

#### The PGCM and its connection to collective states and resonances

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#### Contents

#### Introduction

#### ➢ PGCM

- Ansatz
- Solution of the HWG equation
- New considerations
- Applications
  - Spectra and collectivity
  - Electromagnetic responses





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**NUCLEAR THEORY** — solve the many-body problem (structure, reactions).

Difficulties:

- a. Challenging nature of nuclear interaction
- b. Quantum A-body coupled system

Even if we knew the nuclear interaction: exact energies and wave functions out of reach due to the immense dimensionality of Many-Body Hilbert Space

- > Approximate Methods: variational principle
  - Quasiparticle Random Phase Approximation (QRPA)
  - 0 ...
  - Projected Generator Coordinate Method (PGCM)





#### **PGCM:** symmetry-restored Generator Coordinate Method (GCM)

D. L. HILL AND J. A. WHEELER



Quantum linear superposition of product states





#### **PGCM:** symmetry-restored Generator Coordinate Method (GCM)

First PGCM implementations (SCCM, MR-EDF):

Gogny. R. Rodríguez-Guzmán, J. L. Egido, L. M. Robledo, *Phys Lett. B* 474, 15 (2000)

Skyrme: P.-H. Heenen, A. Valor, M. Bender, P. Bonche, H. Flocard, *Eur Phys J A* **11**, 393–402 (2001)

Relativistic MF: T. Nikšić, D. Vretenar, P. Ring, Phys. Rev. C73, 034308 (2006)

- Even though historically PGCM has been associated with EDF, nowadays it has been extended to other kind of interactions
- Related methods:
  - Discrete non-orthogonal shell model (DNO-SM)
  - Monte Carlo shell model (MCSM)



#### Introduction

- Kind of nuclei
  - even-even nuclei (blocking required if multi-quasiparticle excitations are included)
  - even-odd/odd-even nuclei (blocking mandatory)
  - odd-odd nuclei (blocking mandatory)
- Observables and physical quantities
  - Ground state and excitation energies
  - electromagnetic transition probabilities (low-lying states)
  - Beta-decay rates
  - Electromagnetic responses / resonances (higher-lying states)





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Variational method based on the <u>mixing of configurations</u>. The many-body wave functions of the system is expressed as:

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} \int_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$
  
coefficients intrinsic (projected) states



Variational method based on the <u>mixing of configurations</u>. The many-body wave functions of the system is expressed as:

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

Where:

>  $\{|\Phi(q_i)\rangle\}$  is a set of intrinsic many-body wave functions defined parametrically along the variables, q

- Multipole deformations
- Pairing correlations
- $\circ$  Cranking
- 0...
- Several at the same time



T. R. Rodríguez and J. L. Egido *Phys. Rev. C* **81**, 064323 (2010)

"You are the architect of your own destiny." - Ralph Waldo Emerson (and your PGCM calculations)



Variational method based on the <u>mixing of configurations</u>. The many-body wave functions of the system is expressed as:

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

Intrinsic self-consistent mean-field (HFB-like, Bogoliubov quasiparticle vacuum) states:

$$\beta_b^{\dagger}(q) = \sum_a U_{ab}(q) c_a^{\dagger} + V_{ab}(q) c_a \qquad |\Phi(q)\rangle = \prod_{j=1}^A \beta_j(q) |-\rangle \quad \longrightarrow \quad \beta_k(q) |\Phi\rangle = 0 \ \forall k$$

But these states are not limited to be quasiparticle vacua!  $|\Phi_{k_1k_2}(q)\rangle = \beta_{k_1}^{\dagger}(q)\beta_{k_2}^{\dagger}(q)|\Phi(q)\rangle$ Blocking

> For odd-mass and odd-odd nuclei, blocking must be applied by definition.

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We minimize the (constrained) energy functional:

$$\beta_b^{\dagger}(q) = \sum_{a} U_{ab}(q) c_a^{\dagger} + V_{ab}(q) c_a$$
variational

$$E[|\Phi(q)\rangle] = \frac{\langle \Phi(q) | \hat{H} | \Phi(q) \rangle}{\langle \Phi(q) | \Phi(q) \rangle} - \langle \Phi(q) | \lambda_q \hat{Q} | \Phi(q) \rangle$$

$$E_{\rm PNVAP}'\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^NP^Z|\Phi(q)\rangle}{\langle\Phi(q)|P^NP^Z|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q\hat{Q}|\Phi(q)\rangle$$



Variational method based on the <u>mixing of configurations</u>. The many-body wave functions of the system is expressed as:

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

projection operators

Symmetry restoration (lost at mean-field level):

 $P^J_{MK} \rightarrow$  angular momentum projection operator  $P^N \rightarrow$  neutron number projection operator  $P^Z \rightarrow$  proton number projection operator  $P^{\pi} \rightarrow$  spatial parity projection operator





Variational method based on the <u>mixing of configurations</u>. The many-body wave functions of the system is expressed as:

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where

 $> f_{\sigma;qK}^{JMNZ\pi}$  are the PGCM variational parameters that minimize the energy.

$$\delta E[|\Psi^{\sigma}\rangle] = 0 \Rightarrow \sum_{\substack{q'K'}} \left(\mathcal{H}_{qK,q'K'}^{\Gamma} - E_{\sigma}^{\Gamma}\mathcal{N}_{qK,q'K'}^{\Gamma}\right) f_{\sigma;q'K'}^{\Gamma} = 0$$

$$\Gamma \equiv (JMNZ\pi)$$

Hill-Wheeler-Griffin (HWG) equation

$$\mathcal{H}_{qK,q'K'}^{\Gamma} = \langle \Phi(q) | \hat{H} P_{KK'}^{J} P^{N} P^{Z} P^{\pi} | \Phi(q') \rangle$$
 Generalized  

$$\mathcal{N}_{qK;q'K'}^{\Gamma} = \langle \Phi(q) | P_{KK'}^{J} P^{N} P^{Z} P^{\pi} | \Phi(q') \rangle$$
 Generalized  
eigenvalue problem!





How do we get to the usual eigenvalue problem? Creating an orthonormal basis

1. Finding the eigenvalues and eigenvectors of the norm overlap matrix:

$$\sum_{j=1}^{N_{\text{int}}} \mathcal{N}_{q_i,q_j} u_{\lambda_k,q_j} = \lambda_k u_{\lambda_k,q_i}$$

2. From them, building a set of orthonormal states ("natural basis"):

$$|\Lambda_k\rangle = \sum_{i=1}^{N_{\text{int}}} \frac{u_{\lambda_k, q_i}}{\sqrt{\lambda_k}} |\Phi_{q_i}\rangle \qquad \langle \Lambda_k |\Lambda_{k'}\rangle = \delta_{k, k'}$$

3. Rewriting the HWG equation and the PGCM ansatz wave function:

$$\sum_{k'=1}^{N_{\text{nat}}} \langle \Lambda_k | \hat{H} | \Lambda_{k'} \rangle g_{k'}^{\sigma} = E^{\sigma} g_k^{\sigma} \qquad |\Psi^{\sigma}\rangle = \sum_{k=1}^{N_{\text{nat}}} g_k^{\sigma} | \Lambda_k^{\sigma}\rangle = \sum_{i=1}^{N_{\text{int}}} \sum_{k=1}^{N_{\text{nat}}} g_k^{\sigma} \frac{u_{\lambda_k, q_i}}{\sqrt{\lambda_k}} |\Phi_{q_i}\rangle$$
Regular eigenvalue problem!



## PGCM: solution of the HWG equation

#### The usual analysis: plateau condition

 $N_{\rm nat}$  $\sum \langle \Lambda_k | \hat{H} | \Lambda_{k'} \rangle g_{k'}^{\sigma} = E^{\sigma} g_k^{\sigma}$ 

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- I. Given the states of the natural basis, we sort them by the eigenvalues of the norm overlap matrix from largest (higher contributions) to smallest.
- II. We solve the HWG equation with only one natural basis state and obtain the energy, then with two and so on.
- III. As the eigenvalues decrease, we expect smaller contributions, so that the energy remains fairly constant → plateau condition



## PGCM: solution of the HWG equation

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Actually, we have:

• Initial set of intrinsic states  $\{ |\Phi_{q_i} \rangle \}_{i=1,...,N_{\text{int}}}$ 

Through the norm overlap matrix:  $N_{
m int}$  eigenvalues  $\lambda_k$  and eigenvectors  $u_{\lambda_k}$ :

- Exact linear dependencies such as  $\lambda = 0$
- Approximate linear dependencies such as  $\lambda \neq 0$  but  $\lambda \approx 0$   $\longrightarrow$   $L_{app}$
- Final set of well-defined natural basis states  $\{|\Lambda_k
  angle\}_{k=1,...,N_{
  m nat}}$

$$N_{\rm nat} = N_{\rm int} - L_{\rm exa} - L_{\rm app}$$

Zero is an accumulation point for the norm overlap eigenvalues!



 $N_{\rm int}$ 

 $L_{exa}$ 

### PGCM: solution of the HWG equation

Non-orthogonality and approximate linear dependence

• Let us have two vectors in  $\mathbb{R}^2$  such that:

 $\vec{v}_1 \cdot \vec{v}_1 = 1$ ,  $\vec{v}_2 \cdot \vec{v}_2 = 1$ ,  $\vec{v}_1 \cdot \vec{v}_2 = \mu$ 

• The norm overlap matrix is

$$\mathcal{N}_{ij} = \vec{v}_i \cdot \vec{v}_j = \begin{pmatrix} 1 & \mu \\ \mu & 1 \end{pmatrix} \Rightarrow \text{ Eigenvalues: } \lambda_{\pm} = 1 \pm \mu$$

• Then:

$$\mu = 0 \Rightarrow \vec{v}_1 \perp \vec{v}_2, \quad \lambda_{\pm} = 1, 1 \quad \text{(orthonormal)}$$
  
$$\mu = 1 \Rightarrow \vec{v}_1 = \vec{v}_2, \quad \lambda_{\pm} = 2, 0 \quad \text{(exact linear dependency!)}$$

 For 0 < μ < 1, the natural basis does not contain exact LD. <u>However</u>, if μ ≈ 1, the natural state with λ = 1 − μ could be ill-defined!



**Usually**: cutoff to the eigenvalues,  $\varepsilon_{\lambda}$ 



Problems:

- 1. Cutoff chosen heuristically.
- 2. Ideal value depends on the calculation.
- 3. Big jump is a sign of these approximate linear dependencies, **but there could be more**...





Usual cutoff does not avoid the LD spoiling of the natural basis



J. Martínez-Larraz and T. R. Rodríguez Phys. Rev. C 106, 054301 (2022)

New method: orthonormality condition of the natural states.

- The orthonormality of the natural basis,  $\langle \Lambda_k | \Lambda_{k'} \rangle = \delta_{k,k'}$ , is eventually lost.
- However, we could restore its viability by imposing the condition:

$$\langle \Lambda_k | \Lambda_{k'} \rangle - \delta_{kk'} < \varepsilon_{\text{nat}} \; ; \; \forall k, k'$$

and removing the natural states that do not fulfill it.



Big jump is a sign of these approximate linear dependencies, but there could be more...

> Picket-fence model:

$$\hat{H} = \sum_{k=1}^{N_{lev}} \varepsilon_k \left( c_k^{\dagger} c_k + c_{\bar{k}}^{\dagger} c_{\bar{k}} \right) - G \sum_{k,k'=1}^{N_{lev}} c_k^{\dagger} c_{\bar{k}'} c_{\bar{k}'} c_{k'} \qquad N = 4$$

| k | Orbital    | $\varepsilon_k \; ({\rm MeV})$ |
|---|------------|--------------------------------|
| 5 | $4s_{1/2}$ | 2.0                            |
| 4 | $3s_{1/2}$ | 1.5                            |
| 3 | $2s_{1/2}$ | 1.0                            |
| 2 | $1s_{1/2}$ | 0.5                            |
| 1 | $0s_{1/2}$ | 0.0                            |

✤ Total exact space: 50 0<sup>+</sup> states

✤ PGCM: 46 exact 0<sup>+</sup> states





J. Martínez-Larraz PhD thesis.



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States in the natural basis

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$$|\Psi_{PGCM}^{N,Z;J;\sigma}\rangle = \sum_{k} g_{\sigma}^{N,Z,J}(k) |\Lambda_{k}\rangle \longrightarrow |g_{\sigma}(k)|^{2}$$

characteristic weight distribution

J. Martínez-Larraz PhD thesis.







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- 1. To ensure the orthonormality of the NB is important
- 2. The LD breakdown can be related to spurious states
- 3. Plateau conditions are not a good way of studying convergence
- 4. They only account for the specific distributions of PGCM states
- 5. We could look at the continuity of the weight distributions

J. Martínez-Larraz PhD thesis.



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Once we have found the proper dimension of the natural basis,  $N_{nat}$ , we solve the HWG equation for each angular momentum :

$$\sum_{k'}^{N_{\text{nat}}} \langle \Lambda_k | \hat{H} | \Lambda_{k'} \rangle g_{\sigma}^{N,Z,J}(k') = E_{\sigma}^{N,Z,J} g_{\sigma}^{N,Z,J}(k)$$

retrieving the PGCM nuclear energies of the **yrast state and excited states** on the same footage, besides the wave functions,

$$|\Psi_{PGCM}^{N,Z;J;\sigma}\rangle = \sum_{k} g_{\sigma}^{N,Z,J}(k) |\Lambda_{k}\rangle$$

We can also compute the collective wave functions to obtain an interpretation in terms of the intrinsic states:

$$\left| F_{\sigma}^{N,Z,J}(\vec{q_i}) \right|^2 = \left| \sum_k g_{\sigma}^{N,Z,J}(k) \cdot u_k^{N,Z,J}(\vec{q_i}) \right|^2$$



With the PGCM states defined, we can compute quantities such as the electromagnetic strength functions:

$$B(E\lambda; J_i^{\pi} \to J_f^{\pi}) = \frac{1}{2J_i + 1} |\langle J_f^{\pi}|| \hat{M}_{\lambda}^{\text{elec}} ||J_i^{\pi}\rangle|^2$$
$$B(M\lambda; J_i^{\pi} \to J_f^{\pi}) = \frac{1}{2J_i + 1} |\langle J_f^{\pi}|| \hat{M}_{\lambda}^{\text{mag}} ||J_i^{\pi}\rangle|^2$$

#### Strategy:

- Compute the initial and final states by solving the nuclear many-body problem separately.
- Compute the transition matrix elements between individual states.
- Energies, electromagnetic and decay properties are obtained within the same framework.

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The main goal in the PGCM calculations is to represent the nuclear states as good as possible. However, in some cases it is difficult:

$$J^{\pi} = 1^+$$
 challenge!

Obtaining 1<sup>+</sup> states from HFB-like wave-functions

**Aim**: to reliably reproduce a high density of 1<sup>+</sup> states in PGCM calculations (resonances)

#### **Collaboration**:

- Kamila Sieja
- Thomas Duguet
- Mikael Frosini
- Stavros Bofos
- Benjamin Bally
- Tomás Rodríguez
- Jaime Martínez-Larraz



#### Conclusions

#### PROS

#### CONS

- Applicable to all regions of nuclear chart.
- Adaptable and flexible.
- Continuous and discrete coordinates.
- Beyond-mean-field technique.
- Complete restoration of symmetries.
- Description of nuclear states in terms of collective variables.
- Energies, transitions and decay properties: same framework

- Approximate solutions.
- $\geq$  Depends on the choice of d.o.f.
- Depends on the quality of meanfield wave functions.
- Calculations can be computationally expensive.
- To delimit a proper natural basis can be complex in some cases.







# Thank you for your attention!









The intrinsic HFB-like state can be decomposed in angular momentum eigenstates:

$$|\Phi(q)\rangle = \sum_{\alpha} \sum_{J} \sum_{K=-J}^{J} c_{\alpha,JK}(q) |\alpha,JK\rangle$$

$$\alpha \text{ other quantum numbers}$$

If the intrinsic HFB-like preserves simultaneously:

(typically preserved in self-consistent symmetries imposed in most of the mean-field solvers)

$$\hat{T}|\Phi\rangle = |\Phi\rangle$$

$$\hat{P}|\Phi\rangle = |\Phi\rangle$$

$$\hat{R}_{x}|\Phi\rangle = e^{-i\pi\hat{J}_{x}}|\Phi\rangle = |\Phi\rangle$$

$$- c_{\alpha, J_{odd}K}(q) = 0$$

#### we cannot produce J=1 projected states

- constraints: cranking, isoscalar pairing, etc
- n-quasiparticle states



- Magnetic transitions:
- $B(M1; 1^+_{\sigma} \to 0^+_1)$

$$|J_i\rangle = |1_{\sigma}^+\rangle \quad |J_f\rangle$$

- Nuclei:  $^{20}$ Ne and  $^{24}$ Mg (N=Z)
- USDB shell model interaction (<sup>16</sup>O core)
- Benchmark results from the first one hundred 1<sup>+</sup> states





 $= |0_1^+\rangle$ 

• Generating coordinates (constraints): proton-neutron pairing content





- Generating coordinates (constraints): proton-neutron pairing content
  - In TAURUS, general HFB (real) transformation allows the inclusion of proton-neutron pairing

$$|\Phi(q)\rangle \to \beta_b(q)|\Phi(q)\rangle = 0 \quad \forall \quad b \qquad \beta_b^{\dagger}(q) = \sum_a U_{ab}(q)c_a^{\dagger} + V_{ab}(q)c_a$$

$$U = \begin{pmatrix} U_{pp} & U_{pn} \\ U_{np} & U_{nn} \end{pmatrix}; V = \begin{pmatrix} V_{pp} & V_{pn} \\ V_{np} & V_{nn} \end{pmatrix}$$

Marie Skłodowska-Curie Actions TAURUS (ID:839847)



\* B. Bally, A. Sánchez, T. R. R., EPJA 57, 69 (2021)



- Generating coordinates (constraints): proton-neutron pairing content
  - In TAURUS, general HFB (real) transformation allows the inclusion of proton-neutron pairing

\* B. Bally, A. Sánchez, T. R. R., EPJA 57, 69 (2021)



Generating coordinates (constraints): intrinsic rotations (cranking)







Exploring cranking, pn-pairing (isoscalar and isovector)

 $\{|\Phi(j_x,\delta_{pn}^{T=0},\delta_{pn}^{T=1})\rangle\}$ 



- exact ground state energy
- exact description of low-lying excited energies



Exploring cranking, pn-pairing (isoscalar and isovector)

$$\{|\Phi(j_x,\delta_{pn}^{T=0},\delta_{pn}^{T=1})\rangle\}$$





- convergence of highly excited states can be tricky
- we have to abandon the idea of "plateau condition"

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#### **Projected Generator Coordinate Method**





#### **Projected Generator Coordinate Method**







 Even though historically PGCM has been associated with EDF, nowadays it has been extended to other kind of interactions:



TAURUS (Theory for A Unified descRiption of nUclear Structure)

- B. Bally, T. R. Rodríguez, and A. Sánchez-Fernández, *Zenodo* **99**, 062501 (2020)
- B. Bally and T. R. Rodríguez *Eur. Phys. J. A* **60**, 62 (2024)



