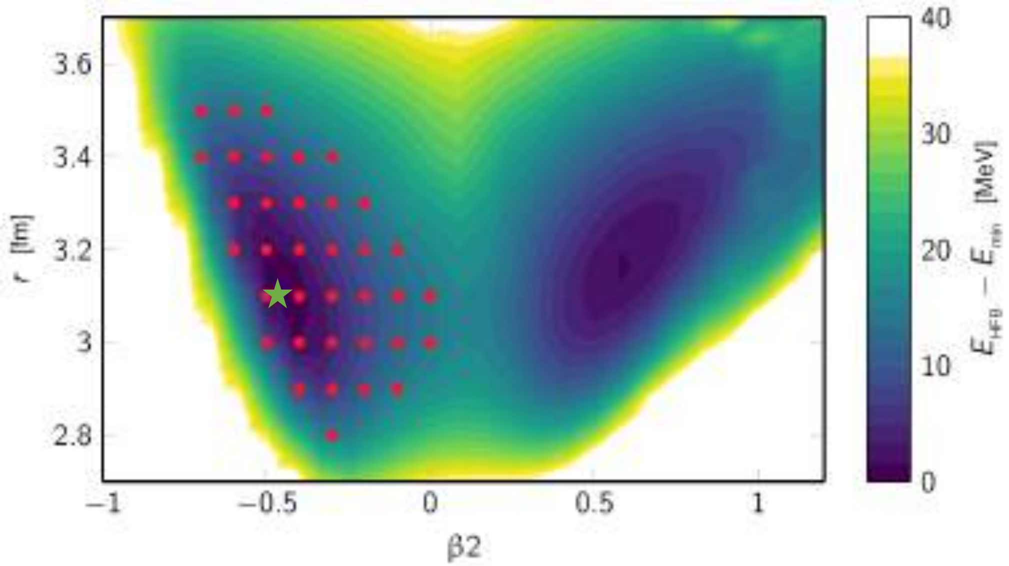
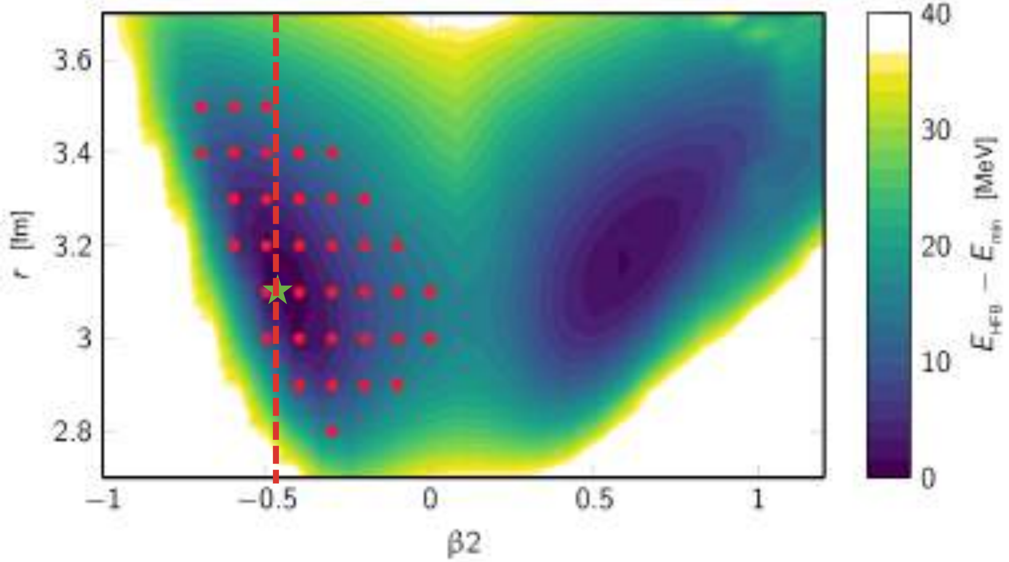


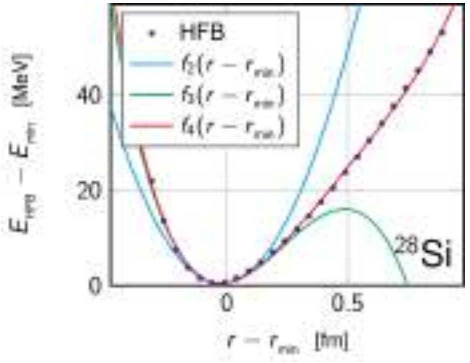
- Quantitative anharmonicities analysis

Anharmonic effects

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



One-dimensional cut



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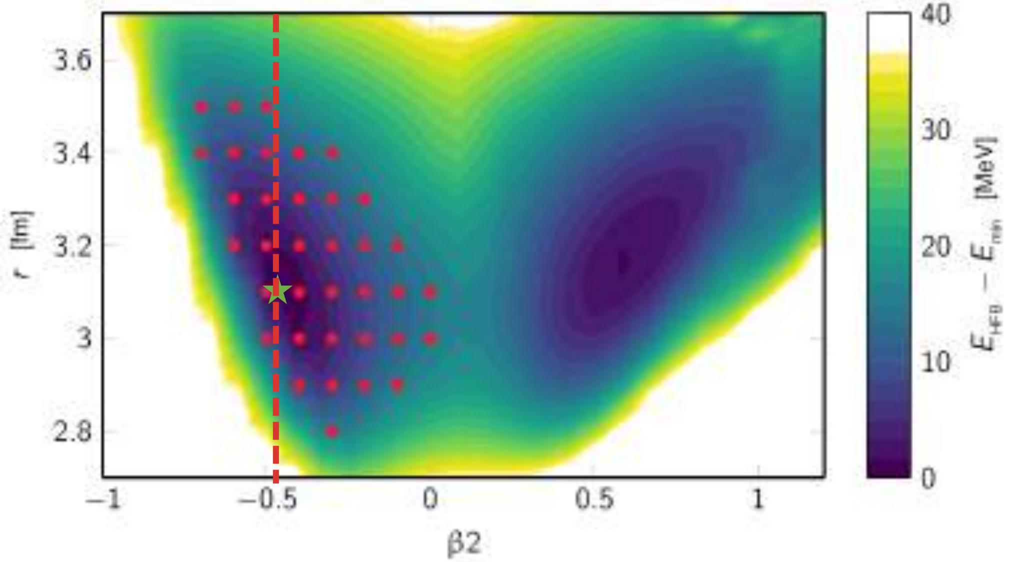

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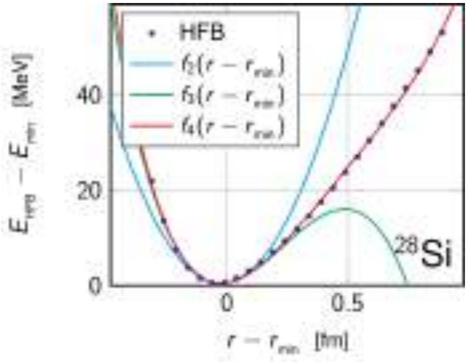

Polynomial fit $f(x) = a_2x^2 + a_3x^3 + a_4x^4$

- Quantitative anharmonicities analysis

Anharmonic effects

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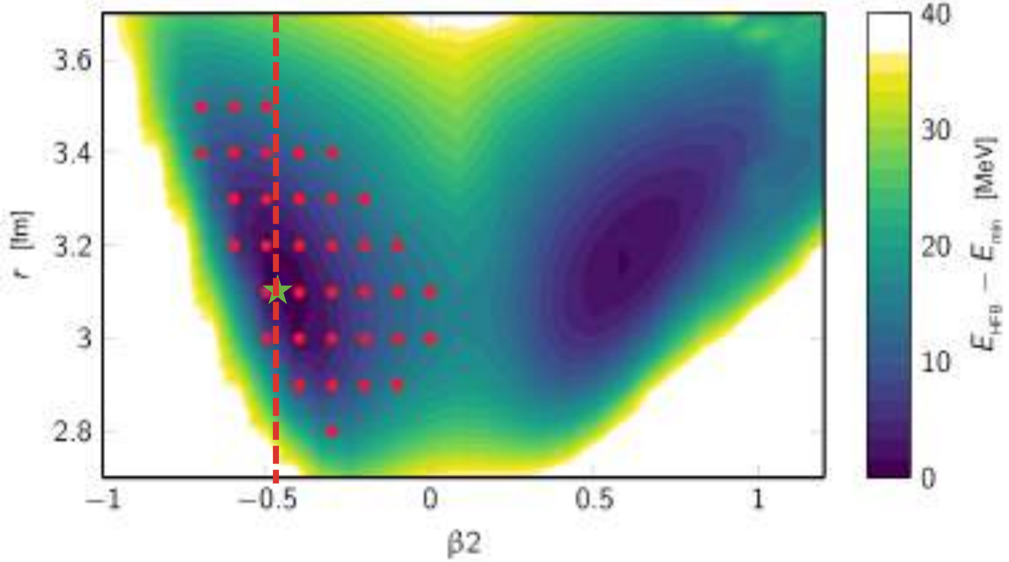

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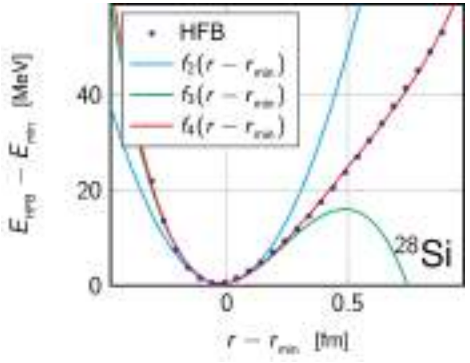

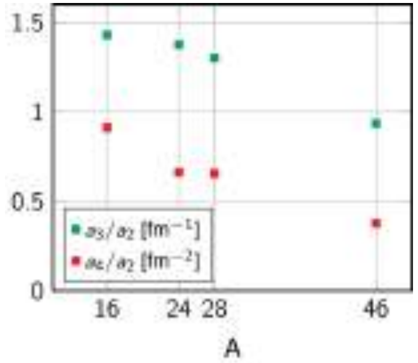

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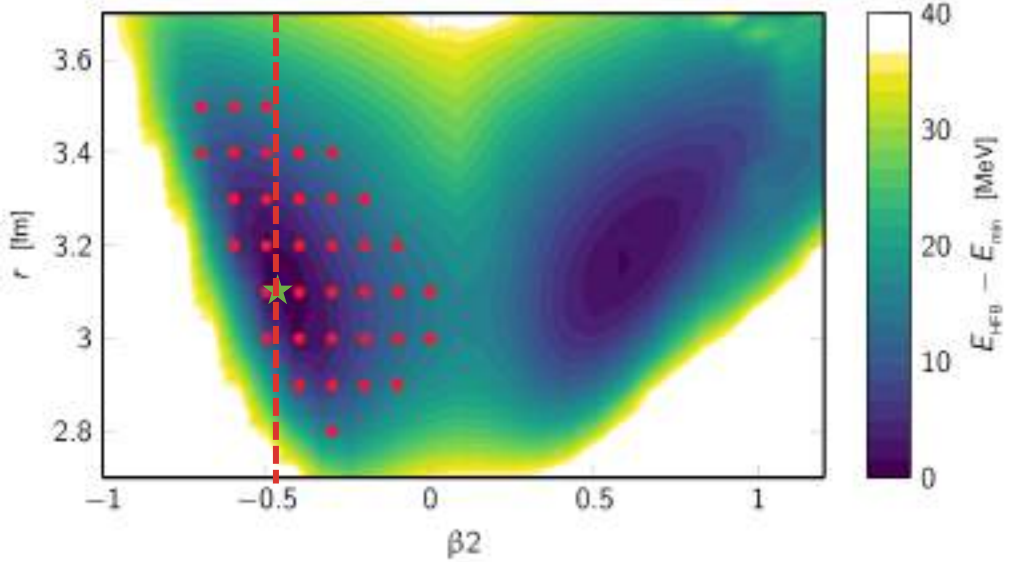
- Quantitative anharmonicities analysis
  - Light nuclei are less harmonic

Anharmonic effects

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



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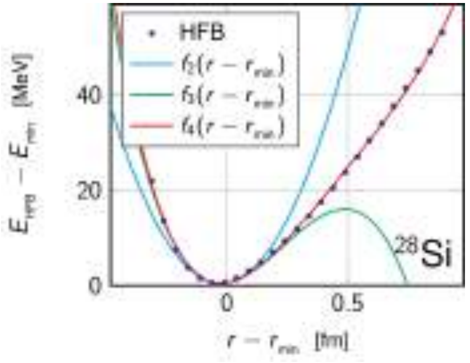

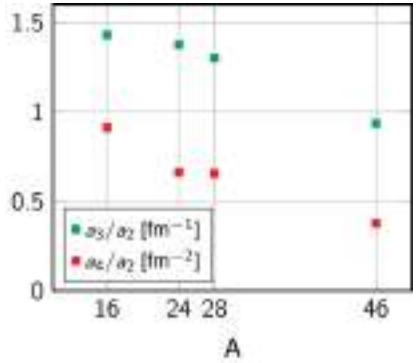

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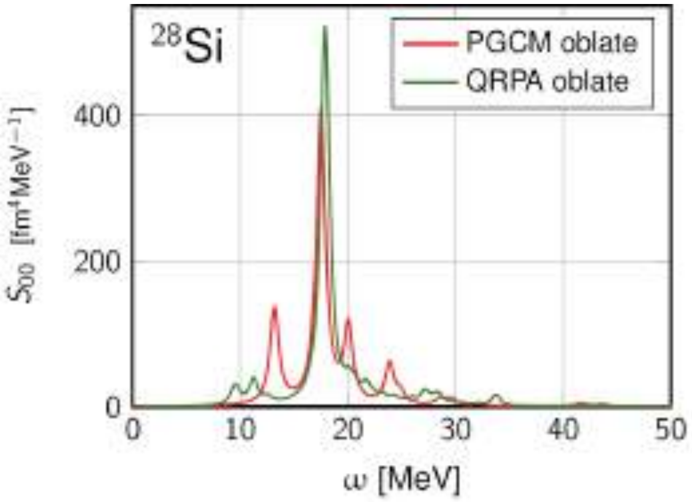
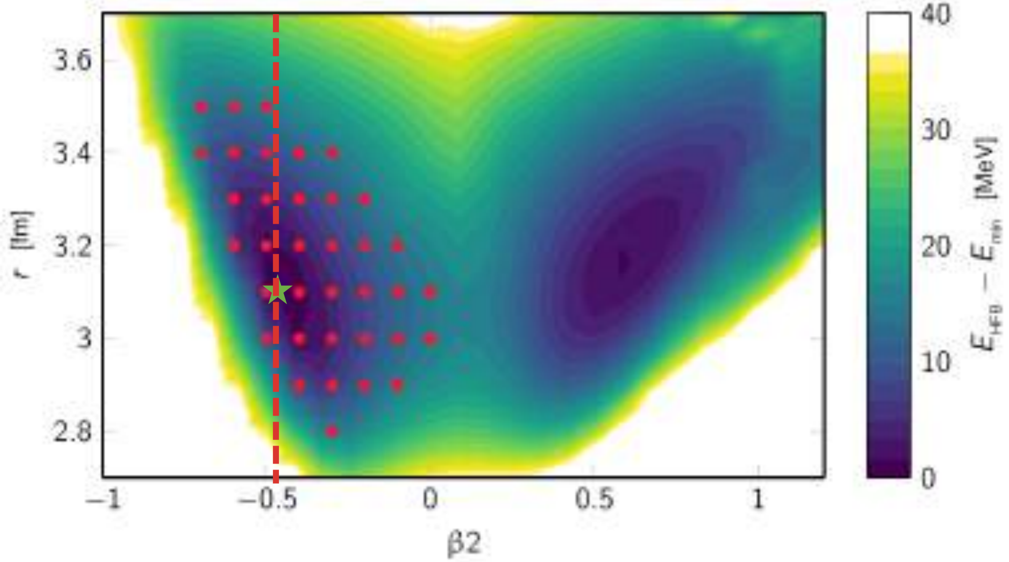


- Quantitative anharmonicities analysis
  - Light nuclei are less harmonic
- Qualitatively similar results QRPA/PGCM

Anharmonic effects

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



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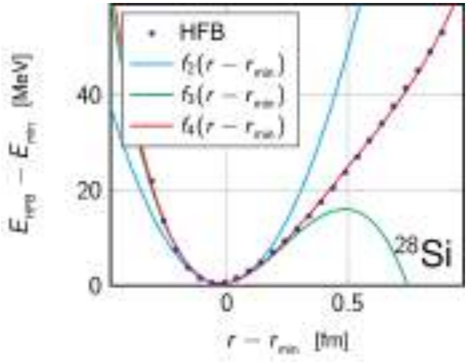

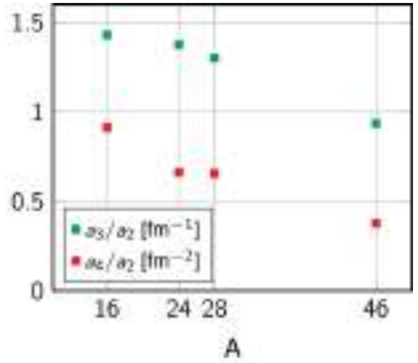

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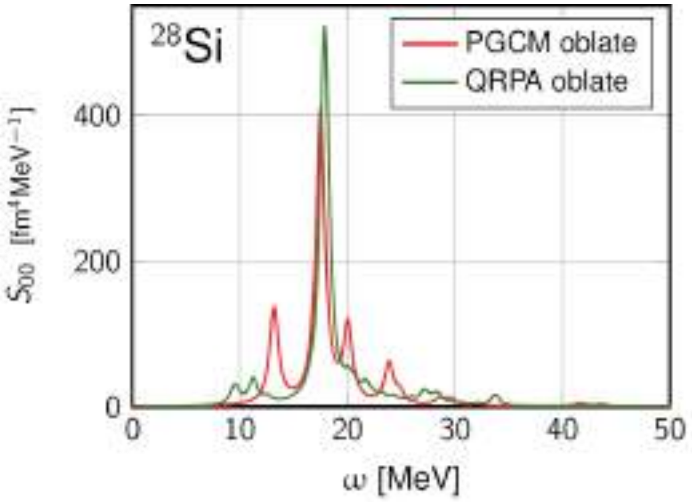
- Quantitative anharmonicities analysis
  - Light nuclei are less harmonic
- Qualitatively similar results QRPA/PGCM
  - Consistent monopole response



Anharmonic effects

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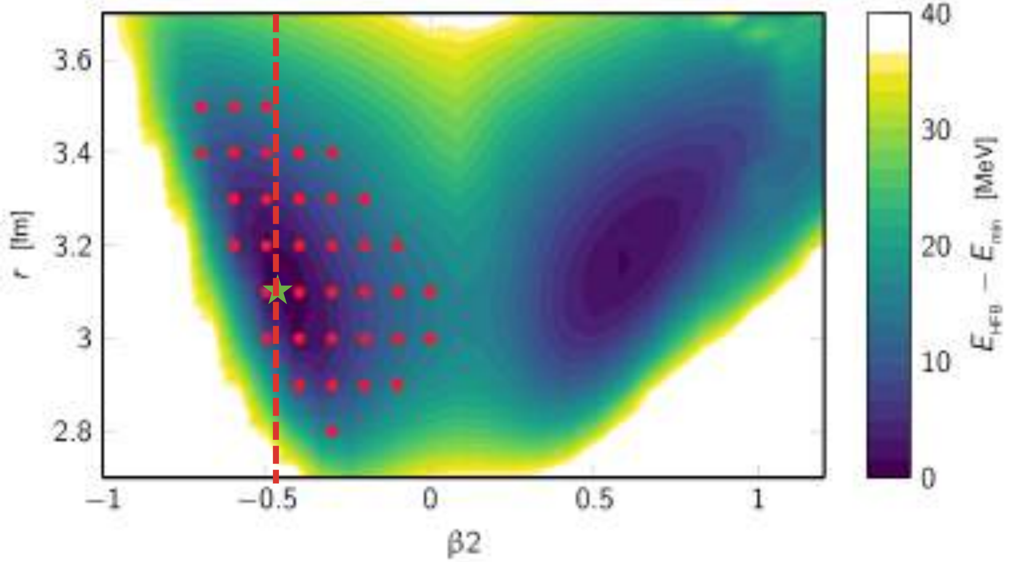

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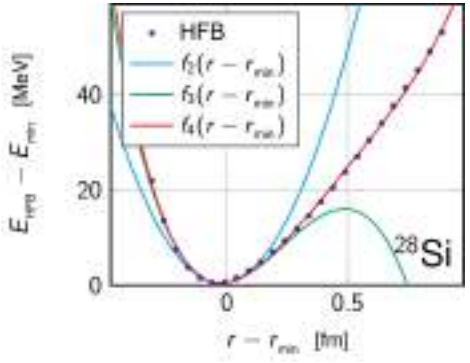

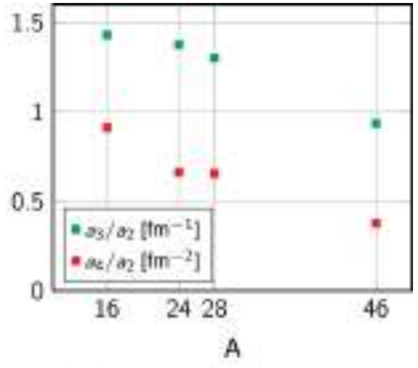

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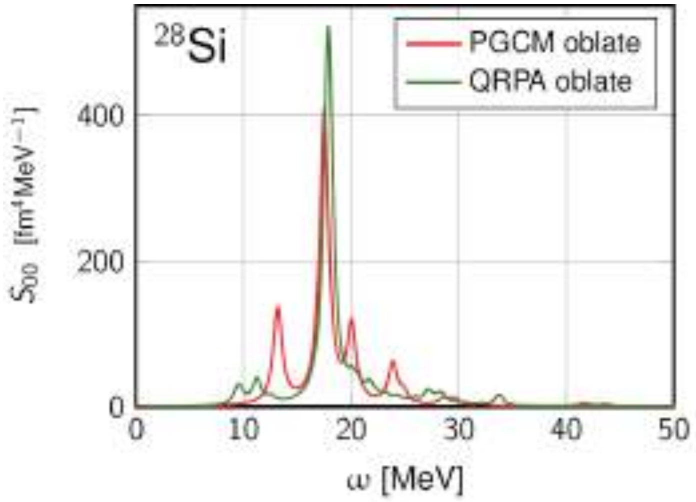
- Qualitatively similar results QRPA/PGCM
  - Consistent monopole response
  - QRPA response less fragmented



Anharmonic effects

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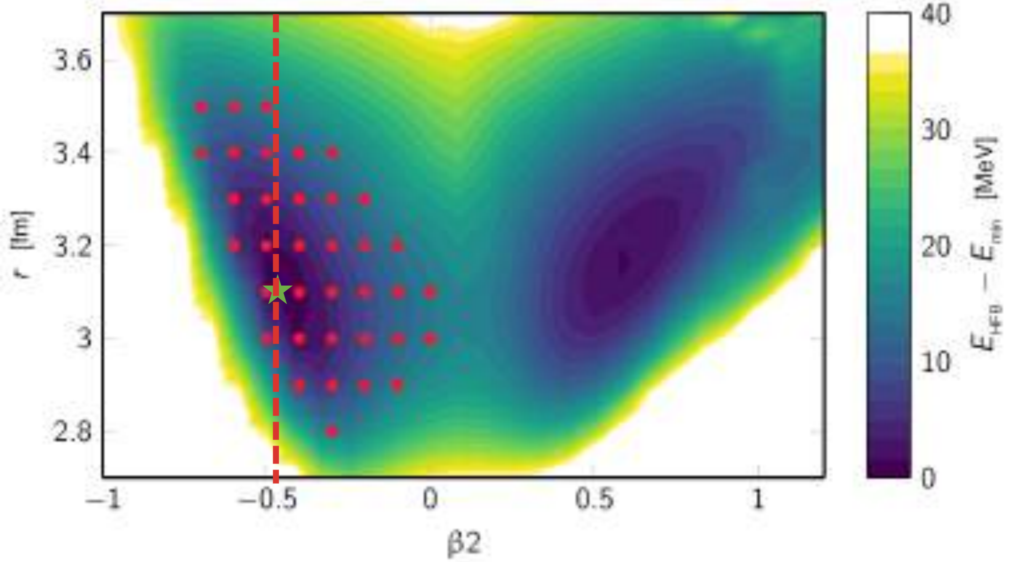

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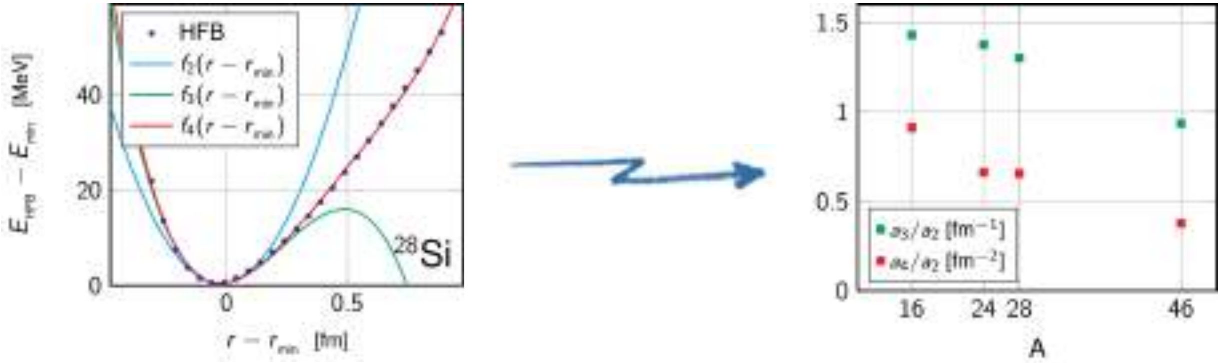

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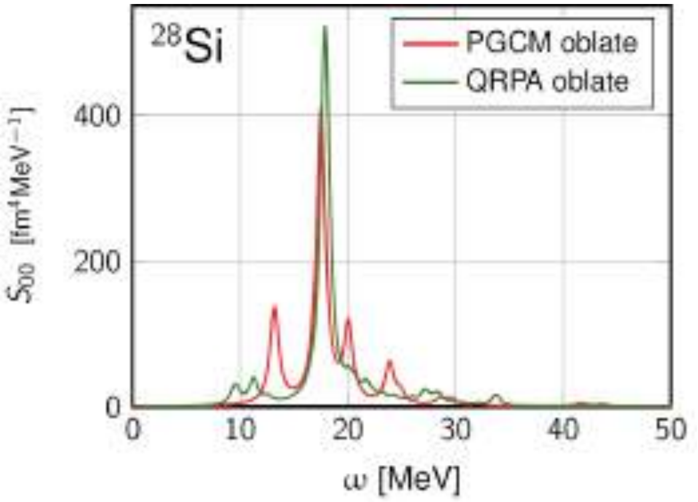

- Quantitative anharmonicities analysis
  - Light nuclei are less harmonic
- Qualitatively similar results QRPA/PGCM
  - Consistent monopole response
  - QRPA response less fragmented
- Case specific fragmentation, no quantitative correlation

Anharmonic effects

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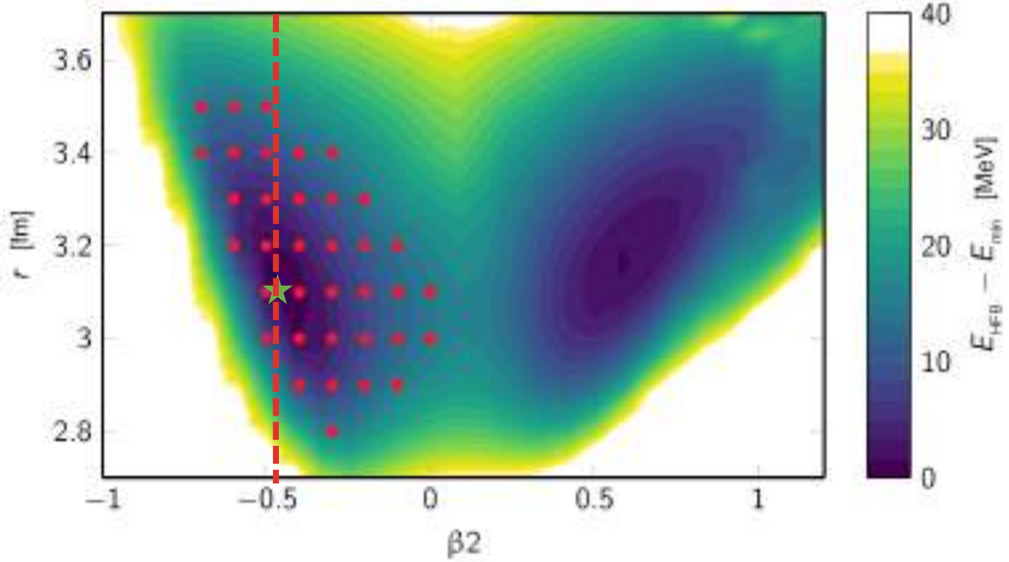

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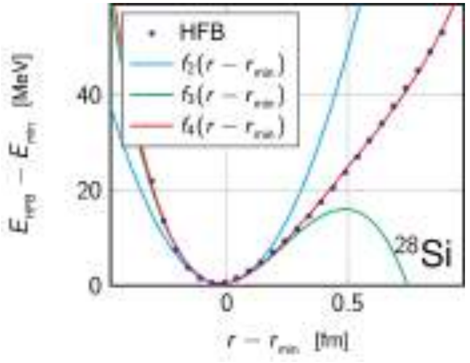

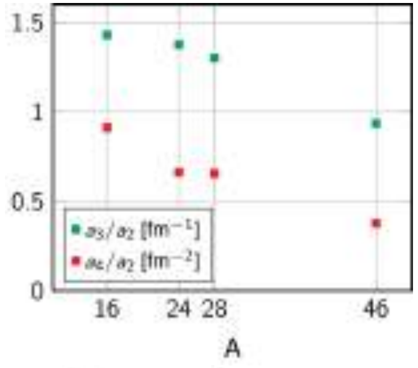

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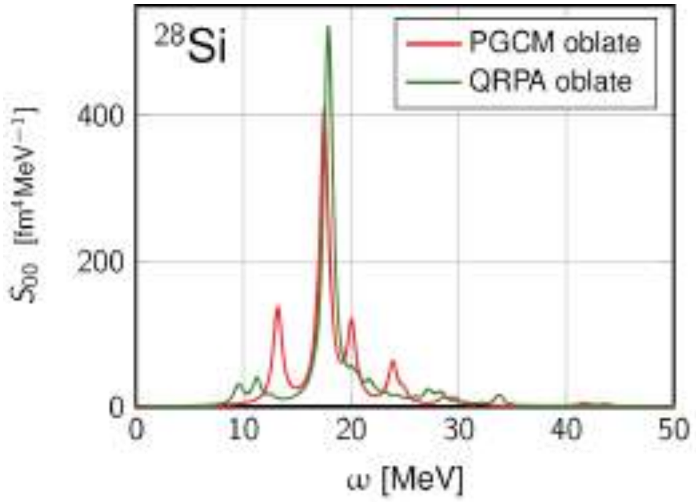

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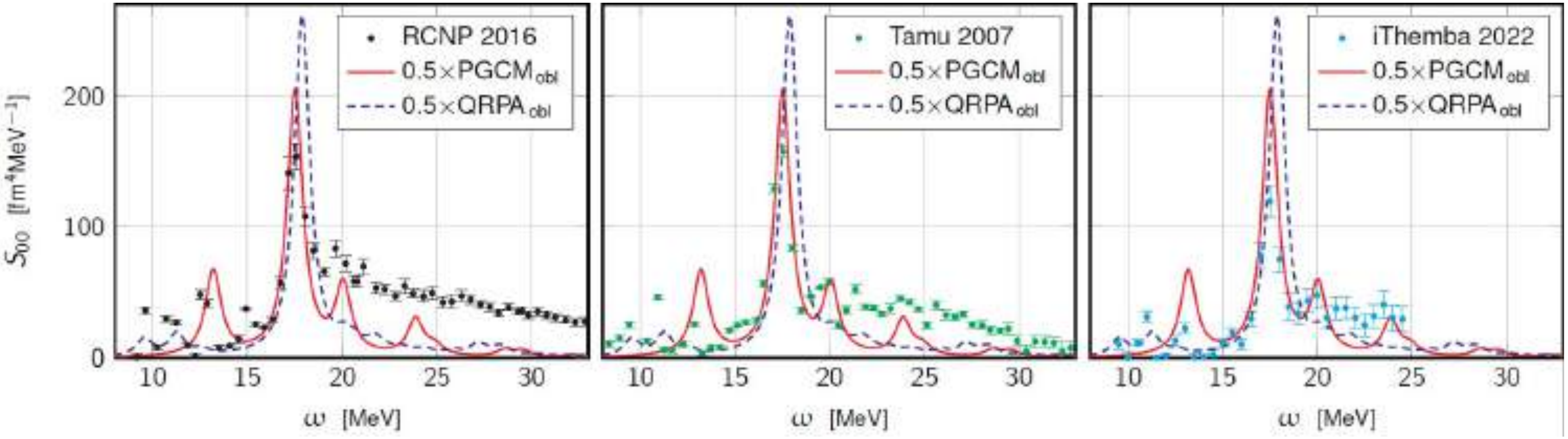
- Qualitatively similar results QRPA/PGCM
  - Consistent monopole response
  - QRPA response less fragmented
- Case specific fragmentation, no quantitative correlation
- Projection contribution to fragmentation

Comparison to experimental data



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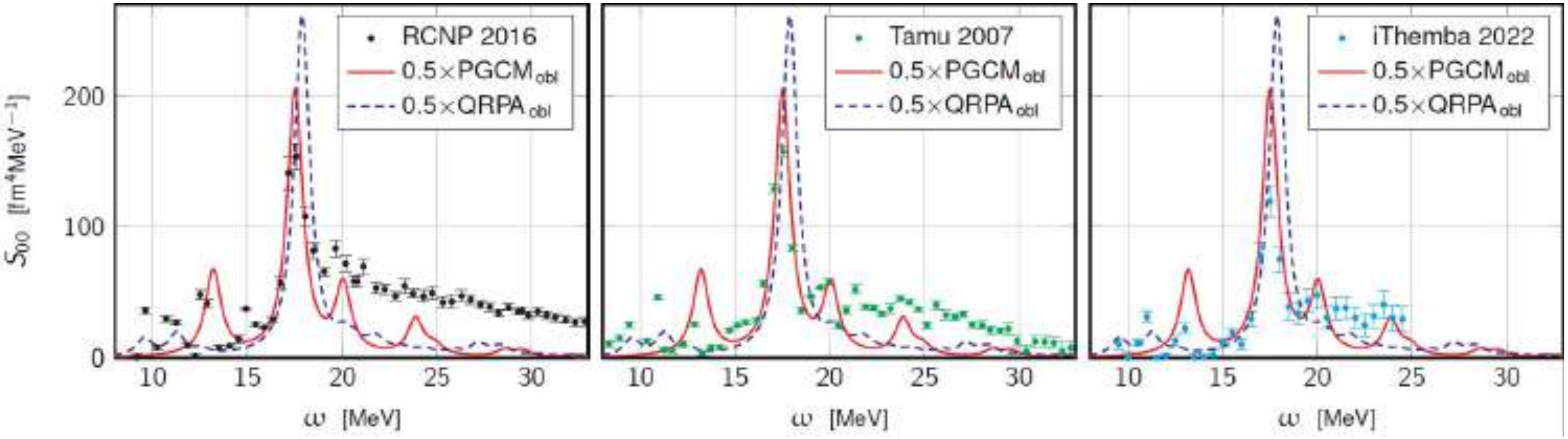


Ab initio PGCM nicely reproduces the experimental data

- Nicer 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 Introduction

- Giant Resonances Physics
- The PGCM
- Link between PGCM and QRPA

2 Systematic study

- Numerical details
- Uncertainty estimate

Conclusions and perspectives

Results 3

Selected applications

- Shape coexistence
- Deformation

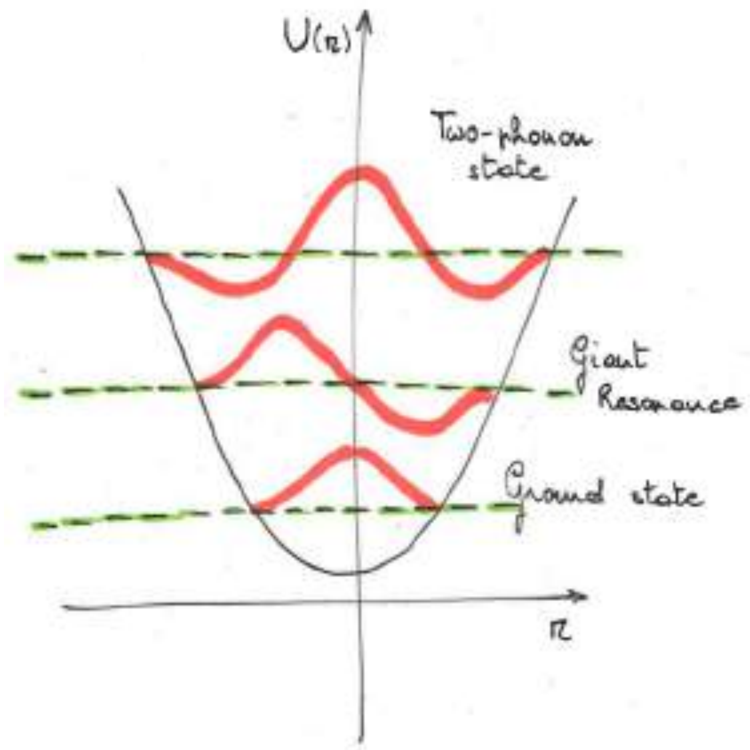
Multi-phonon states

- Proof of principle
- Realistic calculations

From finite nuclei to Astrophysics

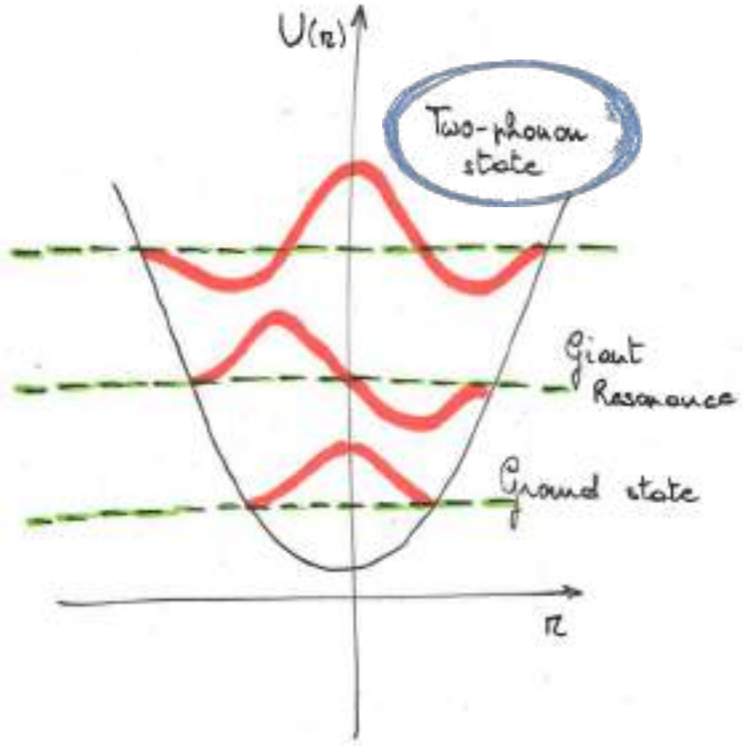
- Preliminary incompressibility results

Multi-phonon states in ^{46}Ti



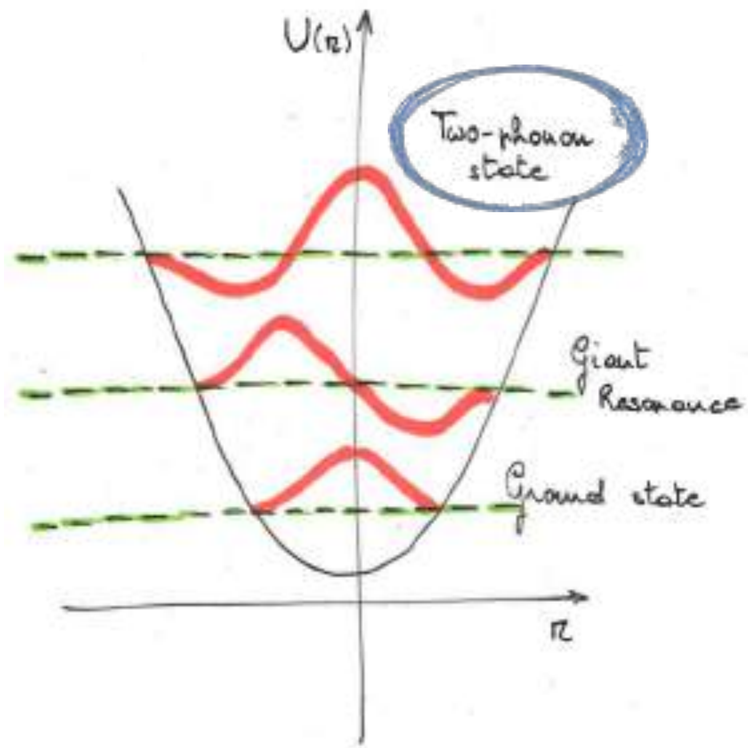
- GRs can be interpreted as the first phonon of a collective excitation

Multi-phonon states in ^{46}Ti



- GRs can be interpreted as the first phonon of a collective excitation
- Higher phonons also exist Multi-phonon states

Multi-phonon states in ^{46}Ti



- GRs can be interpreted as the first phonon of a collective excitation
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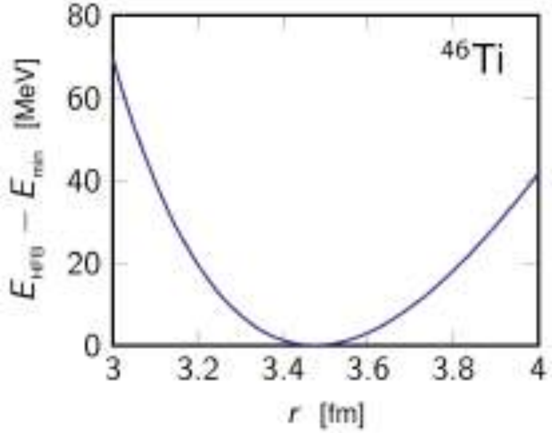
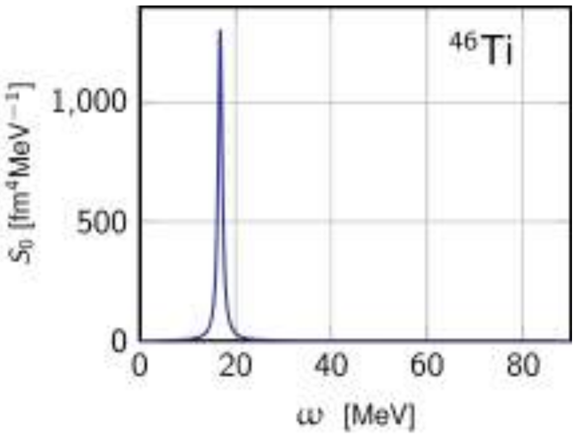
One-dimensional PGCM calculation





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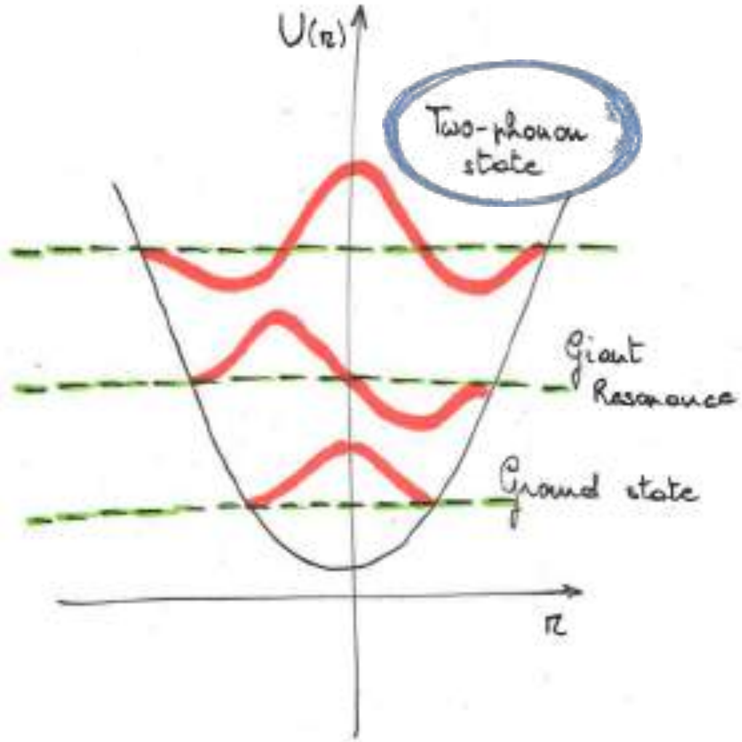

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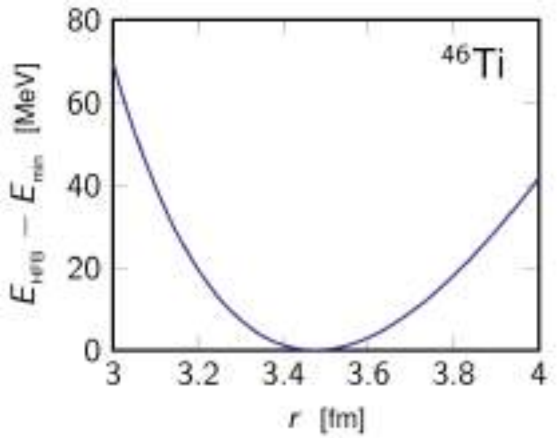
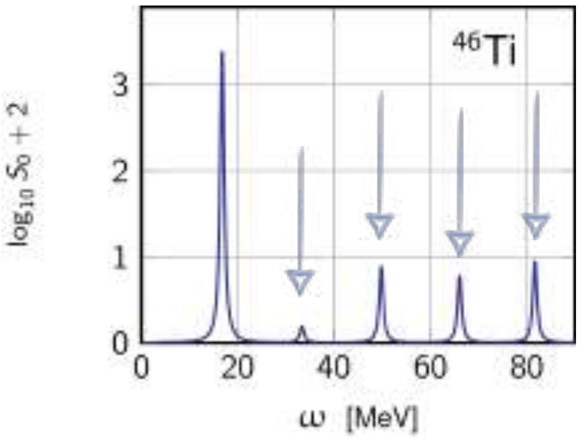
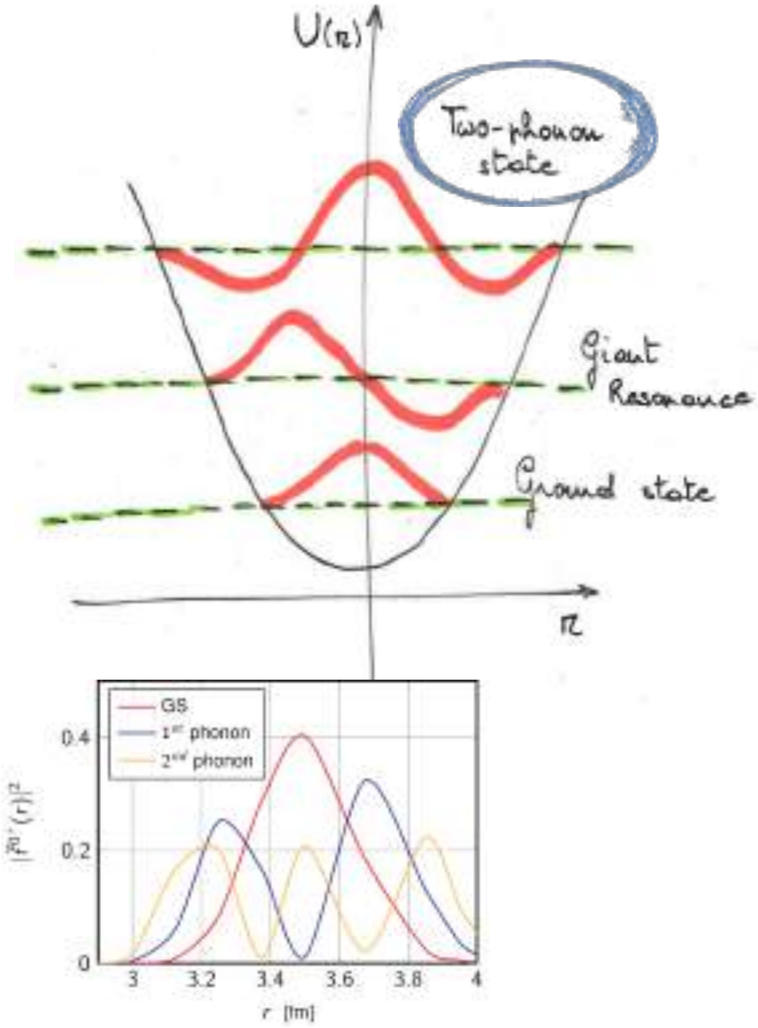




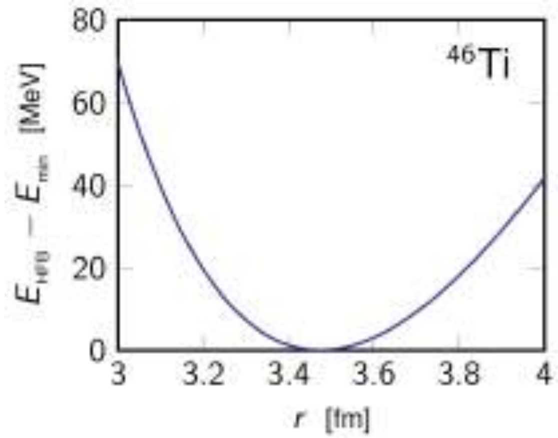
- PGCM predicts high-lying states

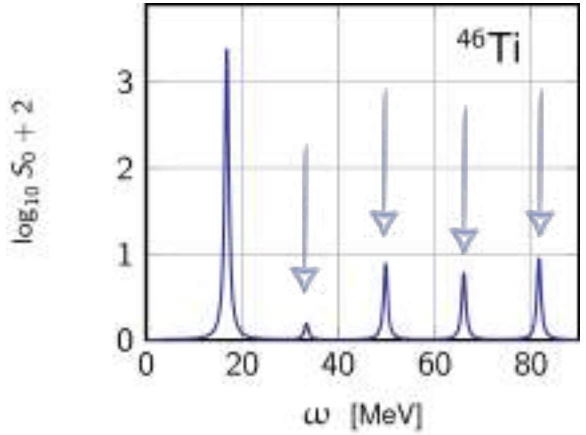
Multi-phonon states in ^{46}Ti

- GRs can be interpreted as the first phonon of a collective excitation
- Higher phonons also exist   Multi-phonon states



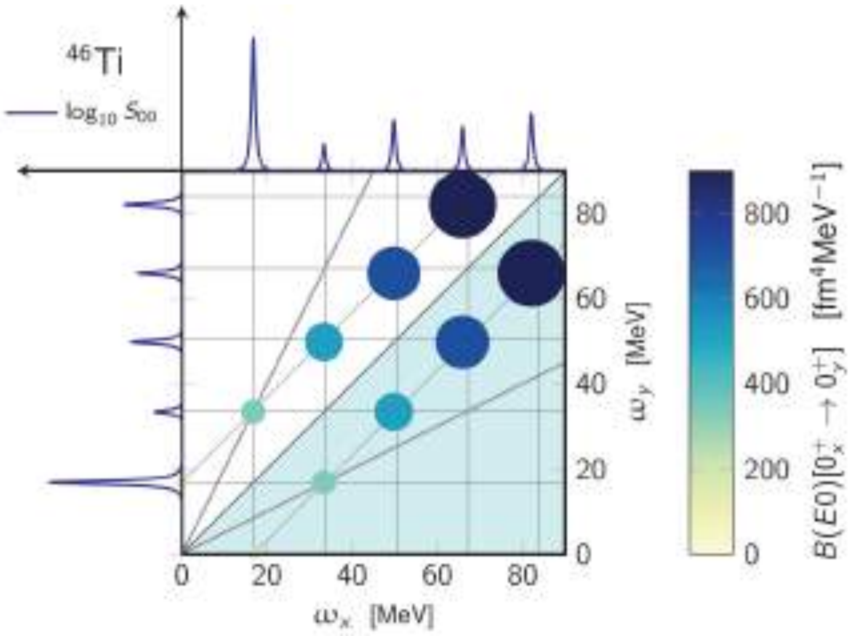
One-dimensional PGCM calculation

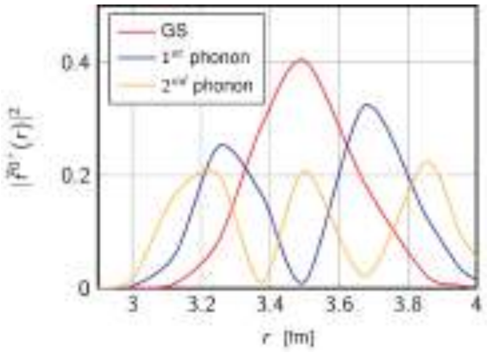




- PGCM predicts high-lying states
- Close to the harmonic oscillator eigen-solutions

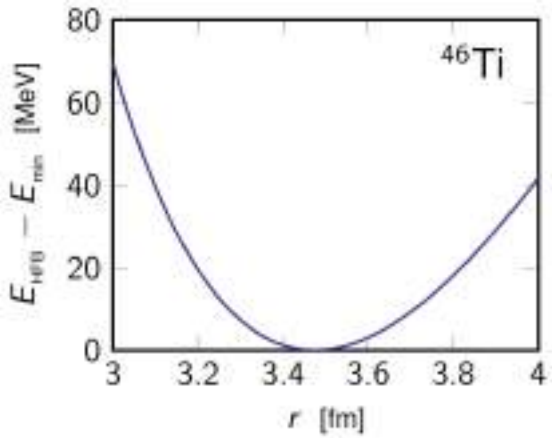
Multi-phonon states in ^{46}Ti

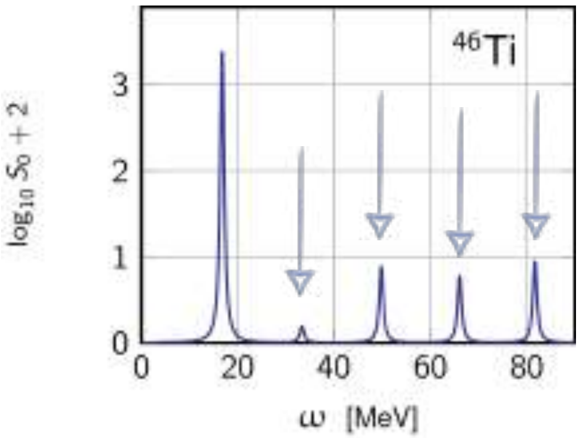




- GRs can be interpreted as the first phonon of a collective excitation
- Higher phonons also exist   Multi-phonon states

One-dimensional PGCM calculation





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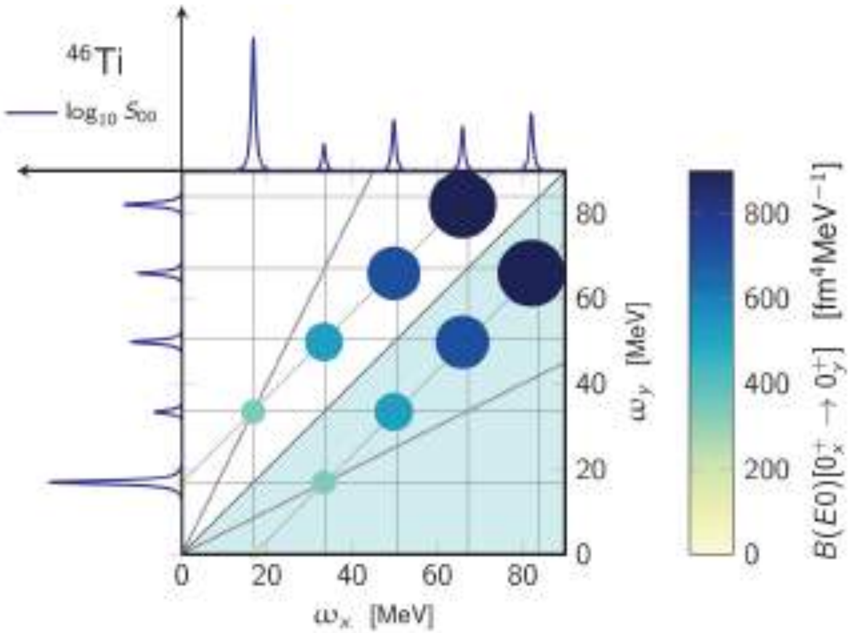

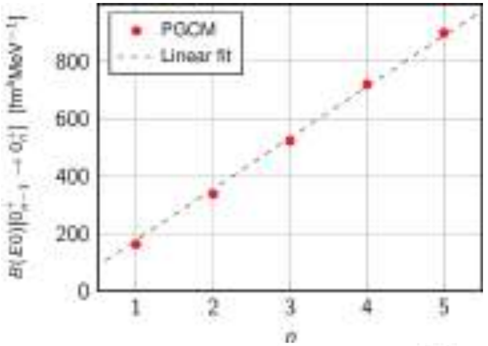

$$|\langle n-1|r^2|n\rangle|^2 = \frac{\hbar}{2m\omega}n$$

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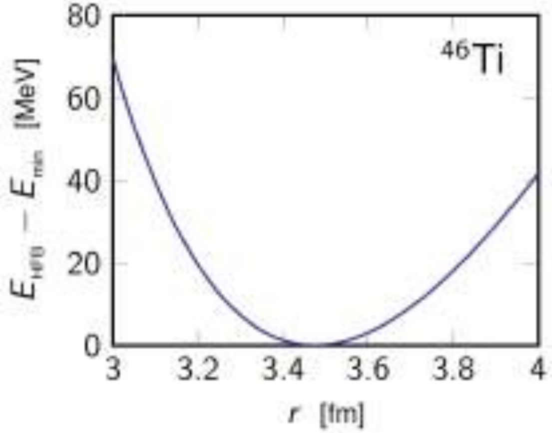
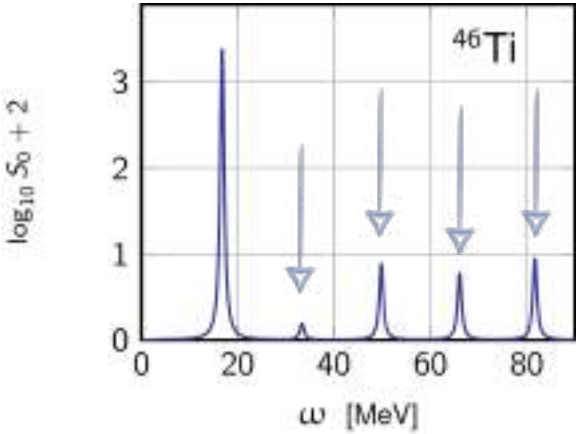
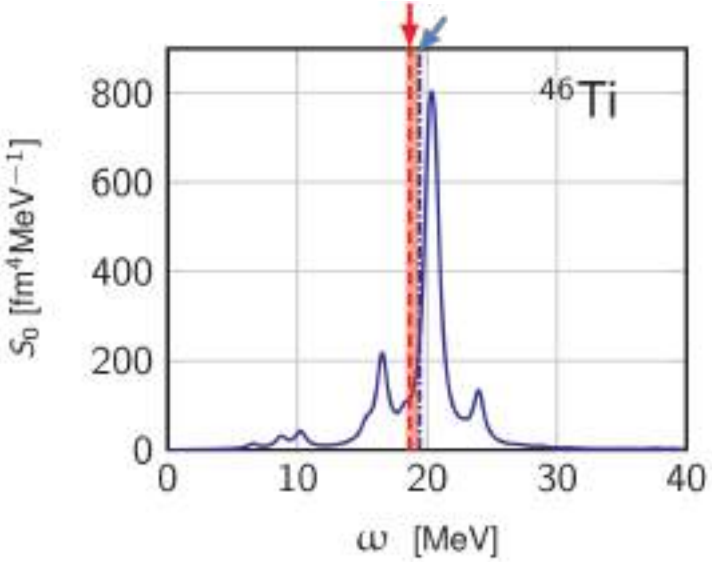




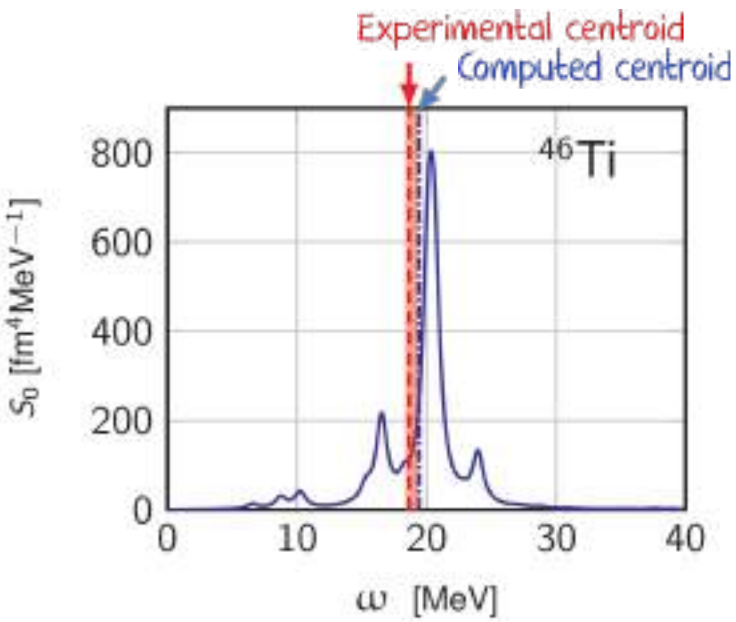
- PGCM predicts high-lying states
- Close to the harmonic oscillator eigen-solutions
- Transitions maximised between neighbouring phonons
  - x Linear trend in the transition strength

Two-dimensional calculations



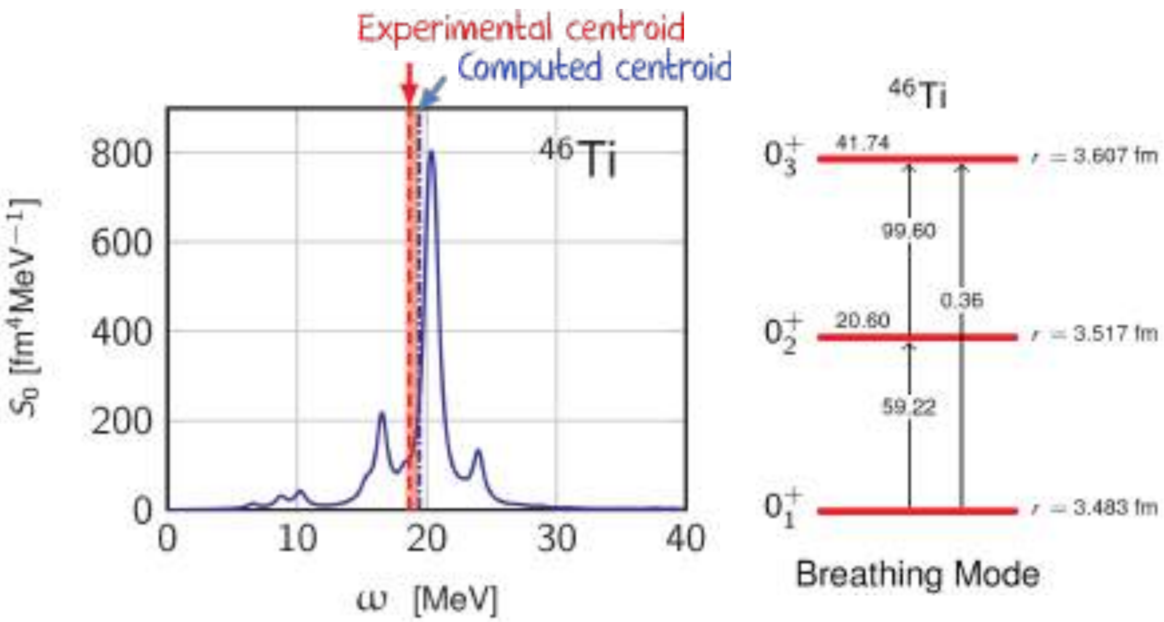
- 2-D PGCM in the (r, β_2) plane

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
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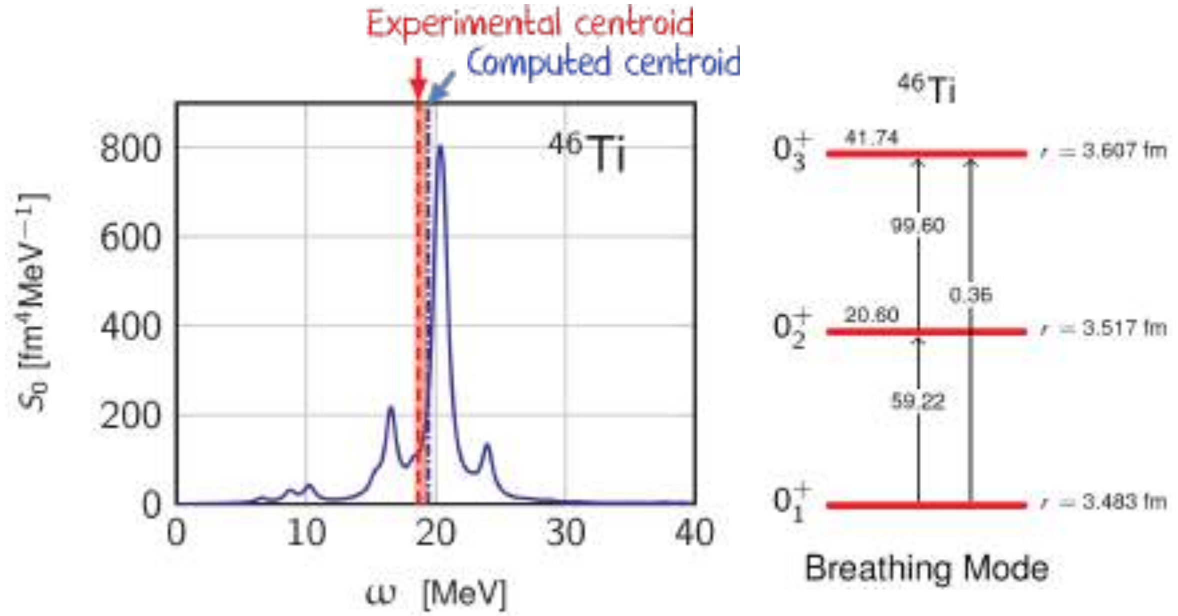
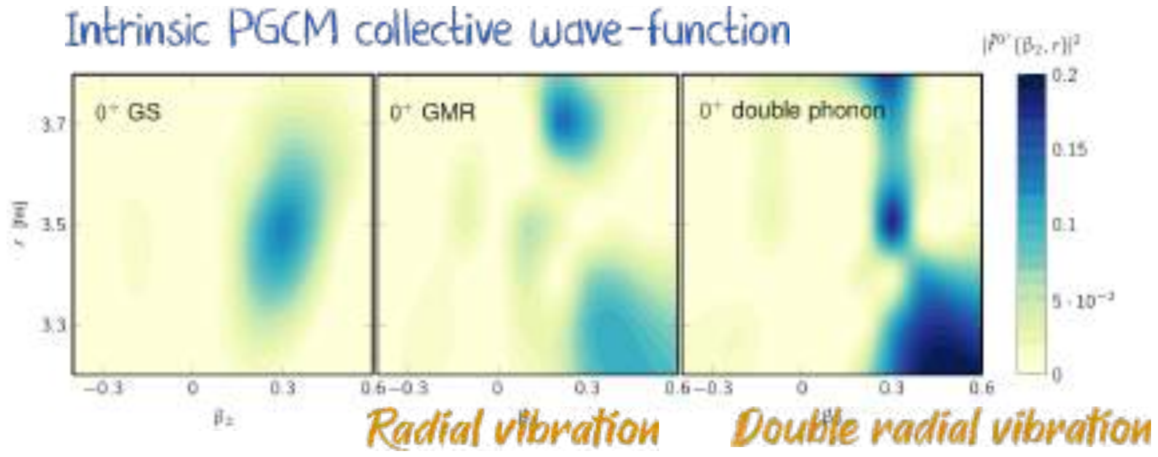
Two-dimensional calculations





- 2-D PGCM in the (r, β_2) plane
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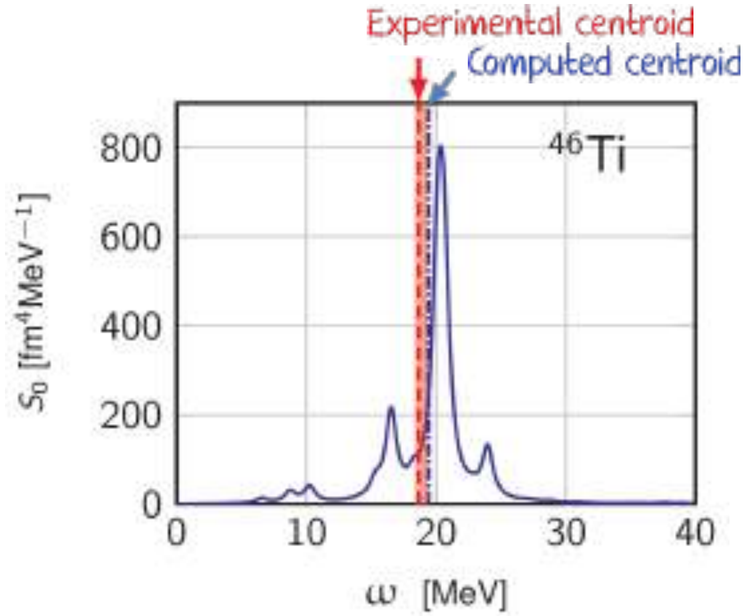

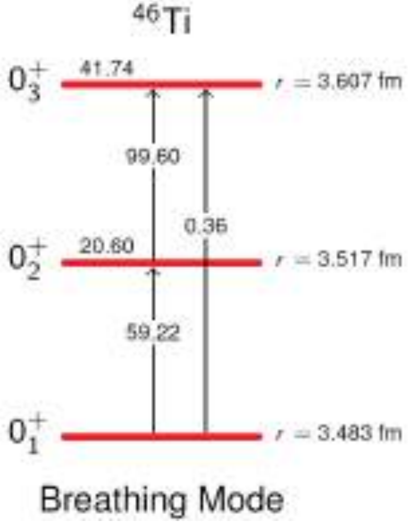

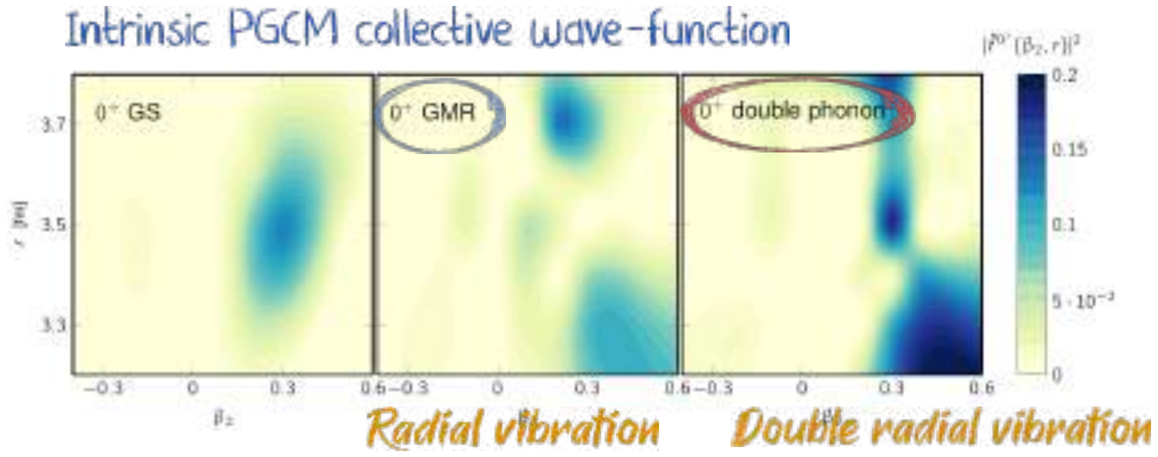

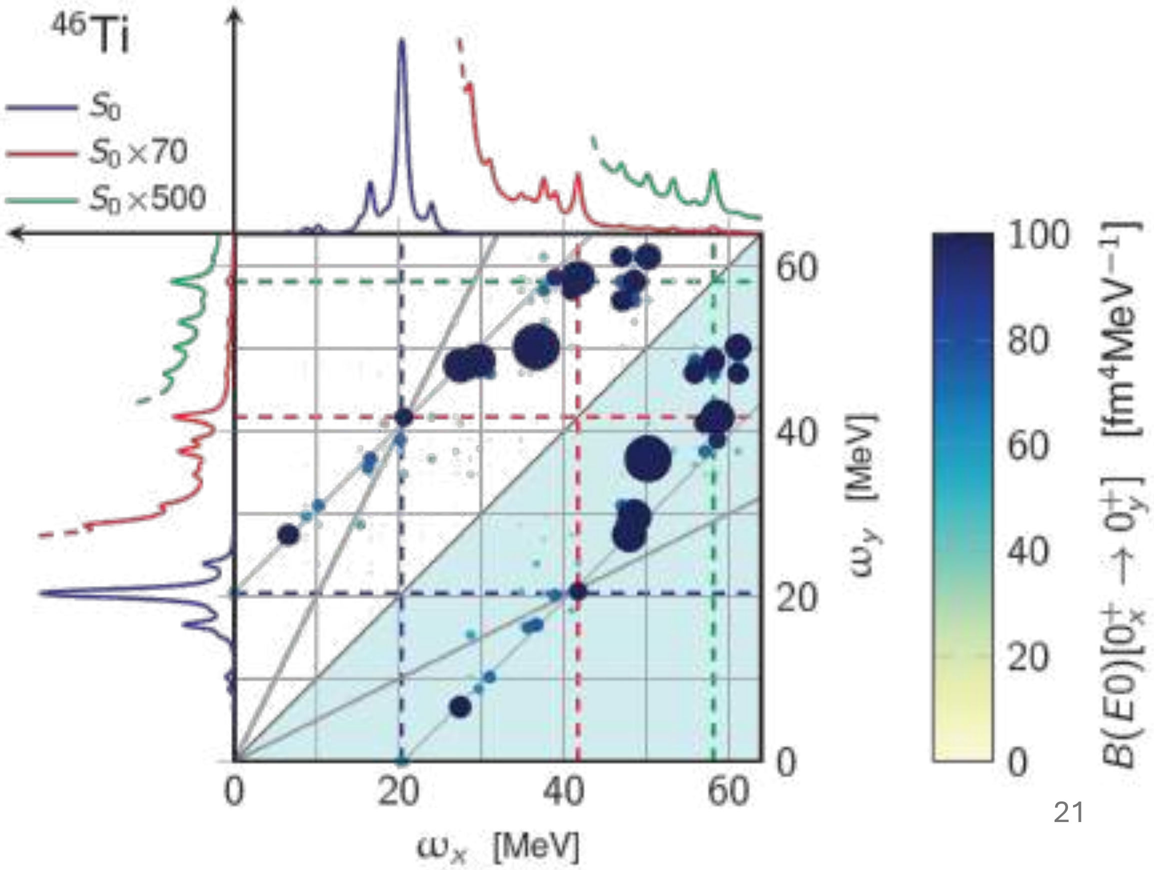

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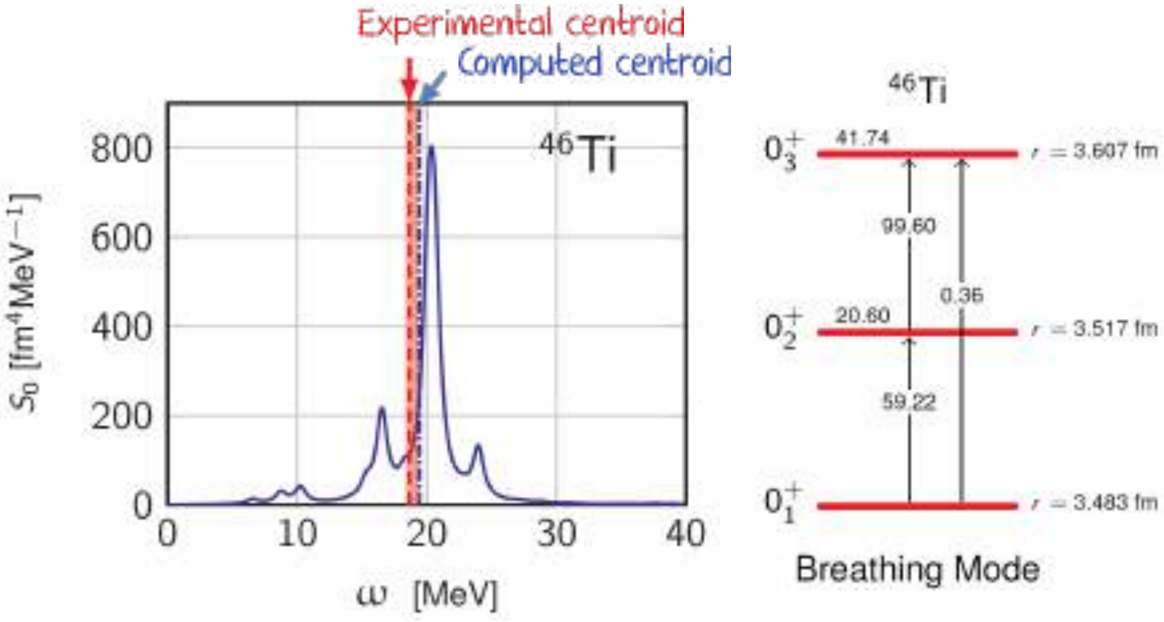

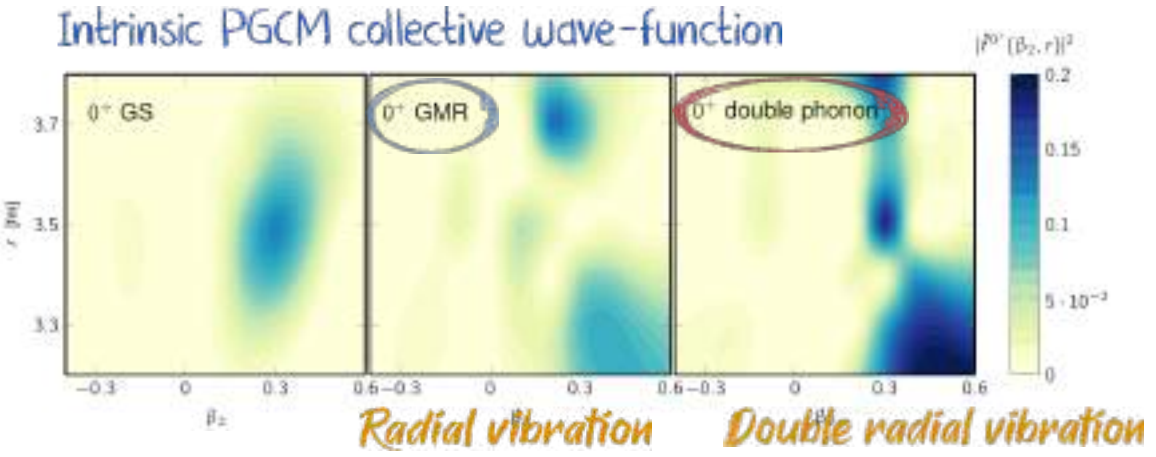

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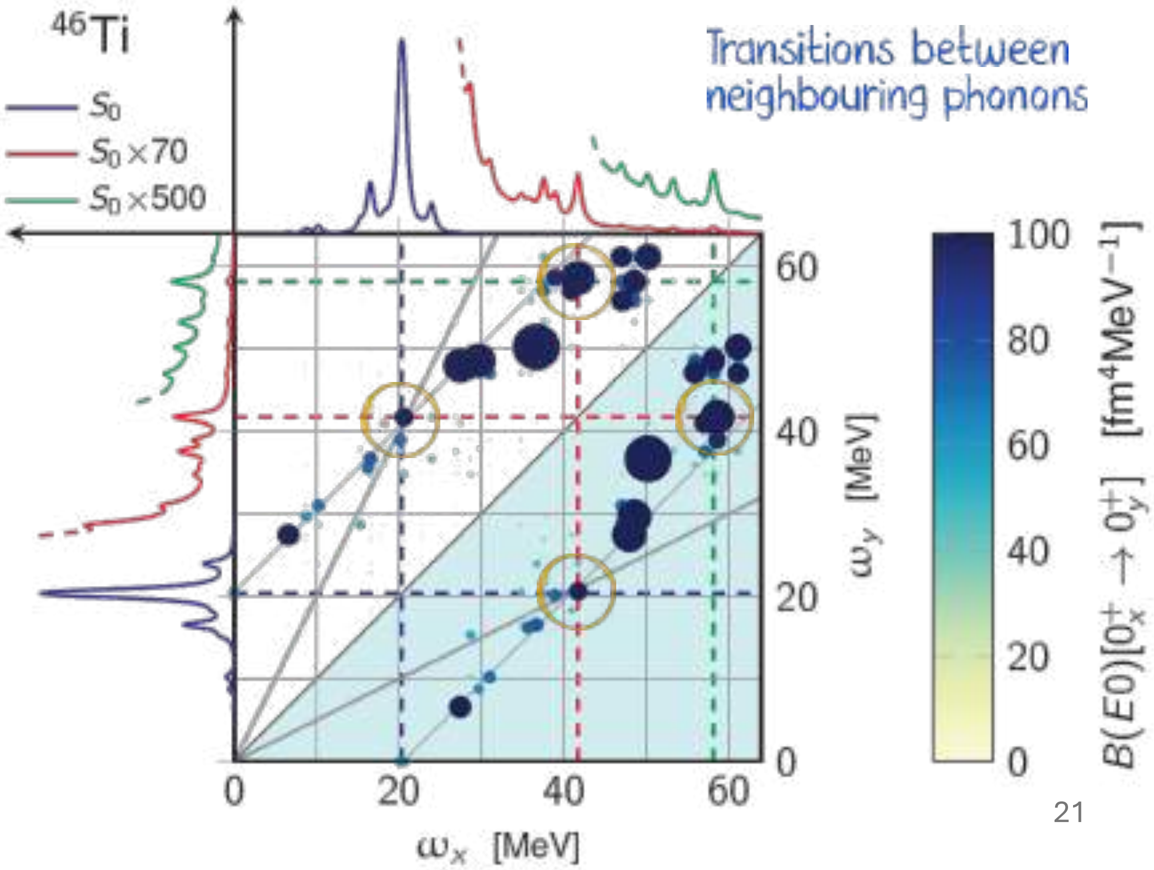

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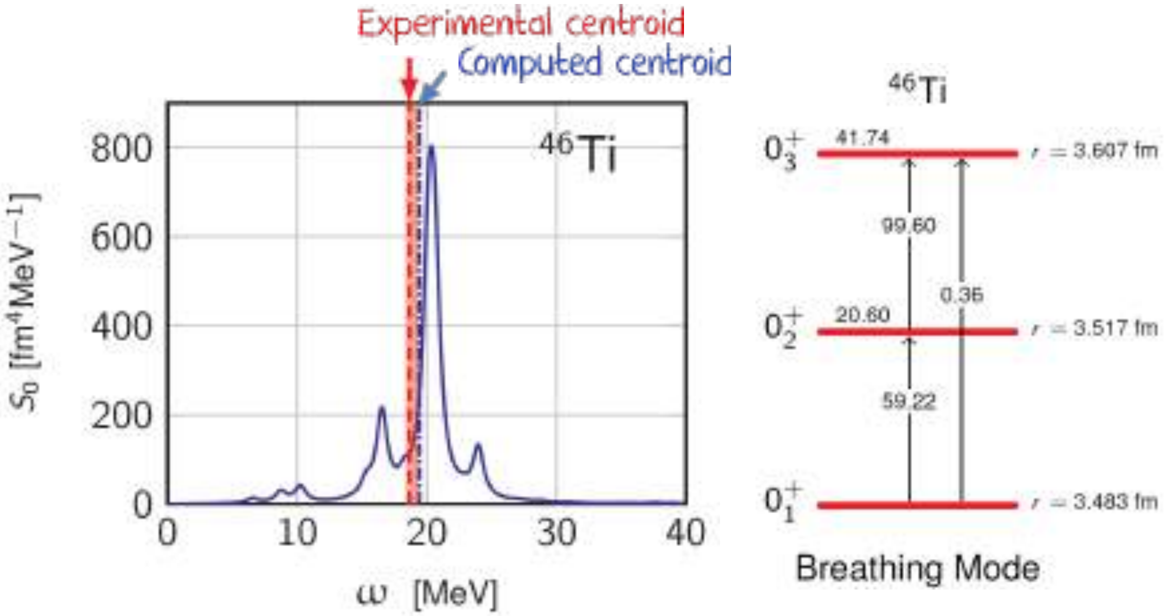
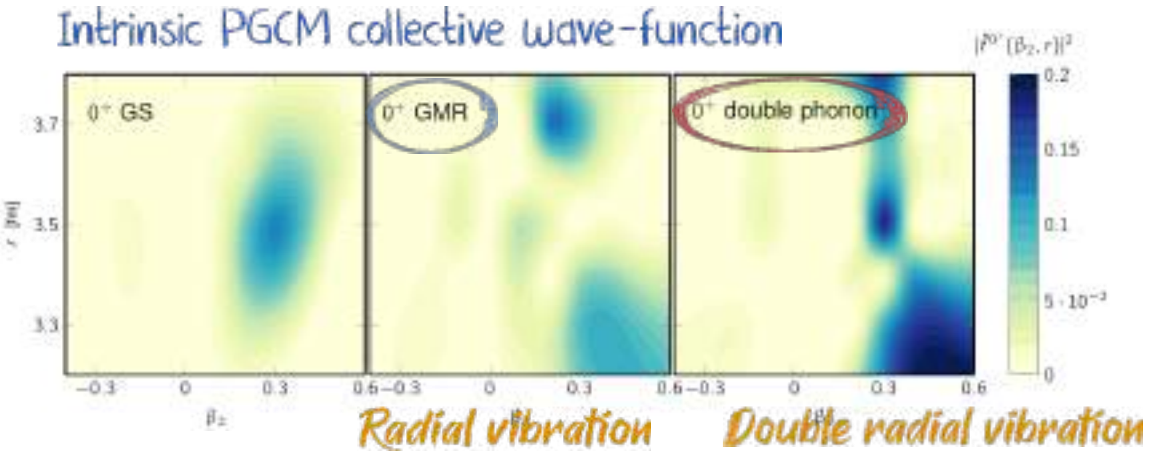
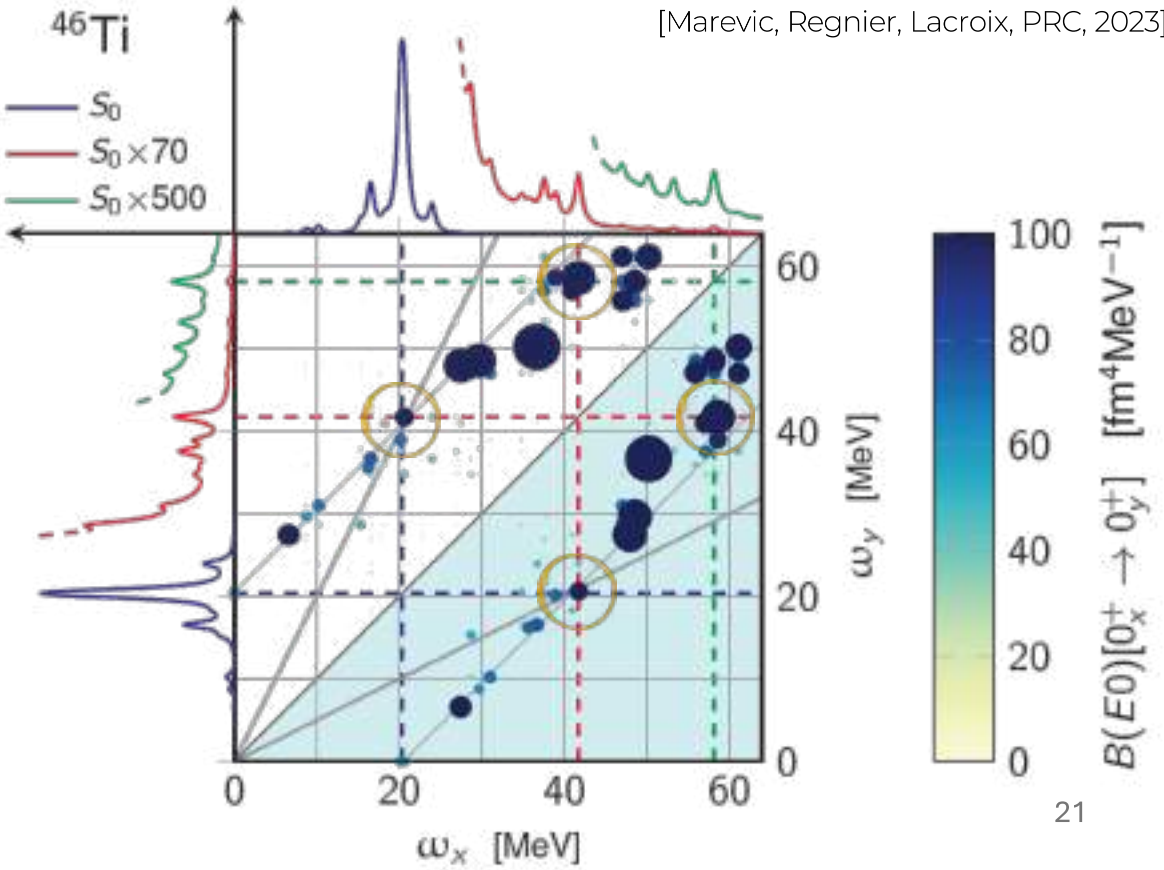




[Marevic, Regnier, Lacroix, PRC, 2023]



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- Giant Resonances Physics
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2 Systematic study
- Numerical details
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Conclusions and perspectives

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From finite nuclei to Astrophysics
- Preliminary incompressibility results

From finite nuclei to Astrophysics

Nuclear compressibility

- GMR

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

From finite nuclei to Astrophysics

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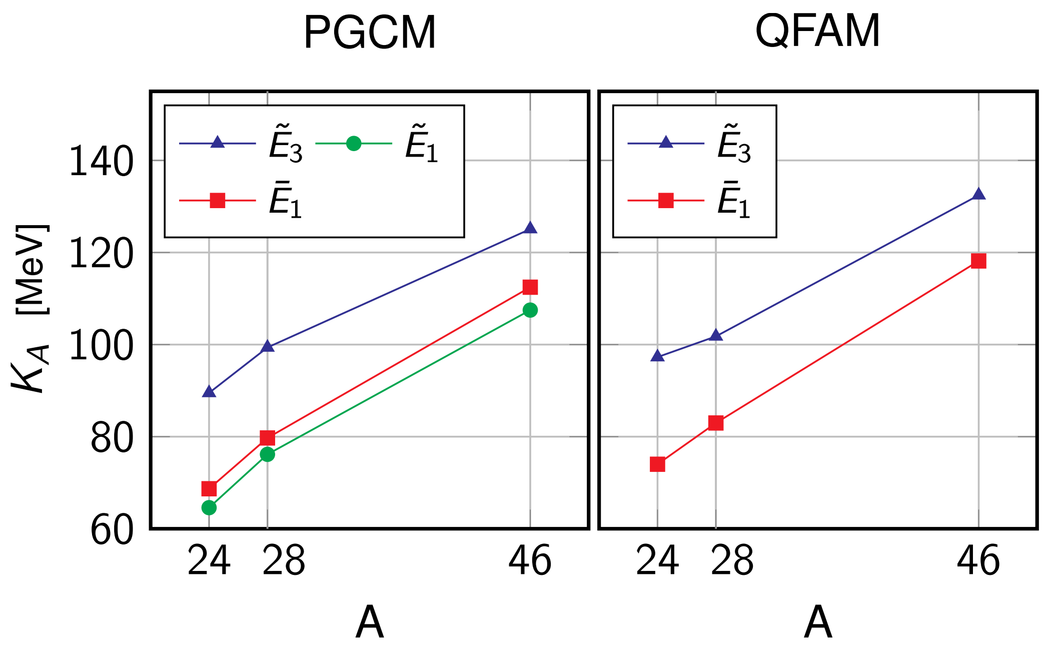
- GMR

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

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



From finite nuclei to Astrophysics

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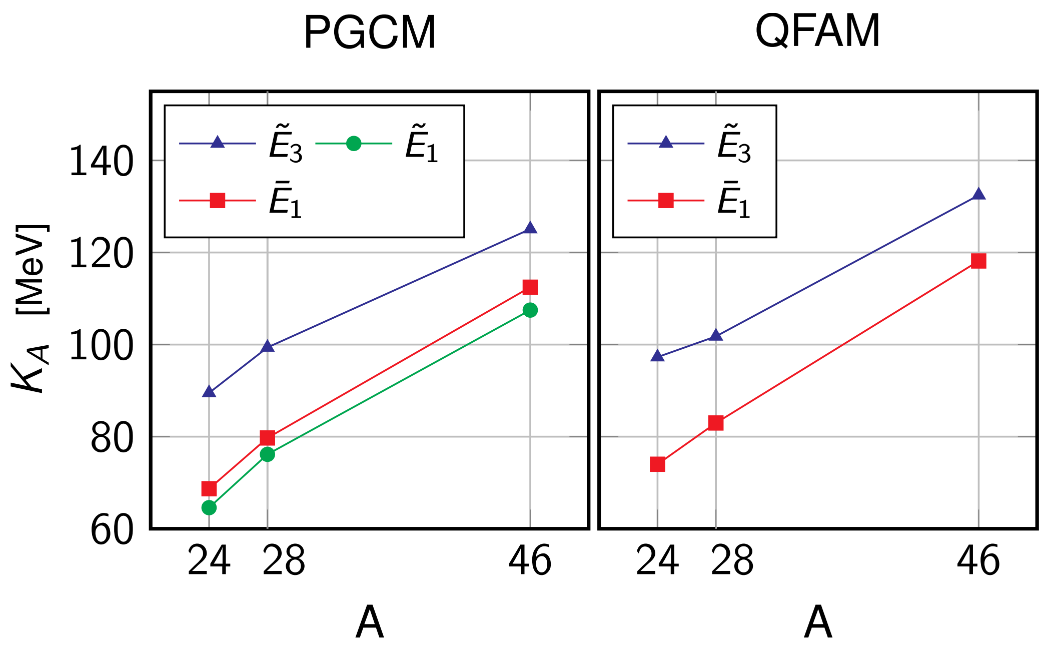
Extrapolation to infinite matter



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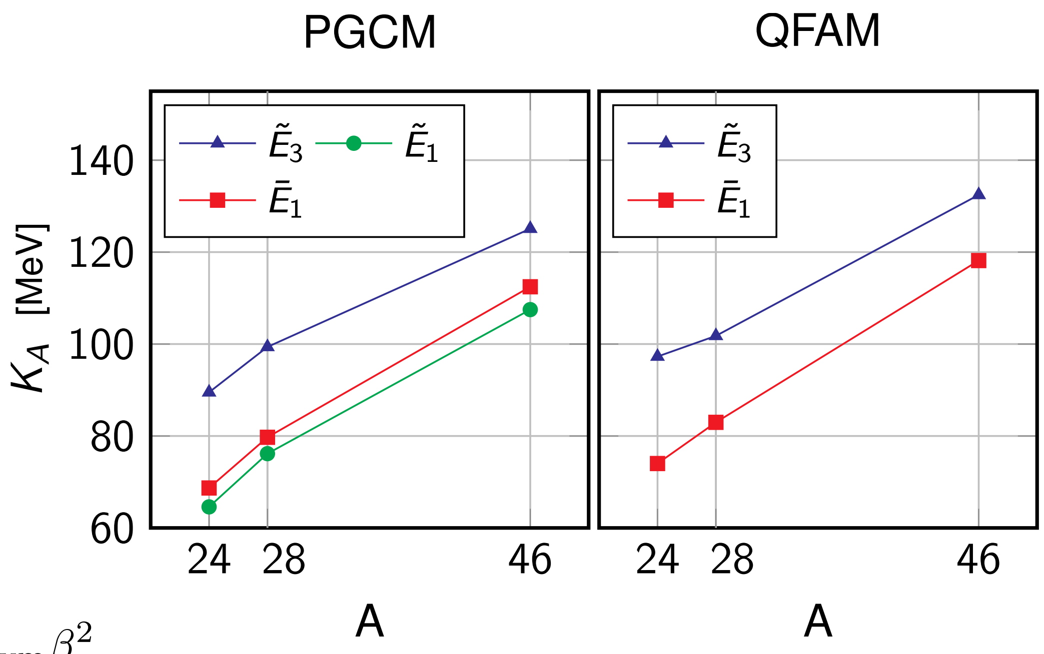

Extrapolation to infinite matter

$$K_A = K_{\mathrm{vol}} + K_{\mathrm{surf}}A^{-1/3} + K_{\mathrm{Coul}}Z^2A^{-4/3} + K_{\mathrm{sym}}\beta^2$$

$$\beta \equiv \frac{N-Z}{N+Z}$$

From finite nuclei to Astrophysics

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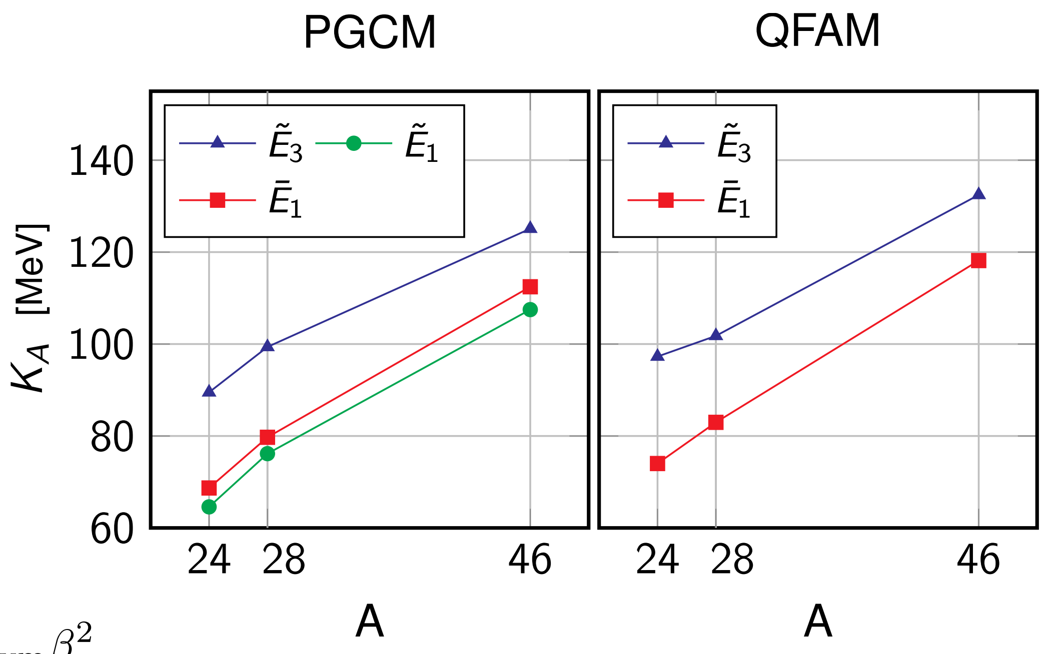

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$$x \equiv A^{-1/3}$$

$$K_A = K_\infty + K_{\mathrm{surf}}\, x$$

[Burrows, Baker, Bacca et al., arXiv:2312.09782]

From finite nuclei to Astrophysics

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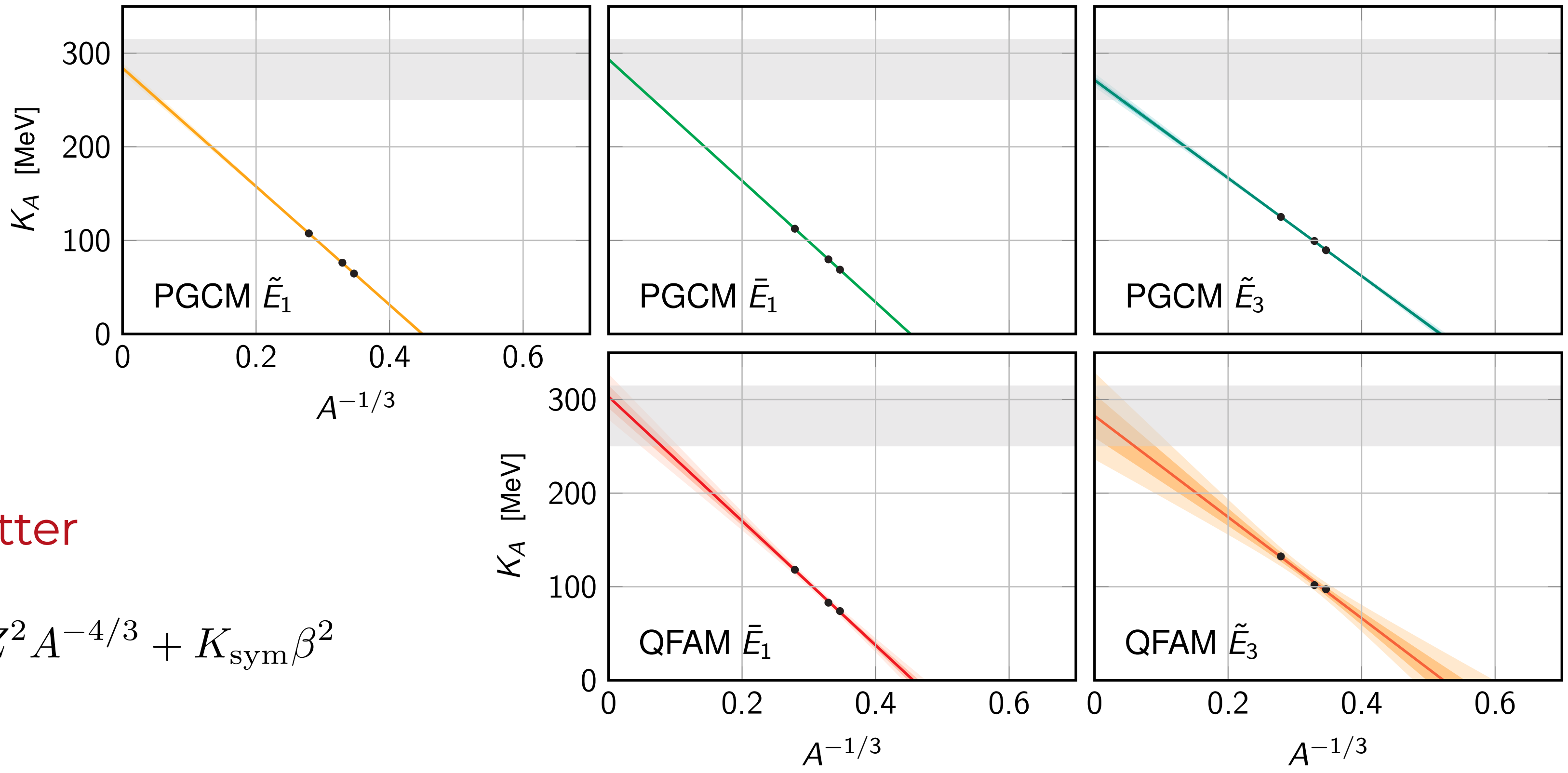

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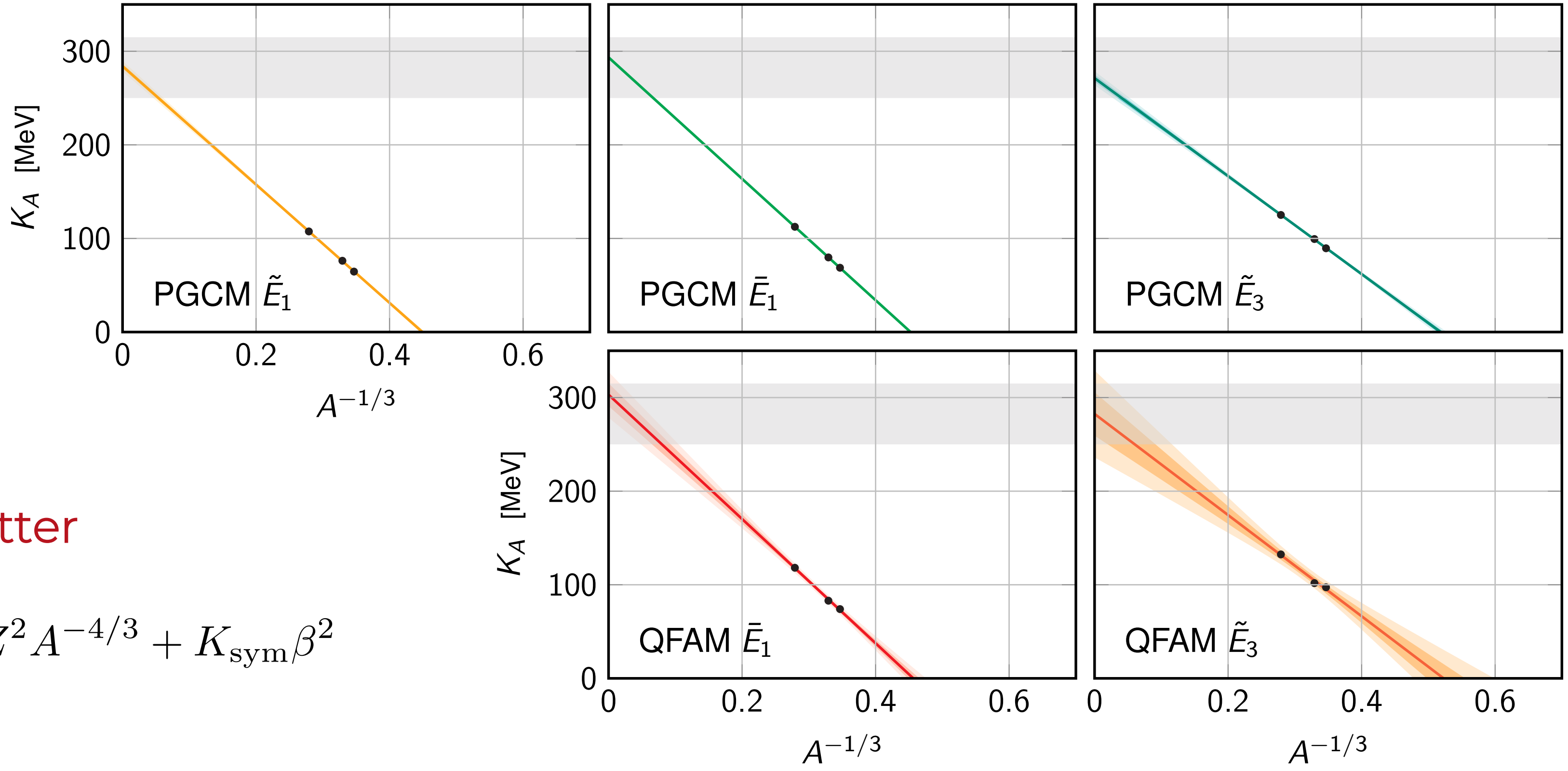

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$$x \equiv A^{-1/3}$$

$$K_A = K_\infty + K_{\rm surf}\, x$$

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)

[Burrows, Baker, Bacca et al., arXiv:2312.09782]

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Current frontiers

SPECTROSCOPY

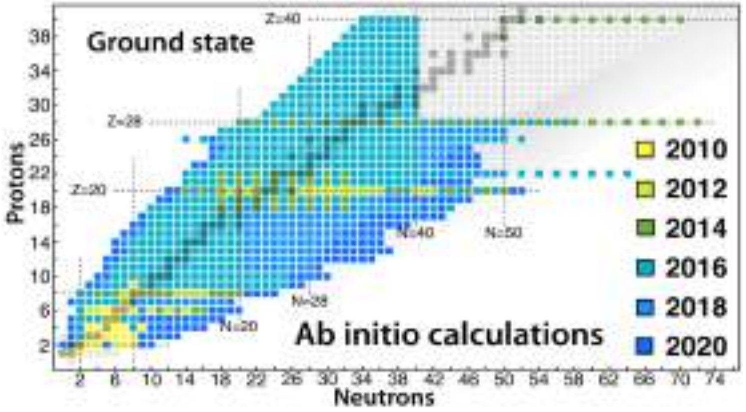
- Single-particle
- Collective excitations

ACCURACY

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

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

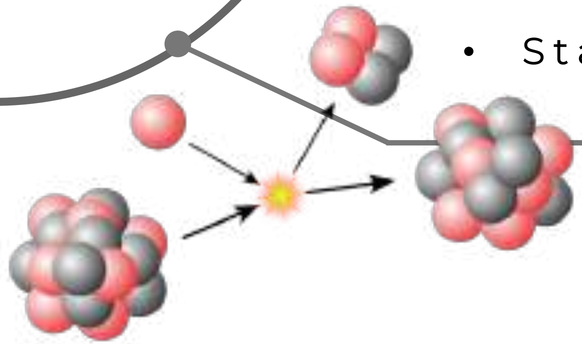
OPEN-SHELL



[Hergert, Front. Phys, 2020]

UNCERTAINTIES

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



REACTIONS

HEAVY-MASS SYSTEMS

Conclusions and perspectives

Perspectives

- Systematic comparison to new and existing exp data
- Deeper uncertainty quantification (EC)
- Develop full symmetry-conserving QRPA
- More systematic choice of the GC

SPECTROSCOPY

OPEN-SHELL

UNCERTAINTIES

Take-away messages

- PGCM reliable tool for *ab initio** spectroscopy
- Access to new observables and phenomena in *ab initio*

How is this even ab initio?

How do you choose the collective coordinates?

Thanks for the attention

Benjamin Bally
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Danilo Gambacurta