

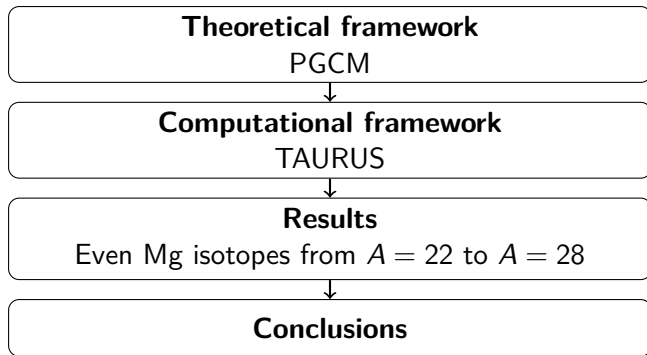
# Nuclear Structure Calculations Including the Effect of Mixing Multi-Quasiparticle Excitations

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The nuclear many-body problem is a **HUGE** problem! Like getting stuck in the elevator...

Even if we *knew* the nuclear interaction the exact nuclear wave functions and energies cannot be obtained in general because of:

- The **exploding dimensionality** of the many-body Hilbert space.
- The huge amount of two-, three-, ...,  $N$ - body matrix elements that are impossible to store.

We depend on approximate methods, in our project we use a **variational approach**.

# Projected Generator Coordinate Method (PGCM)



- This method combines **configuration mixing** with the **variational minimization** of the energy functional while projecting to particle number ( $\hat{P}^N$  and  $\hat{P}^Z$ ) and angular momentum ( $\hat{P}_{MK}^J$ ).

$$|\Psi^{J,M;N,Z,\sigma}\rangle = \sum_{i=1}^{N_{\text{int}}} \sum_K \underbrace{f_{K,q_i}^{J;N,Z,\sigma}}_{\text{Mixing coefficients}} \underbrace{\hat{P}_{MK}^J \hat{P}^N \hat{P}^Z}_{\text{Projectors}} \underbrace{|\phi(\vec{q}_i)\rangle}_{\text{Intrinsic states}}$$

- These **intrinsic states**  $\{|\phi(\vec{q}_i)\rangle\}_{i,\dots,N_{\text{int}}}$  are a set of many-body wave functions that depend parametrically on some collective variables,  $\vec{q}$ , called **generating coordinates**.

# Projected Generator Coordinate Method (PGCM)



- Performing the variation of the energy with respect to the coefficients of  $|\Psi^{J,M;N,Z,\sigma}\rangle$ , we obtain the Hill–Wheeler–Griffin equation:

$$\boxed{\delta E[\Psi^\sigma] = 0} \quad \Rightarrow \quad \boxed{\sum_{j=1}^{N_{\text{int}}} \sum_{K'} \left( \mathcal{H}_{K,q_i;K',q_j}^{J;N,Z} - E^{J;N,Z,\sigma} \mathcal{N}_{K,q_i;K',q_j}^{J;N,Z} \right) f_{K',q_j}^{J;N,Z,\sigma} = 0}$$

Hill–Wheeler–Griffin equation

- Where  $\mathcal{N}_{K,q_i;K',q_j}^{J;N,Z} = \langle \phi_{q_i} | \hat{P}_{KK'}^J \hat{P}^N \hat{P}^Z | \phi_{q_j} \rangle$ , is the **norm overlap matrix** and  $\mathcal{H}_{K,q_i;K',q_j}^{J;N,Z} = \langle \phi_{q_i} | \hat{H} \hat{P}_{KK'}^J \hat{P}^N \hat{P}^Z | \phi_{q_j} \rangle$  is the **Hamiltonian overlap matrix**.

# Projected Generator Coordinate Method (PGCM)



## Hartree-Fock-Bogoliubov

The intrinsic states are constructed as quasiparticle vacua through a Bogoliubov transformation, this is **the most general combination of the single particle operators**, and then a self-consistent **Hartree-Fock** minimization of the energy is performed. This is called the Hartree-Fock-Bogoliubov method, which connects particle and quasiparticle operators:

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

where

- $c_i^\dagger, c_i$  : particle creation and annihilation operators,
- $\beta_q^\dagger, \beta_q$  : quasiparticle creation and annihilation operators,
- $U, V$  : Bogoliubov transformation matrices.

# Projected Generator Coordinate Method (PGCM)



Hartree-Fock-Bogoliubov

The intrinsic state  $|\phi\rangle$  is defined as the quasiparticle vacua:

$$|\phi\rangle = \prod_{q=1}^M \beta_q |-\rangle \quad \rightarrow \quad \beta_k |\phi\rangle = 0, \quad \forall k \in \{1, \dots, M\}$$

By construction, the intrinsic wave function  $\phi$  does **not conserve particle number** or, in general, other symmetries such as **total angular momentum**, even though the Hamiltonian commutes with the corresponding operators.

# Projected Generator Coordinate Method (PGCM)

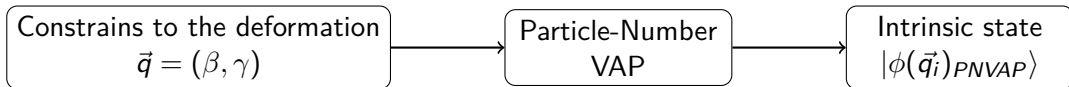


## Particle-Number Variation After Projection (PNVAP)

In order to build the intrinsic states for the PGCM we want to:

- Add **constraints** to create different configurations. We do this by fixing the quadrupole deformations parameters  $\beta$  and  $\gamma$ .  $\rightarrow$  **Collective variables**  $\rightarrow$  **Generating coordinates**.
- And then obtain the wave functions through the minimization of the **projected energy**  $E^{N,Z}[\phi(\vec{q}_i)]$ .

$$E^{N,Z}[\phi(\vec{q}_i)] = \frac{\langle \phi(\vec{q}_i) | \hat{H} \hat{P}^N \hat{P}^Z | \phi(\vec{q}_i) \rangle}{\langle \phi(\vec{q}_i) | \hat{P}^N \hat{P}^Z | \phi(\vec{q}_i) \rangle} - \lambda_{(\vec{q}_i)} \langle \phi(\vec{q}_i) | \hat{\vec{Q}} | \phi(\vec{q}_i) \rangle \xrightarrow{\delta E^{N,Z}=0} |\phi(\vec{q}_i)_{PNVAP}\rangle$$



# Projected Generator Coordinate Method (PGCM)



## Quasiparticle excitations

In this project we include **2 quasiparticle** excitations to the PGCM to **extend the configuration space** and investigate these correlations. The quasiparticle states are constructed as follows:

$$\beta_{\mu}^{\dagger} = \sum_i \left( U_{i\mu} c_i^{\dagger} + V_{i\mu} c_i \right).$$

$\beta_{\mu}^{\dagger}$  is the quasiparticle creation operator, and now we apply them to the PNVAP states.

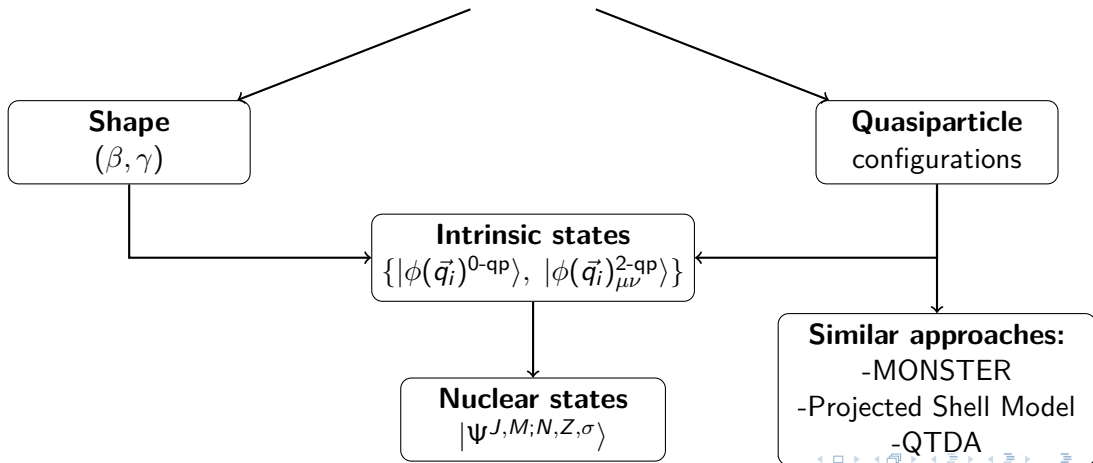
$$\boxed{|\phi(\vec{q}_i)_{\mu\nu}^{2\text{-qp}}\rangle = \beta_{\mu}^{\dagger} \beta_{\nu}^{\dagger} |\phi(\vec{q}_i)_{\text{PNVAP}}\rangle} \quad \mu < \nu$$

$$\text{PNVAP state} \xrightarrow{\beta_{\mu}^{\dagger} \beta_{\nu}^{\dagger}} \text{2-qp configuration}$$

# Projected Generator Coordinate Method

Configuration space

## PGCM configuration space



# Theory for A Unified descRiption of nUclear Structure

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Code Papers

## Symmetry-projected variational calculations with the numerical suite TAURUS

### I. Variation after particle-number projection

B. Bally<sup>1,a</sup>, A. Sánchez-Fernández<sup>1,b</sup>, T. R. Rodríguez<sup>1,2,c</sup>

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THE EUROPEAN  
PHYSICAL JOURNAL A



Code Paper

## Symmetry-projected variational calculations with the numerical suite TAURUS

### II. Configuration mixing of symmetry-projected reference states

B. Bally<sup>1,a</sup>, T. R. Rodríguez<sup>2,3,4,b</sup>

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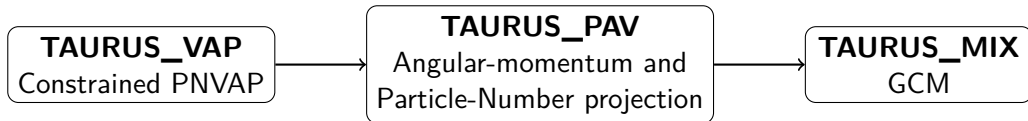
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Communicated by Dario Vretenar

<https://github.com/project-taurus>

# Computational Framework

TAURUS



## Intrinsic states

$$\{|\phi(\vec{q}_i)^{0\text{-qp}}\rangle, |\phi(\vec{q}_i)^{2\text{-qp}}_{\mu\nu}\rangle\}$$

Constrained PNVAP solutions

## Projected kernels

$$\mathcal{H}_{K,q_i;K',q_j}^{J;N,Z}, \quad \mathcal{N}_{K,q_i;K',q_j}^{J;N,Z}$$

Norm and Hamiltonian overlaps

## Physical states

$$|\psi^{J,M;N,Z,\sigma}\rangle$$

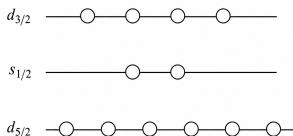
Hill–Wheeler–Griffin solutions

# $^{24}\text{Mg}$ benchmark



## USD interaction

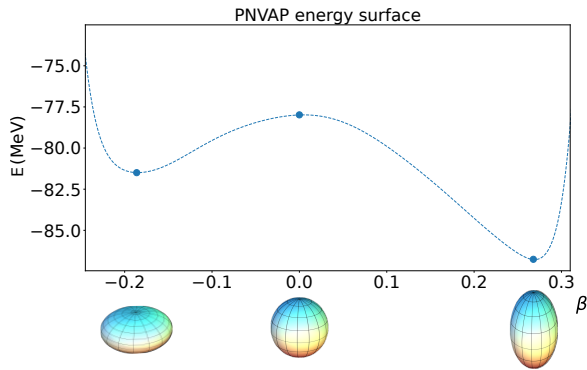
- The model space used to study in this project is a non-interacting  $^{16}\text{O}$  core and valence nucleons in the  $d_{5/2}$ ,  $s_{1/2}$  and  $d_{3/2}$  shells (sd-shells).



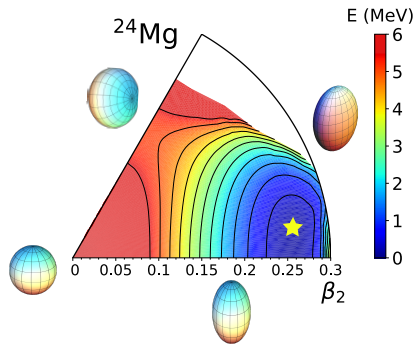
- For this project we have selected  $^{24}\text{Mg}$  as a benchmark to test this approach.
- 0- and 2-qp states were included in the different calculations.

# $^{24}\text{Mg}$ benchmark

## Quadrupole deformations



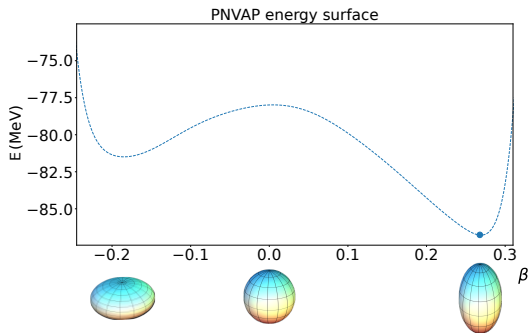
Projected energy vs quadrupole **axial** deformation.



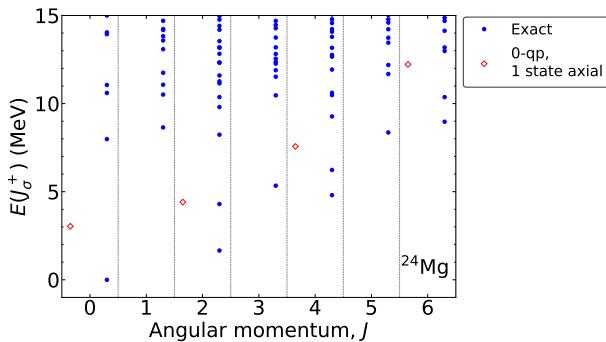
$(\beta, \gamma)$  plane, where the star represents the minimum of the energy corresponding to a **triaxial** deformation.

# $^{24}\text{Mg}$ benchmark

## Axial calculations

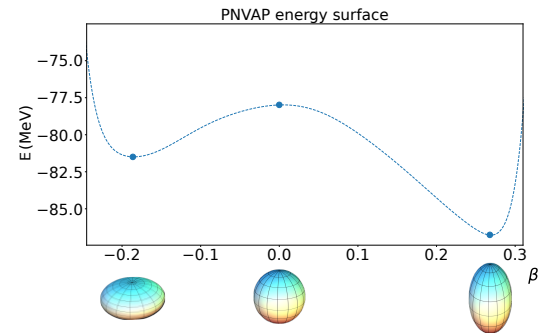


1 0qp state

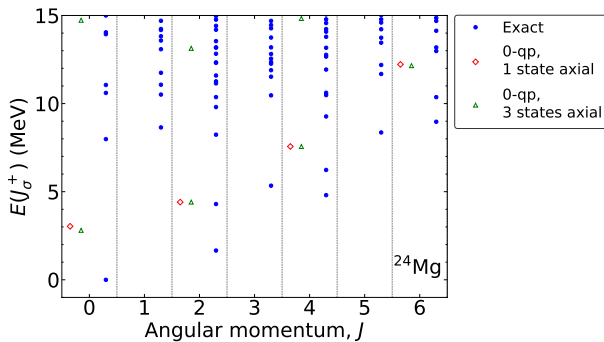


# $^{24}\text{Mg}$ benchmark

Axial calculations

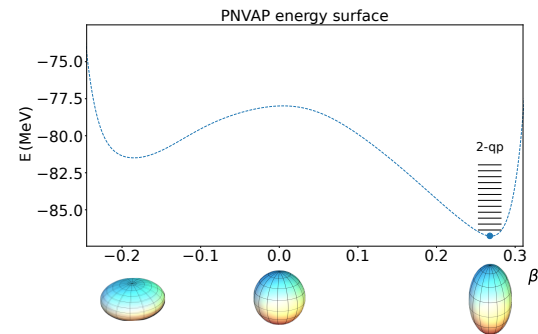


3 0qp states

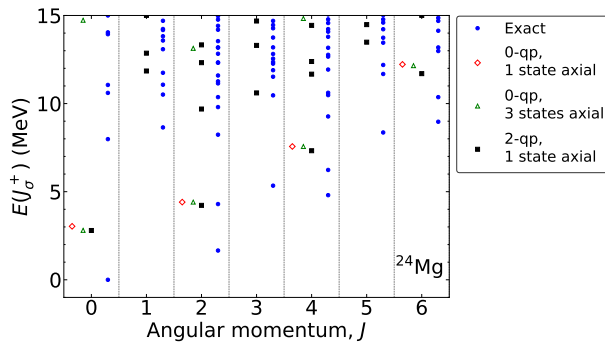


# $^{24}\text{Mg}$ benchmark

## Axial calculations

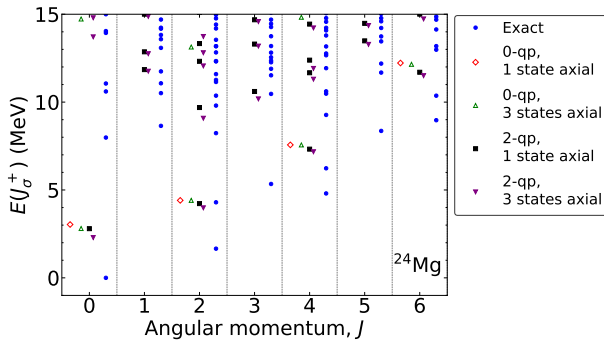
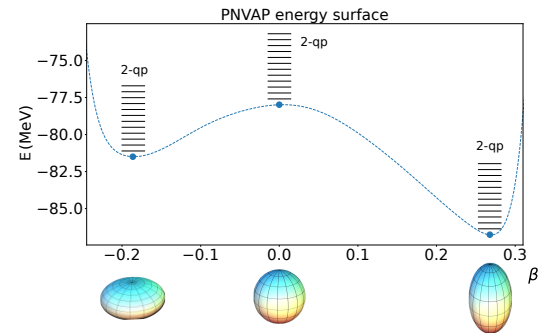


1 0qp state + 66 2qp states



# $^{24}\text{Mg}$ benchmark

## Axial calculations

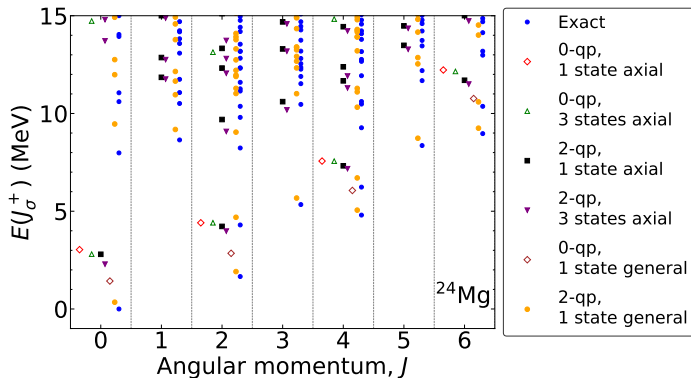


$$3 \text{ 0qp states} + 3 \times \binom{12}{2} = 198 \quad \text{2qp states}$$

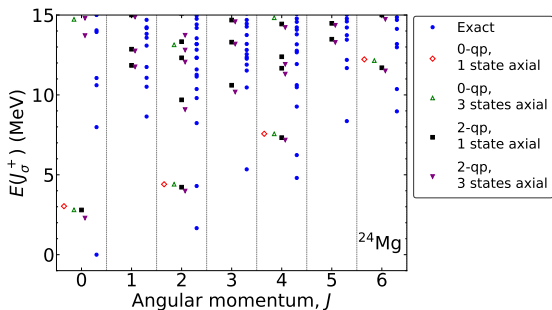
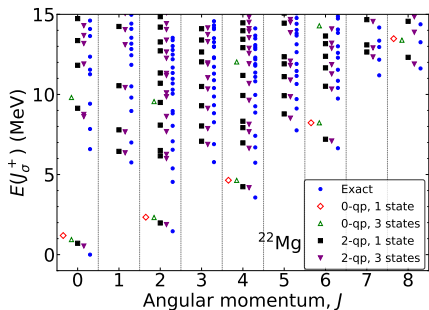
# $^{24}\text{Mg}$ benchmark

## Additional general seed

In orange, the PGCM results with one 0QP state and its 2QP states obtained as the absolute PNVAP minimum without any constraint and using a general symmetry-breaking seed wave function (**triaxiality** and **pn-mixing** is obtained).

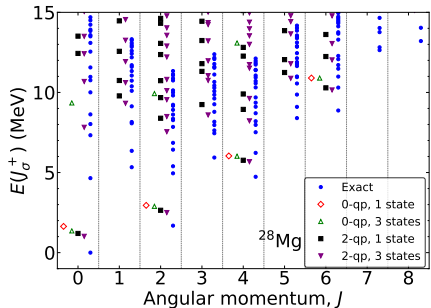
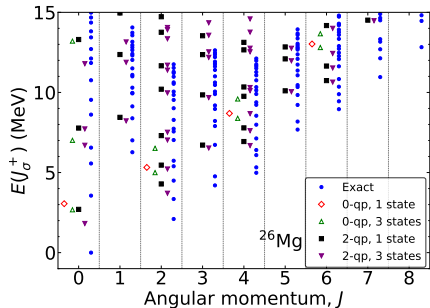


# Energy Spectra: $^{22}\text{Mg}$ and $^{24}\text{Mg}$



**Figure:** Comparative spectra of  $^{22}\text{Mg}$  and  $^{24}\text{Mg}$  calculated for 0 qp and 0 qp + 2qp for 1 and 3 values of  $\beta$ .

# Energy Spectra: $^{26}\text{Mg}$ and $^{28}\text{Mg}$



**Figure:** Comparative spectra of  $^{26}\text{Mg}$  and  $^{28}\text{Mg}$  calculated for 0 q and 0 q + 2q for 1 and 3 values of  $\beta$ .

- Multi-quasiparticle configurations introduce an **additional degree of freedom**, which extends the explored Hilbert space.
- The **axial calculations** were not enough to predict the value of the ground state of  $^{24}\text{Mg}$  very accurately, due to the **lack of proton-neutron pairing and triaxiality**.
- The results show a special good agreement with the exact result for the case of using an **unrestricted Bogoliubov transformation** to build the 0- and 2-qp states.
- The multi-quasiparticle PGCM gives similar results through all the even-even Mg isotopes from  $A=22$  to  $A=28$ .

- Future work will include extending this ansatz to several general 0-q<sub>p</sub> states and n-q<sub>p</sub> configurations.
- Study the effect of triaxiality on the remaining Mg isotopes.
- Study the electromagnetic transitions.
- Compare the multi-quasiparticle configurations calculations with the same amount of intrinsic states and 0 quasiparticles.

# Thank you for your attention

Questions?

# Solving the Hill–Wheeler–Griffin Equation

## 1 Diagonalize the norm kernel

$$\sum_{q'} N^J(q, q') u_k(q') = \lambda_k u_k(q). \quad (1)$$

## 2 Construct the natural basis, removing linear dependencies.

$$|\Lambda_k^J\rangle = \sum_q \frac{u_k(q)}{\sqrt{\lambda_k}} |\phi_q^J\rangle, \quad \langle \Lambda_k^J | \Lambda_{k'}^J \rangle = \delta_{kk'}. \quad (2)$$

## 3 Solve the HWG equation in the natural basis

$$\sum_{k'} \langle \Lambda_k^J | \hat{H} | \Lambda_{k'}^J \rangle g_{\sigma k'}^J = E_\sigma^J g_{\sigma k}^J \quad (3)$$