Collective motion in complex nuclei

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Abstract. We present the implementation in the $(\beta,\gamma)$ plane of the generator coordinate method with full triaxial angular momentum and particle number projected wave functions using the Gogny force. We apply the method to the study of $^{24}$Mg, the calculated energies of excited states as well as the transition probabilities are compared to the available experimental data showing a good overall agreement. In addition we also show preliminary results for the \textsuperscript{126}Xe.

1. Introduction

Self-consistent mean field methods with effective phenomenological interactions and their extensions beyond mean field provide the appropriate theoretical tools for describing many phenomena along the whole chart of nuclides [1]. On the one hand, the success of these methods is related to the high quality of the phenomenological effective interactions used -Skyrme, Gogny or Relativistic Mean Field (RMF). On the other hand, the mean field method by means of the symmetry breaking mechanism allows the inclusion of many correlations within a very simple intrinsic product wave function. Hence, bulk properties such as masses and radii are very well described at the mean field level. However, in some cases this picture fails and methods beyond the mean field approach have to be applied. Furthermore, because the mean field is defined in the intrinsic frame it is mandatory to go beyond this approximation to evaluate excitation energies or transition probabilities in the laboratory system.

There are several methods to incorporate the correlations missing at the mean field level. First, using projection techniques [2], many correlations are obtained by restoring some or all of the spontaneously broken symmetries of the mean field. Second, the mixing of different mean field configurations within the general framework of the Generator Coordinate Method (GCM) [2] allows the inclusion of quantum fluctuations along some relevant collective variables such as the multipole moments.

Most of the currently used beyond mean field calculations with effective forces include two symmetry restoration, i.e., particle number (PN) and angular momentum projection (AMP), and configuration mixing along the axial quadrupole deformation [1, 3, 4]. This approach (axial GCM-PNAMP) has been successfully applied to study many phenomena like, for example, the appearance or degradation of shell closures in neutron rich nuclei [5, 6, 3, 7], shape coexistence in proton rich Kr [8] or Pb [9, 10] isotopes or shape transitions in the $A \sim 150$ region [11, 12]. However, the intrinsic wave functions used there were restricted to have axial symmetry, with $K = 0$, because this assumption simplifies considerably the angular momentum projection and lightens the computational burden significantly. This restriction is one of the major drawbacks
of the method because it limits its applicability to systems where triaxiality does not play an important role. However, many exciting experimental and theoretical phenomena are closely related to the triaxial degree of freedom.

From the theoretical point of view some approaches beyond mean field have been proposed to study the triaxial effects. In particular, one of the most widely used is the collective Hamiltonian [2] given in different versions depending on the interaction used to define the collective potential, namely Pairing-plus-Quadrupole [13], Interacting Boson Model [14], Gogny [15], Nilsson [16], Skyrme [17] or RMF [18]. This model has been applied successfully to describe some of the experimental features mentioned above.

In the past, exact angular momentum projection with triaxial intrinsic wave functions without GCM have been carried out only for schematic forces and/or reduced configuration spaces. Examples are the projection of BCS [19] or Cranked Hartree-Fock-Bogoliubov (CHFB) states [20] with the Pairing-plus-Quadrupole interaction, the projection of Cranked Hartree-Fock (CHF) states (no pairing) with schematic [21] and full Skyrme interactions [22] or angular momentum projection before variation with particle number and parity restoration in limited shell model spaces [23, 24].

However, recent improvement of the computational capabilities enabled the first implementations of the angular momentum projection of triaxial intrinsic wave functions in the whole (β, γ) plane with effective forces. In particular, Bender and Heenen reported GCM calculations with particle number and triaxial angular momentum projection (PNAMP) with the Skyrme SLy4 interaction [25]. In this work, the intrinsic wave functions were found by solving the Lipkin-Nogami (LN) equations. On the other hand, Yao et al presented the implementation of the triaxial angular momentum projection [26] and the extension to the GCM [27] for the Relativistic Mean Field (RMF) framework. In the latter work no particle number projection has been performed and the mean field states are found by solving the RMF+BCS instead of the full HFB or LN equations. These approximations could lead to a poor description of important pairing correlations, especially in the weak pairing regime where even spurious phase transitions appear [28, 3].

Recently [29] we have presented the first implementation of the Generator Coordinate Method with Particle Number and Angular Momentum Projected (GCM-PNAMP) triaxial HFB wave functions with the finite range density dependent Gogny force. The finite range of the Gogny force [30] provides excellent pairing properties and is often used as a benchmark in this respect. Furthermore it is able to provide at the same time both good global as well as spectroscopic properties [31, 32]. The intrinsic HFB states are found by solving the Variation After Particle Number Projection (VAP-PN) equations [33]. This fact constitutes the main methodological difference with respect to the calculations reported in Ref. [25]. This is a very important difference because VAP-PN allows the inclusion of the pairing correlations in a very efficient way yielding a significant improvement of the final results with respect to other approaches [33, 3]. As discussed in [33] there are some problems concerning the restoration of symmetries in energy density functional calculations. The first one has to do with the presence of poles in the calculation of projected matrix elements if some exchange terms of the interaction are missing. In the case of the Gogny force we solved the problem by considering all the exchange terms neglected in earlier calculations. The second problem has to do with the density dependence part of the interaction and the prescription used to calculate its projected matrix elements. In our case we avoided the potential divergencies by using the projected density for the particle number symmetry and the mixed one for the angular momentum projection. See also Ref. [29] for more details in the case of the Gogny force and Ref. [25] and references therein for the Skyrme interaction.

The paper is organized as follows. In Sec. 2 we will give an overview of the theoretical
framework. In Sec. 3 we will focus our analysis on the nucleus $^{24}\text{Mg}$ which has been studied as a test case in earlier implementations of the GCM-PNAMP method with Skyrme and Relativistic interactions and the triaxial nucleus $^{126}\text{Xe}$ which has been used in the past as a test nucleus for comparison of different theoretical models. Then we will show the final results for the calculated spectrum and B(E2) transitions strengths of $^{24}\text{Mg}$ and and $^{126}\text{Xe}$ as well as a comparison with experimental data. Finally, a brief summary and outlook on future work will be addressed in Sec. 4.

2. Theoretical framework

2.1. Generator Coordinate Method with Particle Number and Angular Momentum Projected states (GCM-PNAMP)

In any beyond mean field theory the first step is the determination of the intrinsic HFB states. In our case the wave functions $(|\Phi(\beta, \gamma)\rangle)$ are obtained by minimizing the particle-number projected energy functional $E_{N,Z}[\Phi(\beta, \gamma)]$ (variation after projection, VAP)\cite{33}. This is one of the most relevant parts in the calculation because the quality of the result largely depends on the structure of the intrinsic HFB-type wave functions used. In contrast to other methods like plain HFB or Projected Lipkin-Nogami (PLN), the VAP-PN performs the restoration of the particle number symmetry in an optimal way, including pairing correlations both in the weak and strong pairing regimes \cite{3}. This is especially relevant in GCM-like theories where a large grid of $(\beta, \gamma)$ points is needed. The strength of the pairing correlations has a strong dependence on the single particle level density and the latter one itself with the deformation parameters. This implies that a strongly $(\beta, \gamma)$ dependent oscillating pairing regime appears in the calculations and consequently theories like plain HFB (BCS) or PLN (LN) are unable to cope with this challenge providing wave functions of oscillating goodness. Only a VAP-PN approach warrants high quality solutions independently of the $(\beta, \gamma)$ values.

In our case, we are using the Gogny D1S interaction \cite{30} and in the calculations, all direct, exchange and pairing terms are included \cite{34}. The VAP-PN principle, provides

$$\delta E_{N,Z}[\Phi(\beta, \gamma)]_{|\Phi=\Phi} = 0$$

where:

$$E_{N,Z}[\Phi] = \frac{\langle \Phi|H\hat{P}^{N}\hat{P}^{Z}|\Phi\rangle}{\langle \Phi|\hat{P}^{N}\hat{P}^{Z}|\Phi\rangle} - \lambda_{q_{20}}\langle \Phi|\hat{Q}_{20}|\Phi\rangle - \lambda_{q_{22}}\langle \Phi|\hat{Q}_{22}|\Phi\rangle$$

with $\hat{P}^{N} = \frac{1}{2\pi}\int_{0}^{2\pi} e^{i\varphi(N-N)} d\varphi$ the neutron number projector ( $\varphi$ the associated gauge angle and $\hat{P}^{Z}$ protons the proton number projector).

Furthermore, we see in Eq. 2 that the minimization is performed under constraints on the quadrupole deformation operators $\hat{Q}_{2\mu}$. The Lagrange multipliers $\lambda_{q_{2\mu}}$ ensure that the following conditions are fulfilled in the intrinsic state:

$$\lambda_{q_{20}} \rightarrow \langle \Phi|\hat{Q}_{20}|\Phi\rangle = q_{20}$$

$$\lambda_{q_{22}} \rightarrow \langle \Phi|\hat{Q}_{22}|\Phi\rangle = q_{22}$$

In addition, the deformation parameters $(\beta, \gamma)$ are directly related to $(q_{20}, q_{22})$ by:

$$q_{20} = \frac{\beta \cos \gamma}{C} ; q_{22} = \frac{\beta \sin \gamma}{\sqrt{2}C} ; C = \sqrt{\frac{5}{4\pi}} \frac{4\pi}{3r_{0}^{2}} \frac{1}{A^{5/3}}$$
being \( r_0 = 1.2 \text{ fm} \) and \( A \) the mass number. These constraints allow to explore the \((\beta, \gamma)\) plane to generate the wave functions to be used in the configuration mixing calculations.

The angular momentum projection is performed in the projection after variation (PAV) approach:

\[
|IMK; NZ; \beta\gamma\rangle = \frac{2I + 1}{8\pi^2} \int \mathcal{D}_{MK}^I(\Omega) \hat{R}(\Omega) \hat{P}_N \hat{P}_Z |\Phi(\beta, \gamma)\rangle d\Omega \tag{5}
\]

\( I \) is the angular momentum and \( M, K \) are the projections of \( \vec{I} \) on the laboratory and intrinsic \( z \)-axes respectively. \( \hat{R}(\Omega) \) and \( \mathcal{D}_{MK}^I(\Omega) \) are the rotation operator and the Wigner matrices [? in the Euler angles \( \Omega = (\alpha, b, c) \) \(^1\), respectively. In principle, the ranges for these angles are \((0 \leq a \leq 2\pi, 0 \leq b \leq \pi, 0 \leq c \leq 2\pi)\). However, for intrinsic Hartree-Fock-Bogoliubov (HFB) states \(|\Phi(\beta, \gamma)\rangle\) which are symmetric under time-reversal and simplex symmetries, the intervals for both gauge and Euler angles can be reduced to \((0 \leq \varphi \leq \pi/2)\) and \((0 \leq a \leq \pi/2, 0 \leq b \leq \pi/2, 0 \leq c \leq \pi)\), respectively [25].

The wave functions (Eq. 5) are eigenstates of the particle number and angular momentum operators.

In the configuration mixing approach, the final many-body wave functions that describe the different states of an even-even nucleus with \( Z(N) \) number of protons (neutrons) are written as:

\[
|IM; NZ\sigma\rangle = \sum_{K\beta\gamma} f^{I;NZ,\sigma}_{K\beta\gamma} |IMK; NZ; \beta\gamma\rangle \tag{6}
\]

\( \sigma = 1, 2, \ldots \) labels the levels for a given value of the angular momentum \( I \). The coefficients \( f^{I;NZ,\sigma}_{K\beta\gamma} \) of the linear combination are found by minimizing the energy within the non-orthogonal set of wave functions \(|IMK; NZ; \beta\gamma\rangle\). This leads to the Hill-Wheeler-Griffin (HWG) equation

\[
\sum_{K'\beta'\gamma'} \left( \mathcal{H}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} - E^{I;NZ,\sigma}_{K\beta\gamma} N^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \right) f^{I;NZ,\sigma}_{K'\beta'\gamma'} = 0, \tag{7}
\]

which has to be solved for each value of the angular momentum. The GCM norm- and energy-overlaps have been defined as:

\[
\mathcal{N}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \equiv \langle IMK; NZ; \beta\gamma | IMK'; NZ; \beta'\gamma' \rangle \]
\[
\mathcal{H}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \equiv \langle IMK; NZ; \beta\gamma | \hat{H} | IMK'; NZ; \beta'\gamma' \rangle \tag{8}
\]

For details about the solution of this equations and its convergence as well as for the calculation of transition matrix elements the reader is referred to [29].

3. Results

3.1. The nucleus \(^{24}\text{Mg}\)

The spectrum obtained in the triaxial GCM-PNAMP calculations is shown in Fig.1 (central part). We classify the different levels in three bands according to the corresponding \( \text{B(E2)} \) values. The ground state band is formed by a sequence of even values of angular momentum with a level spacing very similar to a rotational band whereas the second one connects states with \( I = 2, 3, 4, 5 \) as it could be expected from a (quasi) \( \gamma \) band. The third band is built with \( I \)-even states on top of the second \( 0^+_2 \) state. We observe strong electric quadrupole transitions

\(^1\) We choose for the Euler angles the notation \( \Omega = (a, b, c) \) instead of the usual \((\alpha, \beta, \gamma)\) to avoid confusion with the deformation parameters \((\beta, \gamma)\)
between intraband states while the interband B(E2) transitions are much weaker. This fact indicates the different underlying structure for each band and the absence of mixing between those states. We can study the nature of these bands decomposing the collective wave functions into their $K$ components. The results show, see ref. [29], that the first and third bands are rather pure $K = 0$ while the second band corresponds mainly to $K = |2|$ states.

In Fig. 1 we have also compared the triaxial results with GCM-PNAMP axial calculations. In order to understand better the results of this comparison, we investigate first the relationship between the axial and triaxial collective wave functions. The axial states emerge from the $\gamma = 0^\circ - 180^\circ$ path of the $K = 0$ component of the corresponding triaxial states. In particular, we can relate the ground state bands in both approaches and also the axial $0^+_1, 2^+_1, 4^+_2$ with the triaxial $0^+_2, 2^+_3, 4^+_3$ states. Hence, the comparison between the triaxial and axial calculations reveals that both the energies and reduced transition probabilities of the ground state band are very similar in both cases, as expected. Nevertheless, the small $K$-mixing for $I \neq 0$ lowers the excitation energies for higher angular momentum and therefore, the triaxial first band is slightly compressed with respect to the axial band. This effect, although small, helps for giving a better description of the moments of inertia within the GCM-PNAMP framework. The larger differences between the axial and triaxial calculations come out in the second and third bands. Obviously, the axial case is unable to describe the quasi $\gamma$-band but also the energies and B(E2) of the third triaxial band -$K = 0$- are modified with respect to the corresponding ones in the axial case.

Finally we compare the triaxial results with the available experimental data for $^{24}\text{Mg}$ (see Fig. 1). We find a remarkable qualitative agreement between theory and experiment both in energies and reduced transition probabilities. In both cases we observe a rotational ground state band, a second band associated to a $\gamma$-band and a third band with $\Delta I = 2$. In fact, the theoretical description of the measured $\gamma$-band is one of the major achievements of the present model compared to previous implementations. Furthermore, in this particular case $^{24}\text{Mg}$- the excitation energies for the first band are quantitatively very well described with the present calculations as we see in Fig. 1. In addition, it is important to emphasize the quality of the theoretical predictions for the intraband and interband reduced transition probabilities which shows the small mixing between the corresponding bands. Although the improvement on the
results with respect to axial case is evident, the band heads of the $\gamma$- and, especially, third bands are still too high in excitation energy.

![Energy contour plots](image)

**Figure 2.** Energy contour plots of the nucleus $^{126}$Xe in the ($\beta, \gamma$) plane. In panel (a) in the PN-VAP approach and in (b) in the PNAMP. The energy origin has been set in the lowest energy, solid (dashed) lines are 1MeV apart, the dashed contours start at 0.5 MeV and the solid ones at 1MeV.

![Potential energy plot](image)

**Figure 3.** Dotted (dashed) line: Potential energy in the PN-VAP (AMP) approach. Continuous line: wave function in the axial GCM.

### 3.2. The nucleus $^{126}$Xe

In spite of having been used as prototype for all triaxial beyond mean field calculations the nucleus $^{24}$Mg is not a good example of a triaxial nucleus. As a matter of fact it is neither
triaxially deformed nor soft in the gamma degree of freedom. The small $K$ mixing observed in the calculations clearly underline this points and the results obtained by this nucleus can not be generalized for more complex nuclei. To investigate this point we will perform some calculations in a nucleus softer in the gamma degree of freedom. A nucleus which has been used as benchmark for phenomenological models in the past is $^{126}$Xe [35, 36, 37, 38]. In this section we present an exploratory study of the this nucleus, we call it exploratory because in the calculations a configuration space with only with 7 harmonic oscillator shells is used. This space is big enough for $^{24}$Mg but probably not for a precise description of $^{126}$Xe. Nevertheless since its deformation $\beta \approx 0.2$ is not very large we expect to be able to provide a qualitative description of the low spin states.

In panel (a) of Fig. 2 we display the energy contour plot of $^{126}$Xe in the PN-VAP approach, see Eq.2, in the ($\beta$, $\gamma$) plane. We find a very $\gamma$-soft nucleus with a shallow minimum around $\beta = 0.2$, $\gamma = 30^\circ$. In panel (b) the effect of projecting on angular momentum, $I = 0\hbar$, i.e., the energy calculated with the wave function of Eq. 5, is displayed, we observe that the minimum is shifted to larger $\beta$ values and that the triaxial minimum is somewhat deeper, the $\gamma$ softness, however, still persists. In Fig. 3 we present the axial potential energy curves, which obviously coincide with those of Fig. 2 along the $\gamma = 0^\circ$ and $\gamma = 60^\circ$ axes. We can also see in the latter figure that the minima that appear at the oblate and prolate sides, of both, the PN-VAP and the AMP ($I = 0\hbar$) axial calculations, in reality are saddle points.

In Fig. 4 we now present the result of the configuration mixing calculations for the axial and the triaxial calculations. In the triaxial approximation we display the ground band and the quasi $\gamma$-band to be compared with the experimental results [36]. The spectrum is more stretched than the experimental one. This is a well known feature of beyond mean field calculations without time reversal breaking since the variational principle favors the $I = 0\hbar$ ground state. Consequently, we expect the approximation to deteriorate as the angular momentum increases, as a matter of fact we obtain rather good results for both $I = 2^+$ states. Nevertheless one should notice that the ordering of the states of the ground band with respect to the quasi $\gamma$-band is the right
one. The strong odd-even staggering of the levels of the quasi $\gamma$-band is not well reproduced, only the $I = 3h$ display such effect, i.e., the energy separation of the $3^+ - 4^+$ states is smaller than the $2^+ - 3^+$ ones. If we now look at the axial calculations we find that the results for the ground band, at variance to the $^{24}\text{Mg}$ case, looks quite different than the corresponding ones in the triaxial calculations, emphasizing thereby the relevance of triaxial shapes in soft or triaxial nuclei. In Fig. 5 we present the square of the collective wave function of the ground state and of the band head of the quasi $\gamma$-band in the triaxial configuration mixing approach. For the ground state we find a probability distribution centered at $\beta = 0.2 \pm 0.05$ for the $0^+_1$ state, and a somewhat larger $\beta$ deformation that the ground state, and a steeper decrease in the $\gamma$ direction. Both examples illustrate very clearly the relevance of the shape mixing in these calculations.

In Table 1, finally, we show the $B(E2)$ branching ratios in the triaxial configuration mixing calculations and the experimental values [36]. In the table the maximal transition probability of a given state has been set to 100, the other values have been corresponding scaled. It is very remarkable that our results are in very good agreement with the experimental ones. As a matter of fact, with the exception of the transitions which are smaller than 3% of the main transition, all agree with the experimental values within the numerical uncertainties. In this nucleus, at variance with $^{24}\text{Mg}$, we find strong interband transition probabilities.

4. Summary
In summary, we have presented two implementation of GCM-PNAMP method with fully triaxial intrinsic wave functions found by solving the PN-VAP equations with the Gogny interaction. The method has been applied to the study of $^{24}\text{Mg}$ which has been chosen as a test case in previous studies with different interactions. The comparison between axial and triaxial results shows minor changes in the ground state band which is predicted to be an axial rotational band $K = 0$. Only for angular momentum $I \geq 4$ some $K$-mixing is observed giving rise to a small level compression. This result support the use of axial calculations in these cases. However, the
Table 1. $B(E2)$ branching ratios for $^{126}$Xe in the triaxial configuration mixing calculations (third column) compared with experiment (second column).

| $I_i \rightarrow I_f$ | Exp.   | Theory |
|-----------------------|--------|--------|
| $2^+_2 \rightarrow 2^+_1$ | 100.   | 100.   |
| $2^+_2 \rightarrow 0^+_1$ | 1.5 ±0.4 | 0.001 |
| $3^+_1 \rightarrow 4^+_1$ | 35. ±10 | 40.48 |
| $3^+_1 \rightarrow 2^+_2$ | 100.   | 100.   |
| $3^+_1 \rightarrow 2^+_1$ | 2.0±0.6 | 0.000 |
| $4^+_2 \rightarrow 4^+_1$ | 76. ±22 | 80.6   |
| $4^+_2 \rightarrow 2^+_2$ | 100.   | 100.   |
| $4^+_2 \rightarrow 2^+_1$ | 0.4±0.1 | 0.007 |
| $5^+_1 \rightarrow 6^+_1$ | 75. ±23 | 59.6   |
| $5^+_1 \rightarrow 4^+_2$ | 76. ±21 | 90.6   |
| $5^+_1 \rightarrow 3^+_1$ | 100.   | 100.   |
| $5^+_1 \rightarrow 4^+_1$ | 2.9 ±0.8 | 0.02  |
| $6^+_2 \rightarrow 6^+_1$ | 34. ±15 | 27.1   |
| $6^+_2 \rightarrow 4^+_2$ | 100.   | 100.   |
| $6^+_2 \rightarrow 4^+_1$ | 0.49 ±0.15 | 0.003 |
| $7^+_1 \rightarrow 6^+_2$ | 40. ±26 | 45.11  |
| $7^+_1 \rightarrow 5^+_1$ | 100.   | 100.   |

The triaxial calculation is also able to reproduce the second band associated to a $\gamma$-band ($K = 2$) observed in the experimental data. Furthermore, the agreement between the theoretical and experimental results are qualitatively good.

Since the nucleus $^{24}$Mg is not a very good example for studying strong triaxial effects we have performed an exploratory study of the triaxial nucleus $^{126}$Xe. In this work only seven harmonic oscillator shells have been considered and therefore the results have to be considered as preliminary. The fact that the ground-state band in the axial and in the triaxial approaches are quite different indicates that an axial description of this kind of nuclei is unsuitable. A direct comparison of the triaxial and experimental spectra show a qualitative good description, specially the $B(E2)$ branching ratios show a quantitative description of the data.

The fact that our spectra are more stretched than the experimental ones is probably due to the lack of the correlations associated to the angular momentum restoration before the variation and time-reversal symmetry breaking that are not included in this calculation. Additionally, the inclusion of two-quasiparticle states would lower the excitation energies for these band heads. However, all these improvements are beyond the scope of the present work and would lead to a better quantitative description of the experimental results although we do not expect qualitative changes in the general picture. Research in this direction is in progress.

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