Symmetry-projected variational calculations with the numerical suite TAURUS

I. Variation after particle-number projection

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Abstract We present the numerical code TAURUS\textsubscript{vap} that solves the variation after particle-number projection equations for real general Bogoliubov quasiparticle states represented in a spherical harmonic oscillator basis. The model space considered is invariant under spatial and isospin rotations but no specific set of orbits is assumed such that the code can carry out both valence-space and no-core calculations. In addition, no number parity is assumed for the Bogoliubov quasiparticle states such that the code can be used to describe even-even, odd-even and odd-odd nuclei. The variational procedure can be performed under several simultaneous constraints on the expectation values of a variety of operators such as the multipole deformations, the pairing field or the components of the angular momentum. To demonstrate the potential and versatility of the code, we perform several example calculations using an empirical shell-model interaction as well as a chiral interaction. The ability to perform advanced variational Bogoliubov calculations offered by this code will, we hope, be beneficial to the shell model and \textit{ab initio} communities.

Program summary

Program title: TAURUS\textsubscript{vap}  
License: GNU General Public License version 3 or later  
Programming language: Fortran 2008  
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Repository: github.com/project-taurus/taurus_vap

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1 Introduction

Variational methods constitute a cornerstone of quantum many-body methods in general and nuclear theory in particular. Their fundamental principle is to build the best possible approximations to the Hamiltonian eigenstates by determining the states that yield the lowest expectation values for the Hamiltonian within a predetermined set of trial wave functions. There are sophisticated variational techniques that look for a quasi-exact representation of the Hamiltonian eigenstates, such as the Variational Monte Carlo methods [1], but their high computational cost limits their application to the lightest nuclei. In order to be able to address heavier nuclei, and in a systematic fashion, it is necessary to consider far more approximate variational ansätze. Many variational schemes in nuclear physics explore the manifold of
Bogoliubov quasiparticle states by solving self-consistently the Hartree-Fock-Bogoliubov (HFB) equations [2]. These states have the double advantage of possessing a simple product state structure, making them computationally easy to handle, and of naturally incorporating pairing correlations, which are needed as most nuclei exhibit a superfluid character [2–4]. Bogoliubov quasiparticle states, however, in general are not eigenstates of the proton- or neutron-number operators and therefore are not invariant under a gauge rotation in the Fock space [5]. Consequently, they break one of the fundamental symmetries of the nuclear Hamiltonian. Although such a symmetry-breaking scheme is a priori undesirable, it was recognized long ago that this could be advantageous to grasp further correlation energy while conserving the product states as simple variational ansätze. Nevertheless, to avoid the resulting symmetry dilemma pointed out by Löwdin [6], the symmetries broken during the variational minimization have to be eventually restored [7–10].

The concepts of symmetry breaking and restoration have been used for decades in energy density functional (EDF) calculations [11–14]. Nowadays, state-of-the-art multi-reference EDF (MR EDF) schemes include the breaking and restoration of several symmetries concurrently. For example, in addition to the breaking of the gauge invariance, associated with a good number of particles, it is customary to break the rotational invariance, associated with a good total angular momentum, to include deformation correlations [15–17]. Globally, the most important contributions come from the quadrupole deformations [18,19]. Nevertheless, the inclusion of octupole deformations, which requires the use of parity breaking reference states, become crucial to understand the structure of certain isotopes [20,21]. Over the years, the physicists working within the EDF community have developed many sophisticated numerical codes that can solve the HFB equations considering a variety of constraints or intrinsic symmetries for the Bogoliubov reference states. Several of them have been published and are freely available [22–27]. It is interesting to remark that public beyond-mean-field tools, all those codes have the common feature that they were written and optimized specifically for energy density functionals and can not handle natively general Hamiltonians such as the ones constructed from Effective Field Theory (EFT) [29–33] or commonly used in shell-model calculations [34–37]. On that note, we remark that a valence-space finite-temperature HFB solver was recently proposed [38].

Nuclear ab initio methods have experienced great progress in recent years and nowadays routinely describe nuclei in the mid-mass region and even some heavy spherical nuclei [39,40]. This progress is in large part due to the development of a new generation of many-body methods that scale more gently with the number of nucleons or the size of the model space considered [41–45] than the quasi-exact methods previously used in very light systems [1,46]. While the methods vary in their underlying principles, they usually rely either on a diagrammatic expansion on top of a reference state or the diagonalization of the Hamiltonian within a set of reference states. In that regard, the choice of appropriate reference states, i.e. many-body wave functions that capture the most important physical features of the problem, is critical to obtain a rapidly converging theory. For example, the Slater determinant solution of the Hartree-Fock equations can be used to improve the convergence in Many-Body Perturbation Theory (MBPT) calculations [47]. Not so surprisingly, the idea to use symmetry-breaking reference states has thus started to spread in the ab initio community, eventually resulting in the first calculations of open-shell nuclei [41,48–50].

The interacting shell-model (ISM) [34] is another pillar in the modern description of nuclear structure. Diagonalizing exactly the many-body Hamiltonian within a restricted valence space, it offers to this day the most accurate description of nuclear spectra not far away from shell closures. Recently, efforts have been carried out to connect the ISM to the ab initio project with the construction of valence-space effective interactions from first principles [44,51]. Unfortunately, the combinatorial scaling of the ISM is, and will remain for the forseeable future, a major computational limitation. A way to overcome this difficulty might be to consider accurate approximations to the solutions of the Schrödinger equation such as the ones that can be constructed through Monte Carlo methods [52,53] or advanced multi-reference variational calculations in a valence space [54–57].

At the crossing point of these recent developments, we propose in this article the numerical code TAU	extsc{rus}vap that can solve the variation after particle-number projection equations for real general Bogoliubov quasiparticle states represented in a spherical harmonic oscillator basis. This basis is a natural choice in many ab initio or ISM calculations. The code TAU	extsc{rus}vap presented here is actually the first of a new numerical suite, entitled TAU	extsc{rus}, that is under development but was already applied with success using both a shell-model interaction [55] and a chiral interaction evolved through the In-Medium Similarity Renormalization Group (IMSRG) [50]. The other codes of the suite will be the subject of later publications.

The article is organized as follows. In Sect. 2, we give a detailed account of the theoretical framework. Then, in Sect. 3, we perform several example calculations using both an empirical shell-model interaction and a chiral Hamiltonian. In Sect. 4, we present a summary of this work as well as perspectives for the future developments of the numerical suite TAU	extsc{rus}. Finally, Sects. 5 and 6 focus on the most relevant technical details of the program TAU	extsc{rus}vap.
2 Theoretical framework

2.1 Spherical harmonic oscillator

First, let us consider the spherical harmonic oscillator (SHO) Hamiltonian

\[ H_{\text{SHO}} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 , \]

where \( p \) is the momentum operator, \( r \) is the position operator, \( \omega \) is the oscillator frequency, and \( m \) is the average nucleon mass, i.e. \( m = (m_p + m_n) / 2 \) with \( m_p \) and \( m_n \) being the proton and neutron masses, respectively. In addition, we define the oscillator length \( b = \sqrt{\hbar / (m \omega)} \) with \( \hbar \) being the reduced Planck constant.

2.2 Single-particle basis

We consider a model space spanned by a single-particle basis made of a set of eigenstates of \( H_{\text{SHO}} \). The reasons motivating this choice are manifold. First, this is the basis that is usually favoured in \textit{ab initio} and shell-model calculations such that we can directly use the interactions constructed for those approaches and also easily benchmark our results. Second, many expressions, such as the expectation values for the usual operators, are simple and therefore can be coded and debugged with ease. Last but not least, it gives us the generality and flexibility to treat many problems on the same footing. While for specific applications, it is of advantage to use a symmetry-adapted basis in order to reduce the computational cost or improve the convergence, e.g. to use an axial footing. For those approaches and also easily benchmark our results.

The SHO eigenstates \( \phi \) are characterized by their principal quantum number \( n \), orbital angular momentum \( l \), spin \( s \) and their third component \( m \), and isospin \( t \) and its third component \( m_t \). We use as a convention \( m_{-1/2} = -1/2 \) for proton single-particle states and \( m_{+1/2} = +1/2 \) for neutron single-particle states.

Finally, a multiplet containing all values of \( \{ m_j = -j, \ldots, j \} \) will be labeled 
\[ \tilde{a} \equiv (n, l, s, t, m) . \]

The SHO eigenstates form an orthonormal set

\[ \langle \phi_a | \phi_b \rangle = \delta_{ab} , \]

and they can be associated with a set of fermionic annihilation and creation operators \( \{ \hat{c}_a \} \).

Using the spherical coordinates \( (\xi, \theta, \varphi) \), with \( \xi = r / b \) being the dimensionless ratio between the radial distance \( r \) and the oscillator length \( b \), the explicit form of the SHO single-particle wave functions can be written as

\[ \phi_a (\xi, \theta, \varphi) = R_n l a (\xi) Y_{l a} m a s a m s (\theta, \varphi) \chi_{n a m a} , \]

where \( R_n l a (\xi) \) is a normalized radial function, \( Y_{l a} m a s a m s \) a spherical harmonic, and \( \chi_{n a m a} \) is an isospin function. The radial function \( R_n l a (\xi) \) reads

\[ R_n l a (\xi) = \frac{N_{n l a}}{b^{3/2}} \xi^l e^{-\xi^2 / 2} L_{n a}^{l + 1 / 2} (\xi^2) , \]

with \( L_{n a}^{l + 1 / 2} \) being a generalized Laguerre polynomial and \( N_{n l a} \) the normalization constant

\[ N_{n l a} = \sqrt{\frac{2^{n + l + 2} n !}{\pi^{1 / 2} (2 n + 2 l + 1) ! !}} . \]

The tensor spherical harmonic \( Y_{l a} m a s a m s \) reads

\[ Y_{l a} m a s a m s (\theta, \varphi) = \sum_{m = -l}^{l} \sum_{m = -s}^{s} \langle l a s a m s | j a m j a \rangle Y_{l a m} (\theta, \varphi) \chi_{s a m s} , \]

with \( \langle l a s a m s | j a m j a \rangle \) being a \textit{SU}(2) Clebsch-Gordan coefficient and \( \chi_{s a m s} \) a spin function [58].

In this work, we will only consider model spaces that are rotationally invariant, i.e. that includes all the members of a multiplet \( \{ m_j = -j, \ldots, j \} \), and isospin invariant, i.e. with the same single-particle states for protons and neutrons: \( \{ m_j = -1 / 2, 1 / 2 \} \). Apart from that, no other limitation is imposed on the orbitals included. In particular, we will consider both no-core and valence-space model spaces. With that, the model space is entirely specified by the set of orbits \( \mathcal{M} \equiv \{ \tilde{a} \} \) it contains and its dimension can be calculated as

\[ d_{\mathcal{M}} = 2 \sum_{\tilde{a}} (2 j_a + 1) . \]

Finally, let us comment that the single-particle basis is ordered such that the first half of the basis is made of the proton single-particle states while the second half is made of the neutron single-particle states.
2.3 Bogoliubov quasiparticle states

2.3.1 Bogoliubov transformations

We define the Bogoliubov state $|\Phi\rangle$ as the vacuum for a set of quasiparticle annihilation and creation operators $\{\beta_k; \beta_k^{\dagger}\}$ constructed through the unitary linear Bogoliubov transformation

$$\begin{align*}
\begin{pmatrix} \beta_k \\ \beta_k^{\dagger} \end{pmatrix} &= \begin{pmatrix} U^T & V^T \end{pmatrix} \begin{pmatrix} c_k \\ c_k^{\dagger} \end{pmatrix} \equiv \mathcal{W} \begin{pmatrix} c_k \\ c_k^{\dagger} \end{pmatrix}, \quad (8a)
\end{align*}$$

with

$$\mathcal{WW}^\dagger = \mathcal{W}^\dagger \mathcal{W} = 1_{2d_M}, \quad (8b)$$

where $1_m$ refers to the identity matrix of dimensions $m \times m$. The expanded form of Eq. (8a) reads as

$$\begin{align*}
\beta_k &= \sum_i U_{ik}^* c_i + V_{ik}^* c_i^{\dagger}, \\
\beta_k^{\dagger} &= \sum_i U_{ik} c_i^{\dagger} + V_{ik} c_i. \quad (9a, 9b)
\end{align*}$$

In the present work, we allow for general Bogoliubov transformations without any restriction except for the fact that the matrices $(U,V)$ are kept real. From a symmetry perspective, this means that, in the most general case discussed here, we consider wave functions that break all symmetries but the complex conjugation. In particular, angular-momentum, particle-number, and parity symmetry breaking, as well as proton-neutron mixing are allowed. Bogoliubov transformations that conserve a certain quantum number $\mu$ are thus considered only as specific cases where the matrices $(U,V)$ have particular block structures that do not mix single-particles states with different value of $\mu$. Let us remark in particular that starting a calculation with such specific matrices $(U,V)$, their structure will be preserved throughout the minimization procedure if the Hamiltonian and the constraints imposed during the minimization also conserve $\mu$ [2].

2.3.2 One-body densities

A Bogoliubov state $|\Phi\rangle$ can be characterized by its one-body densities defined as

$$\begin{align*}
\rho_{ij} &= \frac{\langle \Phi | c_i^\dagger c_j | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \left(V^* V^T\right)_{ij}, \quad (10a) \\
\kappa_{ij} &= \frac{\langle \Phi | c_i^\dagger c_j^\dagger | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \left(V^* U^T\right)_{ij}. \quad (10b)
\end{align*}$$

1 While we will consider only Bogoliubov matrices, and their related quantities, that are real, we will give the general complex definitions of most quantities.

Additionally, when dealing with two Bogoliubov states, e.g. $|\Phi_L\rangle$ with Bogoliubov matrices $(U_L,V_L)$ and $|\Phi_R\rangle$ with Bogoliubov matrices $(U_R,V_R)$, it is possible to define the so-called transition densities

$$\begin{align*}
\rho_{ij}^{LR} &= \frac{\langle \Phi_L | c_i^\dagger c_j | \Phi_R \rangle}{\langle \Phi_L | \Phi_R \rangle} = \left(V_R^* A^{T-1} V_L^T\right)_{ij}, \quad (11a) \\
\kappa_{ij}^{LR} &= \frac{\langle \Phi_L | c_i^\dagger c_j^\dagger | \Phi_R \rangle}{\langle \Phi_L | \Phi_R \rangle} = \left(V_R^* A^{T-1} U_L^T\right)_{ij}, \quad (11b) \\
\kappa_{ij}^{RL*} &= \frac{\langle \Phi_L | c_i^\dagger c_j^\dagger | \Phi_R \rangle}{\langle \Phi_L | \Phi_R \rangle} = \left(V_L A^{-1} U_R^T\right)_{ij}, \quad (11c)
\end{align*}$$

where

$$A = U_R^T U_L + V_R^T V_L. \quad (12)$$

Let us remark that in the diagonal case where $|\Phi_L\rangle = |\Phi_R\rangle = |\Phi\rangle$, we obtain $A = 1_{d_M}$ due to the unitarity of $\mathcal{W}$ and, therefore, the transition densities reduce to the usual densities defined above.

2.3.3 Quasiparticle excitations

Starting from a Bogoliubov vacuum $|\Phi\rangle$, it is possible to create quasiparticle excitations by applying the quasiparticle creation operators on top of it. A $n$-quasiparticle excitation is defined as

$$|\Phi^{k_1...k_n}\rangle = \beta_{k_1}^{\dagger} \cdots \beta_{k_n}^{\dagger} |\Phi\rangle. \quad (13)$$

In practice, the quasiparticle excitations can be easily performed by interchanging the columns of the $U$ and $V$ matrices [2]

$$(U_{ik}, V_{ik}) \rightarrow (V_{ik}^*, U_{ik}^*), \quad \forall i \in \llbracket 1, n \rrbracket, \quad \forall l \in \llbracket 1, d_M \rrbracket. \quad (14)$$

Note that starting from a Bogoliubov state with a number parity equal to $\pi_A$ (see Sect. 2.3.1), the state $|\Phi^{k_1...k_n}\rangle$ will have a number parity equal to $(-1)^n \pi_A$.

2.4 Nuclear many-body Hamiltonian

Our objective is to develop a versatile approach that can be applied to different type of model spaces and Hamiltonians. Therefore, we will consider a general nuclear Hamiltonian that contains up to two-body terms

2 Here, we assume that all the quasiparticle excitations are distinct.
$H = H^{(0)} + H^{(1)} + H^{(2)}$, 

$$= h^{(0)} + \sum_{ij} h^{(1)}_{ij} c_i^{\dagger} c_j + \frac{1}{(2l)^2} \sum_{ijkl} h^{(2)}_{ijkl} c_i^{\dagger} c_j c_k^{\dagger} c_l,$$

where $h^{(0)}$, $h^{(1)}_{ij}$, and $h^{(2)}_{ijkl}$ are zero-, one-, and antisymmetrized two-body matrix elements, respectively. In particular, we do not constrain the physical content of each term except to require that they respect the symmetries of $H$, such as the rotational and parity invariants, and are kept real. The matrix elements could be obtained from, for example, an empirical shell-model interaction, a normal-order chiral interaction or even a Hamiltonian-based energy functional.\(^3\)

While the inclusion of a three-body term would not present theoretical difficulties, the amount of computer memory required to store all the non-zero matrix elements in the SHO single-particle basis would be prohibitive in most model spaces. Also, \textit{ab initio} calculations have demonstrated that the most important contributions coming from a realistic 3N interactions can be included through the so-called normal order two-body approximation (NO2B) [63,64]. Nevertheless, it might be desirable to include the full three-body term in small model spaces in the future.

To illustrate our discussion, let us first consider the most typical form of an empirical shell-model interaction that is such that

$$h^{(0)} = 0,$$  \hspace{1cm} (16a)

$$h^{(1)}_{ij} = \delta_{ij} \epsilon_i, \hspace{1cm} (16b)$$

$$h^{(2)}_{ijkl} = V_{ijkl}, \hspace{1cm} (16c)$$

where $\epsilon_i$ is a single-particle energy and $V_{ijkl}$ a two-body matrix element obtained from a $G$-matrix and/or a fit. We note that, although considered null here, $h^{(0)}$ could be taken as equal to the energy of the inert core considered for the valence space at hand.

Another relevant example is the case of a typical Hamiltonian constructed from EFT that can be decomposed as

$$H = T^{(1)} - T_{\text{com}}^{(1)} + V^{(2)} - T_{\text{com}}^{(2)} + W^{(3)},$$

where $T^{(1)}$ is the one-body kinetic energy, $V^{(2)}$ and $W^{(3)}$ are the 2N and 3N chiral interactions, respectively, and finally $T_{\text{com}}^{(1)}$ and $T_{\text{com}}^{(2)}$ are the one- and two-body corrections for the center-of-mass motion [65], respectively. Considering the NO2B approximation of the three-body piece with respect to an arbitrary state [66], we obtain the expressions

$$h^{(1)}_{ij} = \left(1 - \frac{1}{A_0}\right) (i \frac{p_i^2}{2m} |j\rangle + \tilde{w}^{(1)}_{ij}, \hspace{1cm} (18b)$$

$$h^{(2)}_{ijkl} = (i j |V^{(2)} - \frac{p_i \cdot p_j}{m A_0} |k\rangle + \tilde{w}^{(2)}_{ijkl}, \hspace{1cm} (18c)$$

where $|k\rangle = |kl\rangle - |lk\rangle$, $A_0$ is the nucleon number of the nucleus we wish to describe, and finally, $\tilde{w}^{(0)}$, $\tilde{w}^{(1)}_{ij}$ and $\tilde{w}^{(2)}_{ijkl}$ are the matrix elements of the zero-, one- and two-body parts of the normal-ordering of the three-body interaction, respectively, whose expressions can be found for example in Ref. [64].

2.5 Particle-number projection

2.5.1 Basic principles

The proton-, neutron-, and nucleon-number operators are defined as

$$Z = \sum_i \delta_{m_i-1/2} c_i^{\dagger} c_i,$$ \hspace{1cm} (19)

$$N = \sum_i \delta_{m_i+1/2} c_i^{\dagger} c_i,$$ \hspace{1cm} (20)

$$A = Z + N.$$ \hspace{1cm} (21)

For the sake of clarity, for the remainder of the section we will consider only the generic particle species $N$ for our definitions but, except told otherwise, all the quantities have to be generalized by replacing $N$ by $Z$ or $A$. With that said, the gauge rotations for the species $N$ in the Fock space are associated with the abelian group $U(1)_N$. In this work, we consider its unitary representation

$$\left\{ R(\varphi_N) = e^{i\varphi_N N}, \varphi_N \in [0, 2\pi]\right\},$$ \hspace{1cm} (22)

with $\varphi_N$ and $R(\varphi_N)$ being the gauge angle and gauge rotation operator, respectively. Any eigenvector $|\Theta^{N_0}\rangle$ of the operator $N$ with eigenvalue $N_0$ represents a one-dimensional irreducible representation (irrep) of $U(1)_N$ such that

$$R(\varphi_N)|\Theta^{N_0}\rangle = e^{i\varphi_N N_0}|\Theta^{N_0}\rangle.$$ \hspace{1cm} (23)

On the contrary, considering an arbitrary many-body wave function $|\Theta\rangle$ that may not be an eigenvector of $N$, it is possible to use a projection operator

$$P^{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi_N e^{i\varphi_N (N-N_0)},$$ \hspace{1cm} (24)

such that

$$N P^{N_0}|\Theta\rangle = N_0 P^{N_0} |\Theta\rangle,$$ \hspace{1cm} (25)

and $P^{N_0} |\Theta\rangle$ is non-vanishing for at least one value of $N_0$.\(^3\)

\(^3\) As demonstrated in [59–62], beyond-mean-field calculations based on general energy functionals are not well defined such that we prefer not to consider them here.
In general, a Bogoliubov vacuum $|\Phi\rangle$ will not be an eigenstate for the particle species $N$. Only when the pairing correlations vanish\(^4\) and the Bogoliubov state reduces to a mere Slater determinant for this species, it is the case. On the other hand, the nuclear Hamiltonian $H$ is always invariant under gauge rotations for particle species $N$, i.e.

$$[H, U(\varphi_N)] = 0, \forall \varphi_N \in [0, 2\pi].$$

(26)

Therefore, to respect the symmetries of $H$, it is necessary to project $|\Phi\rangle$ onto the good number of particles of the nucleus we wish to describe, for example $N_0$.

Obviously, in the general case both the neutron and proton gauge invariances have to be restored, such that we construct the normalized projected state

$$|\psi_{Z0N_0}\rangle = \frac{P_{Z0} P_{N0} |\Phi\rangle}{\sqrt{\langle \Phi | P_{Z0} P_{N0} |\Phi\rangle}}.$$  

(27)

It is important to stress that the projected state $|\psi_{Z0N_0}\rangle$ thus obtained has generally a more complex structure than the one of a mere product state.

While a Bogoliubov state $|\Phi\rangle$ is not in general an eigenstate for any of the particle-number operators mentioned above, it is by construction an eigenstate of the number-parity operator $\Pi_A = e^{i\varphi A}$ with an eigenvalue $\pi_A = +1$ or $-1$. As a consequence, the interval of integration of the projection operator for $A$ can be reduced to $[0, \pi]$

$$P_{A0} = \frac{1}{\pi} \int_0^\pi d\varphi_A e^{i\varphi A (A-A_0)},$$

(28)

which is numerically more efficient \cite{10}. In addition, if there is no proton-neutron mixing in the Bogoliubov matrices $(U, V)$, the state $|\Phi\rangle$ will be an eigenstate of $\Pi_Z$ and $\Pi_N$ individually, thus allowing for similar reductions for $P_{Z0}$ and $P_{N0}$.

In Sect. 6.2, we give the expressions for the discretized projection operators implemented in the code. More generally, further details on the projection on particle-number and its numerical implementation can be found for example in \cite{10,14}.

2.5.2 Gauge-rotated quasiparticle states

Because of the one-body character of gauge transformations, a gauge-rotated Bogoliubov quasiparticle state is still a Bogoliubov quasiparticle state. Therefore, we can define the gauge-rotated state

$$|\Phi(\varphi)\rangle \equiv R(\varphi_Z) R(\varphi_N) |\Phi\rangle,$$ 

(29)

where we used the shorthand notation $\varphi \equiv (\varphi_Z, \varphi_N)$ with $|\Phi(0)\rangle \equiv |\Phi\rangle$. The Bogoliubov matrices $(U^\varphi, V^\varphi)$ of the state $|\Phi(\varphi)\rangle$ can be expressed as

$$U^\varphi = \begin{pmatrix} e^{i\varphi_N} & 0 \\ 0 & e^{i\varphi_Z} \end{pmatrix} U,$$

(30a)

$$V^\varphi = \begin{pmatrix} e^{-i\varphi_Z} & 0 \\ 0 & e^{-i\varphi_N} \end{pmatrix} V,$$

(30b)

where we used our partition of the single-particle basis in terms of the proton (first half) and neutron (second half) single-particle states.

2.5.3 Projected expectation values

Let us consider an operator $O$ that is a scalar regarding gauge rotations, i.e.

$$[O, U(\varphi_N)] = 0, \forall \varphi_N \in [0, 2\pi].$$

(31)

Its expectation value for the projected state $|\psi_{Z0N0}\rangle$ reads

$$O_{Z0N0} \equiv \langle \psi_{Z0N0} | O | \psi_{Z0N0} \rangle = \frac{\langle \Phi | O P_{Z0} P_{N0} |\Phi\rangle}{\langle \Phi | P_{Z0} P_{N0} |\Phi\rangle}.$$ 

(32)

Expanding the numerator and denominator we obtain

$$\langle \Phi | O P_{Z0} P_{N0} |\Phi\rangle = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi_Z \int_0^{2\pi} d\varphi_N e^{-i(\varphi_Z Z_0 + \varphi_N N_0)} \times \langle \Phi | O | \Phi(\varphi) \rangle \langle \Phi | \Phi(\varphi) \rangle,$$

(33)

$$\langle \Phi | P_{Z0} P_{N0} |\Phi\rangle = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi_Z \int_0^{2\pi} d\varphi_N e^{-i(\varphi_Z Z_0 + \varphi_N N_0)} \times \langle \Phi | \Phi(\varphi) \rangle.$$ 

(34)

In the above equations, the fundamental quantities that have to be evaluated are the norm overlap $\langle \Phi | \Phi(\varphi) \rangle$ and the rotated kernel

$$O^{\varphi} \equiv \frac{\langle \Phi | O | \Phi(\varphi) \rangle}{\langle \Phi | \Phi(\varphi) \rangle}.$$ 

(35)

The norm overlap is commonly calculated using the Pfaffian algebra \cite{69,70} (see Sect. 6.3 for more information on the practical implementation). Concerning the rotated kernel, it can be evaluated easily thanks to the Generalized Wick Theorem (GWT) \cite{71} when the overlap does not vanish. In particular, we remark that working within a Hamiltonian-based framework, we consider all the fully-contracted terms appearing in the application of the GWT.

Assuming now that $O$ contains up to two-body terms, i.e.

$$O = O^{(0)} + O^{(1)} + O^{(2)},$$

$$= O^{(0)} + \sum_{ij} O^{(1)}_{ij} c_i^+ c_j + \frac{1}{(2!)^2} \sum_{ijkl} O^{(2)}_{ijkl} c_i^+ c_j^+ c_k,$$

(36)
where $o^{0(0)}$, $o_{ij}^{1(1)}$, and $\bar{\sigma}_{ijkl}^{2(2)}$ are zero-, one-, and antisymmetrized two-body matrix elements, respectively, the rotated kernel reads
\[
O^{0\psi} = o^{0(0)} + \sum_{ij} o_{ij}^{1(1)} \rho_{ji} + \frac{1}{2} \sum_{ijkl} \bar{\sigma}_{ijkl}^{2(2)} \rho_{kl}^{0\psi} \rho_{lij}
\]
\[
\quad + \frac{1}{4} \sum_{ijkl} \bar{\sigma}_{ijkl}^{2(2)} \kappa_{ij}^{0
*\psi} \kappa_{kl}^{0\psi},
\]
(37)
where used the definitions of the transitions densities given in Sect. 2.3.2 setting $|\Phi_L\rangle = |\Phi(0)\rangle$ and $|\Phi_R\rangle = |\Phi(\psi)\rangle$. Let us remark in passing that the expectation value of a one-body operator can be obtained from the above equation by taking $\bar{\sigma}_{ijkl}^{2(2)} = 0$.

In the special case of the Hamiltonian, we define the transition fields
\[
\Gamma_{ij}^{0\psi} = \sum_{kl} \bar{h}_{ijkl}^{(2)} \rho_{lk}^{0\psi},
\]
(38a)
\[
h_{ij}^{0\psi} = h_{ij}^{(1)} + \Gamma_{ij}^{0\psi},
\]
(38b)
\[
\Delta_{ij}^{0\psi} = \frac{1}{2} \sum_{kl} \bar{h}_{ijkl}^{(2)} \kappa_{kl}^{0\psi},
\]
(38c)
\[
\Delta_{ij}^{0\psi*} = \frac{1}{2} \sum_{kl} \bar{h}_{ijkl}^{(2)} \kappa_{kl}^{0\psi*},
\]
(38d)
such that the expression given in Eq. (37) can be written as
\[
H^{0\psi} = h^{(0)} + \sum_{ij} h_{ij}^{(1)} \rho_{ji} + \frac{1}{2} \sum_{ij} \left( \Gamma_{ij}^{0\psi} \rho_{ji} - \Delta_{ij}^{0\psi} \kappa_{ji}^{0\psi*} \right).
\]
(39)
The advantage of the above expressions is that they allow us to confine the use of the two-body matrix elements to the calculation of the fields. Then, the fields can be used to compute the Hamiltonian rotated kernel and other quantities related to the projected gradient.

2.6 Variation after projection

2.6.1 Projected gradient

The variational space explored in this work is the manifold of particle-number projected Bogoliubov quasiparticle states. Therefore, we look for the solution of the variational equation
\[
\delta \langle \Psi^{Z_{0}N_{0}} | H | \Psi^{Z_{0}N_{0}} \rangle = 0.
\]
(40)
This is equivalent to looking for the Bogoliubov reference state $|\Phi\rangle$ that minimizes the projected energy
\[
E^{Z_{0}N_{0}} \equiv \langle \Psi^{Z_{0}N_{0}} | H | \Psi^{Z_{0}N_{0}} \rangle = \frac{\langle \Phi | H P^{Z_{0}N_{0}} | \Phi \rangle}{\langle \Phi | P^{Z_{0}N_{0}} | \Phi \rangle}.
\]
(41)
This approach is called variation after particle-number projection (VAPNP) in the literature [72–75] and is superior to the simpler HFB scheme for several reasons. First, the trial ansatz considered is better on a fundamental level: it possesses a more general structure, being a linear superposition of infinitely many Bogoliubov vacua, and is symmetry adapted, and therefore strictly explores a variational space with the correct number of particles. In particular, by construction, the VAPNP can yield a lower energy than the particle-number projection after variation (PNPAV) scheme within which the Bogoliubov state is obtained by solving the HFB equations first and is projected onto good particle numbers only afterwards. In addition, the VAPNP gives a better description of pairing correlations [72,73,75,76]. Notably, it prevents the frequent and unphysical collapse of the pairing often observed in HFB calculations [77]. This fact has also a practical advantage in configuration mixing calculations as it reduces the chance of finding a pair of orthogonal states, which forbids the use of the GWT usually employed in such calculations.

On the other hand, the VAPNP is more computationally costly than the PNPAV as the particle-number projection has to be performed at each iteration. Even using an efficient discretization of the gauge integrals, such as the one proposed by Fomenko [10,78], the numerical cost generally increases by one or two order of magnitudes compared to traditional PNPAV or plain HFB calculations. Nevertheless, the computational power nowadays at our disposal makes possible such calculations even in large model spaces [13].

Solving Eq. (40) corresponds to finding the state $|\Phi\rangle$ such that the projected gradient [79,80], with matrix elements
\[
G_{ij} = -\frac{\langle \Phi | \beta_{i} \beta_{l} (H - E^{Z_{0}N_{0}}) P^{Z_{0}N_{0}} | \Phi \rangle}{\langle \Phi | P^{Z_{0}N_{0}} | \Phi \rangle} 
\equiv - (H_{ij}^{20} Z_{0} N_{0} - E_{ij}^{20} Z_{0} N_{0}),
\]
(42)
vanishes
\[
||G||_{F} = 0,
\]
(43)
where $||| \cdot |||_{F}$ stands for the Frobenius norm and the superscript 20 indicates the part of the operator when expressed in the quasiparticle basis of $|\Phi\rangle$ [2].

2.6.2 Rotated gradient

To compute the projected gradient, it is necessary to compute the values of the rotated gradient at each gauge angle. After a lengthy but straightforward derivation [72,80], the matrix elements of the rotated gradient at angle $\psi$ can be expressed as
\[
G_{ij}^{0\psi} = (H^{0\psi} - E^{Z_{0}N_{0}}) R_{ij}^{\psi} + \left( \hat{U}^{\psi T} H^{0\psi} \hat{U}^{\psi} \right)_{ij} - \left( \hat{U}^{\psi T} \Delta^{0\psi} \hat{U}^{\psi} \right)_{ij} 
\]
\[+ \left( \hat{U}^{\psi T} \Delta^{0\psi} \hat{U}^{\psi} \right)_{ij} - \left( \hat{U}^{\psi T} \Delta^{0\psi} \hat{U}^{\psi} \right)_{ij} \quad \text{(44)}
\]
where

\[ A^\psi = U^\dagger U^\psi + V^\dagger V^\psi, \]  
\[ B^\psi = V^T U^\psi + U^T V^\psi, \]  
\[ R^\psi = \left( B^\psi A^\psi^{-1} \right)^*, \]  
\[ \bar{U}^\psi = U^* + V R^\psi, \]  
\[ \bar{V}^\psi = V^* + U R^\psi. \]  

### 2.7 Constraints

It is often desirable to perform the energy minimization imposing a constraint on the expectation values of a selected set of operators. In this work, we choose to constrain the expectation values of the Bogoliubov quasiparticle state \(|\Phi\rangle\) rather than those of the projected state \(|\Psi_{Z_0,N_0}\rangle\). There are many reasons motivating this choice. First, it as the advantage of being cheaper from computational point of view as we only to evaluate the expectation values for a product state. Second, it permits us to consider symmetry-breaking constraints, e.g. the constraint on the expectation value of a pair operator that breaks the gauge invariance. Finally, it is the Bogoliubov quasiparticle states, and not the projected states, that are considered as deformed reference states in our calculations. Nevertheless, this strategy has its drawbacks as different Bogoliubov states, obtained by using different constraints, may give the same projected state at the end of the VAPNP minimization. For example, an axially deformed Bogoliubov state may give a spherical particle-number projected state.

First, let us specify that for a general operator \(O\), we will constrain its hermitian average

\[ \bar{O} = \frac{1}{2} (O + O^\dagger), \]  

(46)

to the desired value, let say \(O_0\)

\[ \langle \Phi | \bar{O} | \Phi \rangle = O_0. \]  

(47)

More generally, considering a set of constraints \(C \equiv \{ \bar{O}_k, O_{k,0} \}\), the energy minimum in the hypersurface defined by \(C\) can be obtained by using the modified gradient \([2,81]\]

\[ G = - \left[ \left( H_{ij}^{20, Z_0 N_0} - E_{ij}^{20, Z_0 N_0} \right) - \sum_k^C \lambda_k \bar{O}_k \right], \]  

(48)

where

\[ \bar{O}_{k,ij} = \frac{\langle \Phi | \beta_j \beta_i \bar{O}_k | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \]  

(49)

and the \(\lambda_k\) are Lagrange multipliers that are obtained by solving self-consistently a system of linear equations (see Sect. 2.8.2).

#### 2.7.1 Particle number

The most basic constraints we consider are the ones on the proton- and neutron-number operators. Because the operators are hermitian, the constrained operators simply read

\[ \bar{Z} = Z, \]  

(50)

\[ \bar{N} = N. \]  

(51)

Let us remark that while VAPNP calculations do not require in principle such constraints due to the symmetry restoration embedded in the method, it is desirable to include them in the code for two reasons. First, they have to be used when doing plain HFB calculations. Second, such constraints usually improve the convergence of VAPNP calculations when using a sparse discretization of the gauge integrals and a large step for the gradient descent. Otherwise, the gradient may not converge or change the number of particles to lower the energy. While this particle-number constrained VAPNP is in principle not as general as the unrestricted one, it is an interesting option whenever the computational time becomes problematic. A somewhat similar approach was used in [74]. This is not a necessity though and we will consider in general full VAPNP calculations.

#### 2.7.2 Multipole deformations

Together with pairing, deformation correlations are certainly the most prominent collective correlations exhibited by nuclei throughout the nuclear chart [18]. Therefore, to constrain the total deformation of the state \(|\Phi\rangle\), we use the multipole operators

\[ Q_{lm} = \sum_{ij} (i|Y_{lm}|j)c_i^\dagger c_j, \]  

(52)

where \(Y_{lm}\) is a spherical harmonic. For now, we will consider the cases \(l = 2\) (quadrupole deformations), \(l = 3\) (octupole deformations) and \(l = 4\) (hexadecapole deformations). Considering constraints on higher-order multipole operators would not present any theoretical difficulties. Their physical importance, however, is expected to be much smaller.

Using the property

\[ Q_{lm}^\dagger = (-1)^m Q_{l-m}, \]  

(53)

the hermitian average operators read

\[ \bar{Q}_{lm} = \frac{1}{2} (Q_{lm} + (-1)^m Q_{l-m}), \]  

(54)

and it sufficient to consider them for \(m \geq 0\). Let us also remark in passing that the constraint on \(Q_{21}\) has to be set to zero as it corresponds to the orientation of the state in space rather than a proper shape, as explained in [2].
Instead of constraining the operators $\hat{Q}_{lm}$ directly, we also consider the possibility to constrain the dimensionless operators \([25]\)

$$
\hat{\beta}_{lm} = C_l \hat{Q}_{lm}, \tag{55}
$$

$$
C_l = \frac{4\pi}{3R_0^2A}, \tag{56}
$$

where \(R_0 = 1.2A^{1/3}\) fm.

Also, when dealing with triaxial deformations, it is usually more intuitive to constrain the value of the triaxial parameters \((\beta, \gamma)\) rather than the average values of the multipole operators expressed in spherical coordinates. In that order, we can use the relations

$$
\beta = C_2\sqrt{\langle \hat{Q}_{20} \rangle^2 + 2\langle \hat{Q}_{22} \rangle^2}, \tag{57}
$$

$$
\gamma = \arctan \left( \frac{\sqrt{2}\langle \hat{Q}_{22} \rangle}{\langle \hat{Q}_{20} \rangle} \right), \tag{58}
$$

to determine the values of the constraints on \((\langle \hat{Q}_{20} \rangle, \langle \hat{Q}_{22} \rangle)\) necessary to obtain a state with the desired values of \((\beta, \gamma)\) in the end.

Finally, we want to stress that all the multipole deformations discussed here were defined using the “bare” multipole operators, i.e. using their textbook definitions. While the use of effective operators adapted to the model space \([82]\), or to the value of the flow parameter \([43]\), would be theoretically more appropriate, we are confident that the same variational space can be explored using the simpler bare operators. In addition, it is important to note that these intrinsic deformations are not observable quantities. They are useful intermediate quantities that can be used to gain a physical insight about the collective character of the nucleus and to generate quasiparticle vacua with different intrinsic configurations that can be eventually used in beyond-mean-field techniques, such as the projected Generator Coordinate Method \([2]\).

### 2.7.3 Angular momentum

The variation of Eq. \((40)\) will in priority target the ground state energy. To better optimize the projected energy with respect to the excited states, it is of advantage to use a constraint on the expectation value of the angular momentum components \(J_k, k \in \{x, y, z\}\). Such “cranking” constraints have been used for decades in mean-field calculations to describe rotational bands of heavy nuclei \([2,83]\). More recently, several MR EDF calculations \([12,17,84]\) included cranked Bogoliubov states in their symmetry-projected configuration mixing and obtained a great improvement in the description of the low-lying excited states.

Given that the angular momentum component \(J_k\) is hermitian, we obtain

$$
\hat{J}_k = J_k, \tag{59}
$$

Finally, let us remark that, as we consider only real matrices \(U\) and \(V\), we cannot constrain the real part of the expectation value of the operator \(J_y\) as it has only imaginary matrix elements within our choice of basis.

### 2.7.4 Pair coupling

While the VAPNP offers a better treatment of pairing correlations than HFB, it is still a method built upon a single quasiparticle state which might not be sufficient whenever collective pairing fluctuations around the variational minimum are important. In those cases, the description of the system can be improved by performing a configuration mixing of reference states optimized with a pairing constraint \([55]\). In that order, we consider the constraint on an operator that couples pairs and which we generically label \([P^\dagger]\). The hermitian average operator reads in that case

$$
\left[ \hat{P}^\dagger \right] = \frac{1}{2} \left[ [P^\dagger] + [P] \right]. \tag{60}
$$

Several choices have been used in the literature concerning the precise type of coupling imposed. Frequently, the pairs are coupled in \(JT\)-scheme following the seniority model \([85]\)

$$
\left[ \hat{P}_{sen} \right]^{JT}_{M_J M_T} = \frac{1}{\sqrt{2}} \sum_{\tilde{a}} \sqrt{2j_a + 1} \left[ c_{\tilde{a}}^\dagger c_{\tilde{a}}^\dagger \right]^{JT}_{M_J M_T}, \tag{61}
$$

where the creation operators are \(JT\)-coupled according to

$$
\left[ c_{\tilde{a}}^\dagger c_{\tilde{b}}^\dagger \right]^{JT}_{M_J M_T} = \frac{\sqrt{1 - \delta_{\tilde{a}\tilde{b}}(-1)^J + T}}{1 + \delta_{\tilde{a}\tilde{b}}} \sum_{m_{ja}m_{jb}} m_{ja} m_{jb} c_{\tilde{a}}^\dagger c_{\tilde{b}}^\dagger \times \langle j_a m_{ja}, j_b m_{jb} | J M_J \rangle \langle \frac{1}{2} m_{ja} \frac{1}{2} m_{jb} | T M_T \rangle. \tag{62}
$$

Both isoscalar \((T = 0, J = 1)\) \(pn\)-pairing and isovector \((T = 1, J = 0)\) \(pp\), \(nn\), and \(pn\)-pairing can be explored with these operators.

Another possibility is to adopt a more “agnostic” point of view and consider the coupling

$$
\left[ \hat{P}_{ign}^{\dagger} \right]^{JT}_{M_J M_T} = \sum_{\tilde{a} \tilde{b}} \left[ c_{\tilde{a}}^\dagger c_{\tilde{b}}^\dagger \right]^{JT}_{M_J M_T}, \tag{63}
$$

which can couple states coming from different orbits \(\tilde{a}\) and \(\tilde{b}\).

### 2.7.5 Pairing field

Another possibility to adjust the pairing content of the trial Bogoliubov vacuum is through the direct constraint of its
pairing field, i.e. considering a constraint on the particle-number nonconserving one-body operator

\[ \Delta C = \sum_{ij} \Delta^{ij}_{ij} c_i^\dagger c_j^\dagger, \]

(64)

where \( \Delta^{ij}_{ij} \) is the (state dependent) pairing field defined in Eq. (38c). In that case, the hermitian average operator reads

\[ \bar{\Delta} C = \frac{1}{2} (\Delta C + \Delta C^\dagger). \]

(65)

In practice, this constraint is equivalent to a rescaling of the pairing field, i.e. considering the modified field \( \delta \Delta^{ij}_{ij} \) with \( \delta \in \mathbb{R} \), when performing the iterative minimization [67]. This solution has the double advantage of possessing a straightforward implementation and offering a good numeric stability.

2.8 Iterative procedure

The minimization algorithm used is the combination of two iterative procedures. First, there are the global iterations, labeled with the letter \( i \), that correspond to a new calculation of the particle-number projected energy gradient. Second, there are the local iterations within each iteration \( i \), labeled with the letter \( j \), that correspond to a new evolution of the wave function to enforce the constraints. In the following, the iterations will be labeled \((i, j)\). The iterations start at \((0, 0)\) and the last local iteration \( j \) for a given \( i \) will be noted \( J \).

2.8.1 Heavy-Ball method

The Heavy-Ball algorithm (see Ref. [86] and references therein) is an efficient first-order minimization method that adds a momentum term to the plain gradient in order to achieve a faster, and somewhat more reliable, convergence. More precisely, the gradient matrix used at iteration \((i, 0)\) to evolve the wave function \((U^{(i-1,J)}, V^{(i-1,J)})\) is defined as

\[ \tilde{G}^{(i,0)} = \eta^{(i,0)} G^{(i,0)} + \mu^{(i,0)} \bar{G}^{(i-1,J)}, \]

(66)

with \( \tilde{G}^{(0,0)} = \bar{G}^{(0,0)} = 0 \). The factors \( \eta^{(i,0)} \) and \( \mu^{(i,0)} \) can either be read from the input parameters and have fixed values during the iterative procedure, i.e. \( \eta^{(i,0)} = \eta^{(0,0)} \) and \( \mu^{(i,0)} = \mu^{(0,0)} \), or be evaluated at each iteration using the formulae [86]

\[ \eta^{(i,0)} = \left( \frac{2}{\varepsilon^{(i,0)}_{\max} + \sqrt{\varepsilon^{(i,0)}_{\min}}} \right)^2, \]

(67)

\[ \mu^{(i,0)} = \left( \frac{\varepsilon^{(i,0)}_{\max} - \sqrt{\varepsilon^{(i,0)}_{\min}}}{\varepsilon^{(i,0)}_{\max} + \sqrt{\varepsilon^{(i,0)}_{\min}}} \right)^2. \]

(68)

with \( \varepsilon^{(i,0)}_{\max} \) and \( \varepsilon^{(i,0)}_{\min} \) being approximations to the maximum and minimum eigenvalues of the second derivative of the energy, respectively. The program includes two empirical recipes to build these approximations:

1. Following the idea presented in Ref. [87], the eigenvalues of the HFB stability matrix are approximated using the eigenvalues of \( H^{11}_{11} \), i.e. the 11 part of the of Hamiltonian in the quasiparticle basis of the trial wave function [2]. More precisely, we diagonalize \( H^{11}_{11} \) at iteration \((i, 0)\) and set

\[ \varepsilon^{(i,0)}_{\max} = 4 \max \left[ \text{diag} \left( H^{11}_{11,(i-1,J)} \right) \right], \]

(69)

\[ \varepsilon^{(i,0)}_{\min} = 2 \min \left[ \text{diag} \left( H^{11}_{11,(i-1,J)} \right) \right], \]

(70)

where the factors were determined empirically.

2. We use the same principle but replacing the eigenvalues of \( H^{11}_{11} \) by the ones of the single-particle Hamiltonian \( h^{00}_{i0} \), i.e.

\[ \varepsilon^{(i,0)}_{\max} = 2 \max \left[ \text{diag} \left( h^{00}_{i0,(i-1,J)} \right) \right], \]

(71)

\[ \varepsilon^{(i,0)}_{\min} = 2 \min \left[ \text{diag} \left( h^{00}_{i0,(i-1,J)} \right) \right], \]

(72)

where the factors were determined empirically. This method proved to be somewhat more stable when dealing with odd-even nuclei.

Finally, the iterative procedure stops when the gradient becomes smaller than a predetermined value \( \epsilon_G \)

\[ \frac{\| \tilde{G}^{(i,0)} \|_F}{\eta^{(i,0)}} \leq \epsilon_G, \]

(73)

or if the maximum number of global iterations is reached.

2.8.2 Adjusting the constraints

When imposing constraints during the energy minimization, the gradient has to be constructed according to Eq. (48). The Lagrange multipliers \( \lambda^{(i,j)} \) are calculated solving a system of linear equations

\[ \delta^{(i,j)} \lambda^{(i,j)} = b^{(i,j)}. \]

(74)

First, assuming that the wave function \( |\Phi^{(i-1,J)}\rangle \), which is associated with the matrices \((U^{(i-1,J)}, V^{(i-1,J)})\) in storage at the beginning of iteration \((i, 0)\), satisfies the set of of constraints \( C \), i.e.

\[ \| \langle \Phi^{(i-1,J)} | \tilde{O}_k | \Phi^{(i-1,J)} \rangle - O_{k,0} \| \leq \epsilon_Q, \forall k, \]

(75)

with \( \epsilon_Q \) being a numerical parameter, the system of equations is set with
\[ A_{k}^{(i,0)} = \text{Tr} \left( \hat{O}_{k}^{20}\langle \bar{u}^{-1}, J \rangle \hat{O}_{k}^{20}\langle \bar{u}^{-1}, J \rangle^{T} \right), \]
\[ b_{k}^{(i,0)} = \text{Tr} \left[ \left( H_{ij}^{20} Z_{0N_{0}}\langle \bar{u}^{-1}, J \rangle - E_{ij}^{20} Z_{0N_{0}}\langle \bar{u}^{-1}, J \rangle \right) \hat{O}_{k}^{20}\langle \bar{u}^{-1}, J \rangle^{T} \right]. \]

(76)
(77)

With the Lagrange multipliers \( \lambda_{k}^{(i,0)} \) thus obtained, the projected gradient \( \tilde{G}_{k}^{(i,0)} \) is built according Eq. (48) and a first evolution is performed to obtain the wave function \( |\Phi^{(i,0)}\rangle \) associated with the matrices \( (U^{(i,0)}, V^{(i,0)}) \).

Then, if the evolved wave function \( |\Phi^{(i,0)}\rangle \) does not satisfy the condition (75), we start a local iterative procedure setting the system of linear equations with

\[ A_{k}^{(i,j)} = \text{Tr} \left( \hat{O}_{k}^{20}\langle \bar{u}^{-1}, J \rangle \hat{O}_{k}^{20}\langle \bar{u}^{-1}, J \rangle^{T} \right), \]
\[ b_{k}^{(i,j)} = O_{k,0} - \langle \Phi^{(i,j-1)} | \hat{O}_{k} | \Phi^{(i,j-1)} \rangle \]

and modifying the gradient as

\[ \tilde{G}_{k}^{(i,j)} = \tilde{G}_{k}^{(i,j-1)} + \sum_{j} c_{k}^{(i,j)} \hat{O}_{k}^{20}(\bar{u}^{-1}, J). \]

(80)

After each calculation of the gradient \( \tilde{G}_{k}^{(i,j)} \), an evolved wave function \( |\Phi^{(i,j)}\rangle \) is constructed. The iterative procedures stops whenever \( |\Phi^{(i,j)}\rangle \) satisfies the condition (75) or if the maximum number of local iterations is reached.

2.8.3 Evolution of the wave functions

The matrices \( (U^{(i,j)}, V^{(i,j)}) \) of the evolved quasi-particle state at the end of iteration \( (i, j - 1) \) are obtained as [88]

\[ U^{(i,j)} = \left( U^{(i,j-1)} + V^{(i,j-1)} \tilde{G}_{k}^{(i,j)^{+} \dagger} \right) L_{(i,j)}^{-1 \dagger}, \]
\[ V^{(i,j)} = \left( V^{(i,j-1)} + U^{(i,j-1)} \tilde{G}_{k}^{(i,j)^{+}} \right) L_{(i,j)}^{-1 \dagger}, \]

(81)
(82)

where \( L_{(i,j)} \) is the triangular matrix from the Cholesky factorization

\[ L_{(i,j)} L_{(i,j)}^{\dagger} = 1d_{M} + \tilde{G}_{k}^{(i,j)^{+} \dagger} \tilde{G}_{k}^{(i,j)^{+}}, \]

and we set \( (i, -1) \equiv (i - 1, J) \).

2.8.4 Iterative algorithm

We give here a schematic overview of the iterative algorithm used in the code:

I) Initialization of the global iterative procedure.

1) \( (U^{(0,0)}, V^{(0,0)}) \equiv \) first trial wave function. If the maximum number of iteration \( i_{\text{max}} > 0 \), the initial wave function (read from file or randomly generated) has already been evolved to satisfy the constraints, with their matrix elements in the quasiparticle basis \( O_{20}^{0(0,J)} \) being stored.

2) \( \tilde{G}_{k}^{(0,J)} = 0 \).

II) Loop over the global iteration number \( i \in [1, i_{\text{max}}] \).

1) Computation of the particle-number projected gradient \( \tilde{G}_{k}^{(i,0)} \) using the wave function \( (U^{(i-1,J)}, V^{(i-1,J)}) \), the projected gradient \( \tilde{G}_{k}^{(i-1,J)} \), and the matrix elements for the constraints \( O_{20}^{0(i-1,J)} \).

2) If \( ||\tilde{G}_{k}^{(i,0)}||_{F}/N_{0}^{(i,0)} \leq \epsilon_{G} \): go to III.

3) Evolution of the wave function taking into account the constraints.

a) Loop over the constraint iteration number \( j \in [0, j_{\text{max}}] \)

i) Computes \( (U^{(i,j)}, V^{(i,j)}) \) and then the expectation values \( \langle \hat{O}_{k} \rangle \).

ii) If \( ||\langle \hat{O}_{k} \rangle^{(i,j)} - O_{k}|| \leq \epsilon_{O} \): go to b).

iii) Computes the Lagrange multipliers \( \lambda_{k}^{(i,j)} \) and with them updates \( \tilde{G}_{k}^{(i,j+1)} \).

b) Storage of the final wave function \( (U^{(i,j)}, V^{(i,j)}), \) projected gradient \( \tilde{G}_{k}^{(i,j)} \), and matrix elements of the constraints \( O_{20}^{0(i,J)} \), with \( J \) being the last iteration of a).

III) End of the iterative procedure

3 Examples

3.1 Unconstrained minima of \( ^{24,25}\text{Mg} \) and \( ^{26}\text{Al} \) with the USDB interaction

As first example, we perform unconstrained calculations for three nuclei in \( sd\)-shell with the USDB interaction [36]: the even-even nucleus \( ^{24}\text{Mg} \), the odd-even nucleus \( ^{25}\text{Mg} \) and finally the odd-odd nucleus \( ^{26}\text{Al} \). All three nuclei are located in the middle of the \( sd\)-shell and exhibit quadrupolar deformations in their ground state. In particular, \( ^{24}\text{Mg} \) is found to have a triaxial minimum in valence space mean-field calculations [38, 89] as well as EDF calculations that include angular momentum projection [15, 90, 91]. Similarly, \( ^{25}\text{Mg} \) is found to be triaxial after the restoration of the rotational invariance within the EDF framework [16, 92]. Unfortunately, advanced mean-field calculations of odd-odd mass nuclei are scarce but axial calculations with the Gogny EDF found a prolate deformed minimum [93].

The oscillator frequency \( \hbar \omega \) used in the calculations of each nucleus was determined using the formula\(^{5}\) [94]

\[^{5}\text{Note that the code uses this formula by default if no value of } \hbar \omega \text{ is entered in the hamiltonian file (with hamil_type = 1 or 2). See the file manual_hamiltonian.pdf for more information.}\]
\[ h\omega = \left( 45A^{-1/3} - 25A^{-2/3} \right), \] (84)

where \( A \) is the number of nucleons of the nucleus studied, and which gives the values \( h\omega = 12.60 \text{ MeV} (b = 1.81 \text{ fm}) \) for \( ^{24}\text{Mg} \), \( h\omega = 12.47 \text{ MeV} (b = 1.82 \text{ fm}) \) for \( ^{25}\text{Mg} \) and \( h\omega = 12.34 \text{ MeV} (b = 1.83 \text{ fm}) \) for \( ^{26}\text{Al} \).

We also specify that the triaxial deformations \((\beta, \gamma)\) were computed using the bare multipole operators, as explained in Sect. 2.7.2. In particular, this means that we did not use any effective operators or charges. This definition allows us to benchmark our results to the ones of Gao et al. [89] who made a similar choice. On the other hand, it is important to remember that the values of \((\beta, \gamma)\) thus obtained will differ from the ones computed in no-core calculations of the same nuclei. In this case, the difference does not come from the definition of the quadrupole operators but from the particles and orbits involved in their evaluation.

The calculations were carried out considering real general trial wave functions and the initial states were randomly generated. For \( ^{25}\text{Mg} \), a quasiparticle was blocked on top of the random initial wave function. For \( ^{26}\text{Al} \), we tried with and without the blocking of two quasiparticle excitations during the generation of the initial state. The two procedures gave the same results. It is important to remember that our general scheme allows the mixing of protons and neutrons such that the wave function already includes odd-odd components even without an explicit blocking. To bypass the problem of local minima, we repeated the calculations ten times before selecting the state giving the lowest energy for each nucleus. In particular, we remark that in VAPNP calculations with wave functions that include proton-neutron pairing, we frequently found many local minima very close in energy.

In Table 1, we give the values of the total HFB energy \( E_{\text{HFB}} \), the pairing part of the energy \( E_{\text{pair}}^{\text{HFB}} = -\text{Tr}(\Delta\kappa^+) / 2 \), and the triaxial deformation parameters \((\beta_{\text{HFB}}, \gamma_{\text{HFB}})\) for the unconstrained minima of the three nuclei. Also, for comparison, we give the value of the exact energy of the ground state \( E_{\text{exact}} \) as obtained from the full diagonalization performed with the shell model code ANTOINE [34]. As expected, all HFB energies are above the exact ones. More surprisingly, the HFB energies of \( ^{25}\text{Mg} \) (odd-even) and \( ^{26}\text{Al} \) (odd-odd) are in better agreement with the exact results than the HFB energy of \( ^{24}\text{Mg} \) (even-even). One problem with the \( ^{24}\text{Mg} \) calculations is that the pairing collapses entirely as can be seen from its vanishing pairing energy. All nuclei are found to be well deformed and to have a triaxial minimum.\(^6\) In particular, the minima of \( ^{25}\text{Mg} \) and \( ^{26}\text{Al} \) are about \( 22^\circ \) away from the closest axial axis.

|                | \(^{24}\text{Mg}\) | \(^{25}\text{Mg}\) | \(^{26}\text{Al}\) |
|----------------|------------------|------------------|------------------|
| \( E_{\text{exact}} \) | -87.101          | -94.399          | -105.749         |
| \( E_{\text{HFB}} \)   | -80.960          | -89.192          | -103.288         |
| \( E_{\text{Gao}} \)   | -80.965          | -82.847          | -90.732          |
| \( E_{\text{VAPNP}} \) | -82.831          | -90.732          | -102.711         |
| \( \beta_{\text{HFB}} \) | 0.282            | 0.240            | 0.236            |
| \( \beta_{\text{Gao}} \) | 0.281            | 0.268            | 0.214            |
| \( \beta_{\text{VAPNP}} \) | 0.260            | 0.214            | 0.184            |
| \( \gamma_{\text{HFB}} \) | 11.98            | 21.9             | 277.7            |
| \( \gamma_{\text{Gao}} \) | 11.96            | 240.16           | 145.3            |
| \( \gamma_{\text{VAPNP}} \) | 21.9             | 355.7            | (25.3)           |
| \( \gamma_{\text{VAPNP}} \) | 0.09             |                  |                  |

\(^6\) Note here that the orientation of the nucleus is not fixed to correspond to a particular sextant of the \((\beta, \gamma)\) plane. Therefore, the amount of triaxiality has to be determined relatively to the closest axial axis located at \( n \times 60^\circ \), with \( n \) an integer.

Finally, we note that our results for \( ^{24}\text{Mg} \) are in very good agreement with the ones of Gao et al. [89] also obtained with the USDB interaction. In particular, using our definition for the deformation (see the caption of Table 1) and considering the same number of digits, we obtain for the deformation \( \beta = 0.282 \) and \( \gamma = 11.98^\circ \) (relatively to the axis at \( 120^\circ \)) which are very close to their values. The energy is also well reproduced, differing only by 5 keV. Although one could expect an even better agreement between the two HFB calculations, we remark that the value they give for the exact energy of \( ^{24}\text{Mg} \) also differ from ours by 4 keV [89]. We do not know the origin of this discrepancy. It might comes from a slight difference in the matrix elements of the USDB interaction (we used the file provided on the webpage of the code ANTOINE).

Considering now the VAPNP calculations, the same properties, but now computed as expectation values for the projected state giving the lowest energy, are also given in Table 1. The first observation is that the total energies of \( ^{24}\text{Mg} \) and \( ^{25}\text{Mg} \) are lowered compared to the HFB calculations and therefore get closer to the exact values. By contrast, the
energy of $^{26}\text{Al}$ is increased such that it gets worst at the VAPNP level. This is a surprising result as VAP calculations are commonly thought as decreasing the energy compared to HFB calculations, which is indeed true in the vast majority of cases. But there is no contradiction with the variational principle as only VAPNP calculations consider the variational space with the correct number of particles. A particle-number projection analysis of the HFB minimum shows that the components ($Z = 5, N = 5$) has an energy equal to $-101.147$ MeV that is above the value obtained from the VAPNP. Interestingly, the two other leading contributions\(^7\) comes from the $N = Z$ even-even neighbors $(6, 6)$ with an energy equal to $-131.697$ MeV and $(4, 4)$ with an energy equal to $-79.055$ MeV.

We note also that, in contrast with the HFB results, the pairing energy integrated over the gauge angles is non-zero for all nuclei. It is a well-known fact that the methods based on the VAP for particle numbers provide a better description of the pairing correlations, in particular avoiding its frequent collapse observed at the HFB level.

Concerning the deformation, we observe that the projected minima of the three nuclei are much less deformed than their HFB counterparts and in the case of $^{24}\text{Mg}$ and $^{25}\text{Mg}$ also become almost purely axial. Only $^{26}\text{Al}$ conserves a large amount of triaxiality at the VAPNP level. This reduction of triaxility for $^{24}\text{Mg}$ was also observed by Gao et al. in their so-called VAP-TA calculations that include the isospin and particle-number projections in the variational process. In Table 1, we compare their values to ours using our definition of the deformation parameters. Indeed, we work here with general (real) quasiparticle states whereas their framework conserves the time-reversal invariance and the separation between protons and neutrons. In particular, we note that our VAPNP solution displays some proton-neutron mixing.

### 3.2 Analysis of the Heavy-Ball algorithm for $^{24}\text{Mg}$

For our second example, we study the convergence of the Heavy-Ball (HB) algorithm for different choices for the parameters $\eta$ and $\mu$. The calculations are performed using the same model space, interaction and oscillator parameters as the ones used in Sect. 3.1. Taking the calculations of the HFB and VAPNP unconstrained minima of $^{24}\text{Mg}$ as examples, we display in Fig. 1 the evolution of the number of iterations required to reach convergence as a function of the parameter $\eta$ for different gradient schemes. Bottom: Same for VAPNP calculations. The convergence criterion is fixed at $\epsilon_G = 10^{-4}$. The dashed lines represent the (optional) empirical recipes pre-implemented in the code.

\[\text{Fig. 1} \quad \text{Top: Evolution of the number of iterations required to converge a HFB calculation of the unconstrained minimum of} \, ^{24}\text{Mg} \, \text{as a function of the parameter} \, \eta \, \text{for different gradient schemes. Bottom: Same for VAPNP calculations. The convergence criterion is fixed at} \, \epsilon_G = 10^{-4}. \, \text{The dashed lines represent the (optional) empirical recipes pre-implemented in the code.} \]

\(^7\) The components $(Z = 5, N = 5)$, $(6, 6)$ and $(4, 4)$ have weights approximately equal to 0.493, 0.256 and 0.244, respectively. The two other smaller components are $(3, 3)$ and $(7, 7)$. 

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Adding a momentum term, i.e. $\mu \neq 0$, has two main effects. First, for a given $\eta$, the calculations tend to converge faster. This is not a general rule however as the calculations with $\mu = 0.9$ are globally outperformed by the pure gradient descent with $\mu = 0$. The second benefit of the presence of a momentum term is that it stabilizes the calculations by pushing up the value of $\eta$ over which the calculations do not converge anymore.

Comparing the HFB and VAPNP calculations, we see that the latter requires in general more iterations to converge than the former and also that the critical value $\eta_c$ is slightly smaller. Strangely, the calculation with $\mu = 0.9$ behaves better in the VAPNP calculation. Another remark, less apparent on the plot, is that the VAPNP calculations do not always converge to the exact same minimum. Indeed, there are two minima that are very similar (e.g. same deformation) but differ by 40 keV such that the calculations will transition from one to the other. On the curves, the transitions can be seen as small steps at $\eta \approx 0.02$ for the calculation with $\mu = 0.6$ and at $\eta \approx 0.07$ for the calculation with $\mu = 0.3$.

Finally, we notice that the two empirical recipes introduced in Sect. 2.8.1 perform similarly in the two calculations. In the HFB case, they are extremely efficient and allow to reach convergence with less than 100 iterations. In the VAPNP case, however, they are not nearly as good and are outperformed by most of the other schemes. The lesser performance of these recipes can be understood as they have been designed to use the quasiparticle/single-particle energies of the Bogoliubov state at hand to optimize the unprojected gradient. Obviously, these quantities are not necessarily as well adapted to optimize the projected gradient built from the same state. Nevertheless, the two recipes still converge with an acceptable number of iterations without the need to manually fix the parameters.

3.3 No-core calculations of $^{24}$Mg with a Chiral EFT interaction

As final example calculation, we consider again the nucleus $^{24}$Mg but this time performing a no-core calculation in a model space characterized by $\epsilon_{\text{max}} = (2n + l)_{\text{max}} = 8$, i.e. containing 9 major oscillator shells, and $\hbar \omega = 20$ MeV. The chiral Hamiltonian used contains a 2N interaction at next-to-next-to-leading order (N3LO) [31], a 3N interaction at N2LO [95], and was evolved through Similarity Regularization Group (SRG) techniques [63]. In addition, the 3N part of the Hamiltonian was recasted following the procedure explained in [96] using as reference state a spherical HFB state constructed for $^{24}$Mg. In this special case, this procedure is similar in spirit to the well-known NO2B [63].

In Fig. 2, we display the HFB energy surface in the first sextant of the triaxial $(\beta, \gamma)$ plane. All calculations were started from randomly generated wave functions breaking all symmetries but the parity$^9$ and were constrained to have $\langle \hat{O}_{21} \rangle = 0$. As can be seen, the HFB minimum is triaxial with a deformation $(\beta = 0.404, \gamma = 12.62^\circ)$ and an energy $E_{\text{HFB}} = -152.937$ MeV. Interestingly, the value for $\gamma$ is in very good agreement with the one obtained in the valence-space USDB calculations discussed previously. On the other hand, the value for $\beta$ is slightly larger, which is not totally surprising as we consider now all the nucleons as being active in a much larger model space. In other words, a fair comparison between the values of $(\beta, \gamma)$ obtained in the valence-space and no-core calculations would have required the use of proper effective quadrupole operators in the valence-space calculations. We also recall that state-of-the-art EDF calculations only obtain an axial minimum at the HFB or VAPNP level [15,90,91]. Here, a VAPNP calculation for the minimum gives a very similar result for the deformation $(\beta = 0.403, \gamma = 12.45^\circ)$, but with an energy $E_{\text{VAPNP}} = -157.010$ MeV. Therefore, we do not observe any reduction of the triaxiality, contrary to the valence-space calculations. We remark in passing that while the pairing collapses in the wave function of the HFB minimum, the pairing energy (integrated over the gauge angles) of the VAPNP solution is completely dominated by the neutron-proton contribution even if the chiral Hamiltonian breaks explicitly the isospin.

The energy of the HFB and VAPNP minima are more than 40 MeV above the experimental ground-state energy, $E_{\text{exp}} = -198.257$ MeV [97]. This is not surprising because these methods miss many important correlations as shown, for example, in many-body perturbation theory calculations performed on top of HFB minima [49]. This deficiency could be corrected by unitarily transforming the Hamiltonian to include the necessary correlations, as done in Ref. [50] using the In-Medium Similarity Renormalization Group method [43]. Nevertheless, it is interesting to remark that the energy surface is very similar to what can be obtained in EDF calculations at the multi-reference level [15,92]. It might be that even if absolute quantities (e.g. the total energy) are not well reproduced at the HFB level, relative quantities (e.g. the energy difference between deformed states and thus the deformation adopted by the minimum) are.

Finally, we remark that an $\epsilon_{\text{max}} = 10$ calculation gives a minimum with a deformation $(\beta = 0.407, \gamma = 12.65^\circ)$ and an energy $E_{\text{HFB}} = -153.179$ MeV, thus the calculation

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$^9$ When starting from parity breaking states, most of the calculations converge towards positive parity wave functions at the end of the minimization, such that the energy surface is mostly unchanged. However, a few final wave functions break the parity and would require a subsequent parity projection that is outside the scope of the present article.
Fig. 2 Energy surface in the first sextant of the $(\beta, \gamma)$ plane for the HFB calculations performed in a model space with $e_{max} = 8, \hbar \omega = 20$ and using the chiral Hamiltonian described in the text. The black lines are separated by 1 MeV, starting from the minimum represented by a black dot.

is relatively well converged as a function of the number of shells (for a fixed value of $\hbar \omega = 20$ MeV).

4 Conclusions

In this article, we presented the numerical code TAUROSVAP that solves the variation after particle-number projection equations for real general Bogoliubov quasiparticle states represented in a spherical harmonic oscillator basis. We explained the theoretical framework within which the code operates and outlined its principal features. Additional information can also be found on the GitHub repository associated with this article.

We hope that making this advanced variational solver publicly available will be of interest to the nuclear structure community in general. In particular, TAUROSVAP can be used to carry out constrained variational calculations in both valence-space and no-core model spaces with general Hamiltonians containing up to two-body terms. Moreover, the MPI implementation included in the code allows one to use parallel supercomputers to run large model space calculations.

While the numerical code TAUROSVAP already allows the realization of advanced variational calculations, many developments are possible in the future such as the inclusion of additional symmetry projections in the variational scheme or the use of the full three-body interaction. Nevertheless, the next logical step will be the publication of the companion code TAUROSPAV that, considering the same theoretical framework, performs various symmetry projections using the output wave functions produced by TAUROSVAP.

5 Using the code

5.1 Source files and compilation

The numerical code TAUROSVAP is divided into different files containing the main program, the various modules, and specific mathematical routines. The list all the files, in the order of which they should be compiled, is the following:

- module_constants.f90
- module_mathmethods.f90
- module_parallelization.f90 (only if MPI)
- module_nucleus.f90
- module_basis.f90
- module_hamiltonian.f90
- module_wavefunctions.f90
- module_fields.f90
- module_particlenumber.f90
- module_pairs.f90
- module_angularmomentum.f90
- module_multipoles.f90
- module_radius.f90
- module_operators.f90
- module_projection.f90
- module_constraints.f90
- module_gradient.f90
- module_initialization.f90
- subroutines_pfaffian.f
- taurus_vap.f90

To use the MPI implementation, it is first required, before compilation, to remove the comment flags “!cmpi” present in the Fortran files. This can be done easily using the command

```
  sed -i "s/!cmpi//g" src/*f90
```

while being in the main directory of the repository.

On the GitHub repository, we provide a makefile to compile the code that takes in entry two arguments: FC to specify the compiler and TH to specify if we want to include OpenMP threading or not. If no argument is entered, the script will use some default values. The correct values for the argument FC are: gfortran (default), ifort, mpiifort and

10 On BSD-based systems, it is necessary to use instead `sed -i "s/!cmpi//g" src/*f90`

11 As this command changes the source files in an irreversible manner, we recommend to first create a temporary copy of the source files before using it. Otherwise, it will be necessary to discard the changes in the local git repository before the next compilation of the code in sequential mode (i.e. without MPI).
mpif90. On the other hand, the argument TH can take the values omp or none (default). For example, if one wants to compile TAUROSVAP using the gfortran compiler and without OpenMp, one has to execute the command

make FC=gfortran TH=none

For completeness, we also provide in the repository a bash script that offers comparable compilation capabilities. More information about how to use this script or the makefile can be found in the file README.md present in the main directory of the repository.

5.2 Execution

Once in the directory containing the executable file, the code can be run by typing the command

```bash
./taurus_vap.exe < input.txt
```

where input.txt is the STDIN file containing the input parameters. The details concerning the format of STDIN can be found in the file manual_input.pdf present in the directory extras. The code also requires, in the same directory, the file defining the Hamiltonian (and model space), the name of which is written in the STDIN, and the various files containing its matrix elements. The details concerning the format of Hamiltonian files can be found in the file manual_hamiltonian.pdf present in the directory extras.

To simplify the execution of the code, we provide the script launch.sh that performs all the necessary steps to run a calculation. To use it, go to the main directory of your copy of the repository and type the command

```bash
bash launch.sh
```

During its execution, the code prints various information (e.g. inputs and model space used, expectation value of the energy at each iteration, etc.) in the STDOUT. We recommend to store the printing in a file, for example output.txt, by typing

```bash
./taurus_vap.exe < input.txt > output.txt
```
or

```bash
bash launch.sh > output.txt
```

Additionally, the code will produce other files containing relevant information such as the occupation numbers or the eigenvalues of the single-particle Hamiltonian. More importantly, the code will write the final wave function obtained at the end of the iterative procedure in a file. The names of all the files produced during a run are recalled in the STDOUT. See the file extras/manual_input.pdf for more details.

5.3 Time and memory requirements

The runtime of the code will depend on three main factors:

1. The number of non-zero two-body matrix elements of the Hamiltonian stored, which is related to the size of the model space considered.
2. The number of discretization points used in the particle-number projection.
3. The number of iterations required to converge the calculation, which will depend on the initial wave function and the parameters used for the calculation (e.g. the criterion for the convergence of the gradient).

For that reason, it is difficult to give a precise estimate for the time required to complete a run. Nevertheless, from experience we can say that a run in a valence space will take between a few tenths of a second and a few minutes. Similarly, no-core calculations including only a few shells, e.g. \( e_{\text{max}} = 8 \), will be take only a few minutes. Computations in larger model space, however, may take several hours or even days to complete.

On the other hand, the amount of memory required for a calculation is almost entirely driven by the number of non-zero two-body matrix elements of the Hamiltonian stored. In Fig. 3, we give the maximum amount of memory required to store the two-body matrix elements (2BME) of \( H \) in single-precision as a function of the number of oscillator shells \( N_{\text{SHO}} \) included in a no-core calculations. The results were obtained using the storage strategy explained in Sect. 6.4 assuming that all matrix elements not forbidden by symmetry reasons are non-zero. As can be seen, the memory required grows rapidly with the number of shells but remains manageable even for large values of \( N_{\text{SHO}} \) especially considering the parallelization capabilities of our modern computers (see Sect. 5.4).

As a conclusion, we will remark that a run in a small valence space has, for all intents and purposes, no system requirements and can be completed in a short amount of time even on a laptop. By contrast, no-core calculations in large model spaces are computationally heavy and will require the use of a parallel supercomputer or computing cluster.

5.4 Parallelization

In order to make the large model space calculations possible, the code integrates three layers of parallelization, based on MPI and OpenMP, that can be used separately or together. The parallelization scheme depends on three parameters that are handed to the code: the total number of MPI processes \( N_{\text{worldsize}} \), the desired number of MPI processes in a team \( N_{\text{teamsize}} \), and the number of OpenMP threads per MPI proc-
The number of processes assigned to each team is defined as

\[ N_{\text{myteamsize}} = \begin{cases} N_{\text{teamsize}} & \text{[first (}N_{\text{teams}} - 1\text{) teams]} \\ r + \delta r N_{\text{teamsize}} & \text{[last team]} \end{cases} \]  

(87)

The sets of \( N_{\text{teamsize}} \) processes are assigned sequentially according to their global rank.

### 5.4.2 Distribution of the angles

To distribute the \( N_{\text{angles}} = M_{\phi N} M_{\phi Z} \) (see Sect. 6.2) angles among the teams, the code computes the euclidean division

\[ N_{\text{angles}} = p N_{\text{teams}} + r \quad (0 \leq r < N_{\text{teams}}). \]  

(88)

Then, the number of angles attributed to each team is defined as

\[ N_{\text{myangles}} = \begin{cases} p + 1 & \text{[first } r \text{ teams]} \\ p & \text{[last } (N_{\text{teams}} - r) \text{ teams]} \end{cases} \]  

(89)

The sets of \( N_{\text{myangles}} \) angles are assigned sequentially according to their order in the loop over gauge angles.

### 5.4.3 Distribution of the matrix elements

To distribute the \( N_{\text{2BME}} \) two-body matrix elements of \( H \) among the members of a team, the code computes the euclidean division

\[ N_{\text{2BME}} = p N_{\text{myteamsize}} + r \quad (0 \leq r < N_{\text{myteamsize}}). \]  

(90)

Then, the number of matrix element assigned to each member is defined as

\[ N_{\text{my2BME}} = \begin{cases} p + 1 & \text{[first } r \text{ members]} \\ p & \text{[last } (N_{\text{myteamsize}} - r) \text{ members]} \end{cases} \]  

(91)

The sets of \( N_{\text{my2BME}} \) matrix elements are assigned sequentially according to their order of reading in the Hamiltonian input file.

### 5.5 Dependencies

The code requires the BLAS and LAPACK libraries. In addition, it is recommended to use a recent compiler as the code includes a few Fortran 2003/2008 commands that might not be implemented in compilers that are too old.
6 Additional technical details

6.1 Seed generation

The wave function that is used as initial guess in the iterative procedure can either be read from a file or generated randomly, depending on the value of the input parameter seed_type (see the manual). If the user chooses to start the calculation from a random initial state, the following strategy is used for its generation:

1. The seed of the pseudorandom generator is initialized by executing "call random_seed()", which generates a seed based on the system’s time.
2. The occupations \( v^2 \) in the SHO basis, assumed for now to be the canonical basis, are generated randomly and from them the matrices \( U_c \) and \( V_c \) of the Bogoliubov transformation.
   i) In the case of a BCS or general state, the occupations correspond to a fully paired vacuum \((0 ≤ v^2 < 1)\) and the single-particle states are paired with their time-reversal partners \((α \text{ with } -α)\). In addition, if the state is a spherical BCS wave function, there is an equal filling of all single-particle states belonging to the same orbit. At the end of the process, the occupations are scaled such that the states have the correct numbers of particles \(Z\) and \(N\) on average.
   ii) In the case of a Slater determinant, \(Z/N\) randomly selected proton/neutron single-particle states are fully occupied \((v^2 = 1)\).
3. A random orthogonal transformation \( D \) is generated by diagonalizing a randomly generated real symmetry matrix \( S \) and forming the matrix made of its eigenvectors.
   i) In the case of a BCS state (spherical or not), \( D \) is assumed to be the identity matrix \(I_{d_M} \).
   ii) In the case of a general state, the symmetric matrix \( S \) has the dimensions \(d_M × d_M \).
   iii) If some symmetries are to be conserved (such as parity or the separation between protons and neutrons), several smaller matrices \( S_i \) with the dimensions of the symmetry blocks are generated and diagonalized. Ultimately, \( D \) is built from the combinations of their eigenvectors.
4. A random orthogonal transformation \( C \) is generated following the same principles. In the case of a Slater determinant, \( C \) is assumed to be the identity matrix \(I_{d_M} \).
5. The final Bogoliubov matrices of the initial state in the SHO basis are generated, using the Bloch-Messiah-Zumino theorem [2], as \( U = DU_cC \) and \( V = D^*V_cC \).\(^{12}\)

6.2 Discretization of the particle-number projection operator

The integral over gauge angles appearing in the particle-number projection operator is discretized following the idea of Fomenko [78]. More precisely, taking the neutrons as example (the exact same discretization is used for protons), we use the \(M_N\)-point quadrature

\[
P_N^{M_N} = \frac{1}{M_N} \sum_{m=1}^{M_N} e^{iαπf(m, M_N)}(N - N_0),
\]

where

\[
α = \begin{cases} 
1 & \text{if no } p-n \text{ mixing} \\
2 & \text{otherwise,}
\end{cases}
\]

\[
f(m, M_N) = \begin{cases} 
\frac{m-1}{M_N} & \text{if } M_N \text{ is odd,} \\
\frac{m-1/2}{M_N} & \text{if } M_N \text{ is even.}
\end{cases}
\]

The selection of a different discretization for the angles as a function of the parity of \(M_N\) is done to avoid the numerical evaluation of the rotated quantities at angle \(\frac{π}{2}\) whatever the value of \(M_N\). Indeed, when going through the angle \(\frac{π}{2}\), one might have to evaluate a fraction where both the numerator and denominator can become arbitrarily close to zero, which is numerically dangerous [72].

More details on the mathematical aspects of the discretized operator \(P_N^{M_N} \) as well as an analysis of its convergence behavior can be found in Ref. [10].

6.3 Evaluation of overlaps

The projection onto good particle numbers \(Z\) and \(N\) requires the evaluation of the overlap \(\langle \Phi | \Phi(\varphi_Z, \varphi_N) \rangle\) between the state \(|\Phi⟩\) and the gauge rotated state \(|\Phi(\varphi_Z, \varphi_N)⟩\) for all the discretized values of \((\varphi_Z, \varphi_N)\). The evaluation of overlaps between general quasiparticle states can be performed using the Pfaffian algebra [69]. In this work, we use the particular formula given in Eq. (60) in Ref. [70] that presents several advantages, the first of which being that fully occupied/empty single-particle states, once identified, can be treated rather straightforwardly.\(^{13}\)

\(^{12}\) Note that for a state with proton-neutron mixing, only the average number of nucleons \(A\) will be conserved after applying the transformations \(D\) and \(C\) defined above.

\(^{13}\) We remark that Slater determinants, which represent the special case where all the single-particle states are either fully occupied or fully empty, can also be treated using this formula.
The most direct way to identify those single-particle states is by constructing the canonical basis of $|\Phi\rangle$. To do so, we first diagonalize the one-body density $\rho$ and transform the one-body pairing tensor $\kappa$ in this basis. This change of basis is sufficient to transform all the blocks of $\kappa$ corresponding to non-degenerate eigenvalues of $\rho$ into their canonical form. In case there are remaining blocks of $\kappa$ that are not yet in their canonical form, we proceed to a Schur decomposition of each of these blocks, which automatically put them in their canonical form given $\kappa$ is a real antisymmetric matrix. In the end, both $\rho$ and $\kappa$ are transformed in this new basis that both diagonalize $\rho$ and put $\kappa$ in its canonical form.

Once the canonical basis has been constructed, it is easy to identify the fully occupied/empty states of $|\Phi\rangle$ in this basis by searching for the states $i$ that have an occupation $v_i^2$, i.e. an eigenvalue of $\rho$, above/below a desired numerical value. In the code, a state $i$ is considered fully occupied if $v_i^2 \geq 1 - \epsilon$, with $\epsilon$ being a numerical parameter set by default to $10^{-8}$ but that can also being chosen via the parameter seed_occup in the input file. On the other hand, a state $i$ is considered fully empty if $v_i^2 \leq \epsilon$.

After identification, the fully occupied/empty single-particle states in the canonical basis are removed from the calculations of the Pfaffian following the methodology presented in Ref. [70]. The big advantage of removing the empty states is that it reduces the dimensions of the matrices and therefore reduces the computational time required to calculate the Pfaffian. Nevertheless, in some rare occasions, it becomes necessary to include the empty states to avoid having an overlap matrix of the single-particle states that is non-invertible.

On the numerical side, the Pfaffian is computed using the efficient routines provided in the library PFAPACK [98]. We integrated the routines required for our calculations in the file subroutines_pfaffian.f.

6.4 Two-body matrix elements of the Hamiltonian

The number of two-body matrix elements of the Hamiltonian in the SHO single-particle basis can be very large when the model space considered is made of many oscillator shells. Unfortunately, a large number of matrix elements poses several difficulties. First, the amount of memory required to store the matrix elements is directly proportional to the number of matrix elements and can rapidly represent hundreds of gigaoctets or more. Second, in no-core calculations, the run-time within a single iteration is entirely dominated by the calculations of the fields ($r^{0w}$, $\Delta^{0w}$ and $\Delta^{1w}$) and is computationally intensive. Finally, the decoupling of the $J$-scheme matrix elements read in the input files to the $m$-scheme matrix elements used in the calculation, i.e. [94]

$$h_{abcd}^{(2)} = \langle ab|\hat{h}_{cd}^{(2)}|cd\rangle = \sum_{JM_j} (j_a m_{j_a} j_b m_{j_b} |JM_j)(j_c m_{j_c} j_d m_{j_d} |JM_j) \times [N_{\hat{a}\hat{b}}(J)N_{\hat{c}\hat{d}}(J)]^{-1} \langle \hat{a}\hat{b}, J|\hat{h}_{cd}^{(2)}|\hat{c}\hat{d}, J \rangle$$

(95)

where $\langle \hat{a}\hat{b}, J|\hat{h}_{cd}^{(2)}|\hat{c}\hat{d}, J \rangle$ is a $J$-scheme matrix element and

$$N_{\hat{a}\hat{b}}(J) = \frac{\sqrt{1 + \delta_{\hat{a}\hat{b}}(-1)^J}}{1 + \delta_{\hat{a}\hat{b}}}$$

(96)

is a normalization factor, can also become prohibitively long. Similar expression is used when decoupling a $JT$-scheme matrix elements.

To overcome these problems, the main strategy is to store and use in the calculations the minimal number of matrix elements possible. The first obvious step is to store only the non-zero matrix elements $h_{abcd}$ and keep track of the corresponding indices $a, b, c, d$. In that order, for each $m$-scheme matrix element $\tilde{h}_{abcd}$ above a certain numerical cutoff (by default $10^{-16}$), we store:

1. The matrix element $\tilde{h}_{abcd}$ in a one-dimensional 4-byte real array.
2. The quartet of indices $(a, b, c, d)$ in a one-dimensional 2-byte integer array. The quartets are stored sequentially, i.e. the array elements read $a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2, \ldots$, to reduce the memory swap when reading/writing the indices.
3. A permutation number $-8 \leq p \leq 7$ in a one-dimension integer 1-byte array. As explained below, this index is used to reconstruct rapidly the time-reversed matrix elements of $\tilde{h}_{abcd}$ with the indices in the right order.

With that, each matrix element takes 13 bytes of memory. The number of matrix elements itself is stored as a single 8-byte integer.

One could argue that it would be preferable to store the matrix elements as double precision 8-byte real numbers. While it is true to some extent, our tests show that the difference in energy resulting from the two choices is below the keV level, i.e. much below the accuracy of any many-body method or interaction available. In addition, the matrix elements are never used to perform sensitive numerical operations. Indeed, they are only used in the program in the calculations of the fields where they are multiplied by the matrix elements of the one-body densities. Nevertheless, the code

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14 When performing valence-space calculations, the matrix elements are read in $JT$-scheme and decoupled using the adapted expression [94].
can be easily switched to a double precision storage of the matrix elements by setting "$rH2 = real64$" in the file module_constants.f90 and in that case, each matrix element will take 17 bytes of memory.

The vast majority of two-body matrix elements in the SHO basis will vanish due to the symmetries of the Hamiltonian such as the rotational and parity invariances or the conservation of the number of neutrons and protons. These symmetries translate into the relations

\begin{align}
(-1)^{l_a+l_b} &= (-1)^{l_a+l_d} \\
m_{j_a} + m_{j_b} &= m_{j_c} + m_{j_d} \\
m_{l_a} + m_{l_b} &= m_{l_c} + m_{l_d}
\end{align}

that can be used to reduce the loops over the indices when decoupling the $J$-scheme matrix elements.

In addition, it is possible to reduce the number of matrix elements to be stored by considering their antisymmetry under the exchange of two particles, in the bra or the ket, and their symmetry\textsuperscript{15} under the exchange of the bra and the ket. More precisely, we have

\begin{align}
\bar{h}_{abcd} &= -\bar{h}_{abde} \\
&= \bar{h}_{badc} \\
&= -\bar{h}_{bcad} \\
&= \bar{h}_{cdab} \\
&= -\bar{h}_{cdba} \\
&= \bar{h}_{dcb} \\
&= -\bar{h}_{dca},
\end{align}

such that only a subset of the matrix elements have to be stored. Indeed, the non-stored matrix elements can be reconstructed on the fly during the calculations of the fields by permuting the indices and multiplying by the appropriate phase factor. In the code, the single-particle basis states are labeled according to their index $\in [1, d_M]$. With that said, the matrix elements stored are such that

\begin{align}
a &\in [1, d_M], \\
c &\in [a, d_M], \\
d &\in [c + 1, d_M], \\
b &\in [a + 1, b_{\text{max}}] \quad \text{with} \quad \begin{cases} b_{\text{max}} = d & \text{if } c = a, \\
b = d_M & \text{otherwise.} \end{cases}
\end{align}

Furthermore, it is possible to use the time-reversal invariance of $H$ to obtain

\begin{equation}
\bar{h}_{abcd} = (-1)^{l_a+l_b+l_c+l_d} \bar{h}_{-a-b-c-d}.
\end{equation}

\textsuperscript{15} The matrix elements are considered real.

As the trial wave functions considered in TAUROS\textsubscript{vap} may break the time-reversal invariance, it is not possible to use this relation to its full extent, i.e. reducing the sum over the single-particle states in the calculation of the fields. Nevertheless, it allows us to store only the matrix elements that are such that $m_{j_a} + m_{j_b} \geq 0$.

at the cost of reconstructing the time-reversed matrix elements when calculating the fields. Given the possible large number of matrix elements and the fact that the reconstruction has to follow the rules of Eq. (99), this takes a non negligible amount of time. Therefore, to reduce the time needed for the reconstruction, we store for each matrix element $\bar{h}_{abcd}$ an extra permutation index $p$ in a one-dimensional 1-byte integer array that can be used by the code to rapidly determine the correct order of indices and the appropriate phase factor when reconstructing its time-reversed matrix element. This permutation index is calculated only once after the decoupling of the $J$-scheme matrix elements.

While efficient, this strategy is not sufficient by itself to tackle very large model spaces. Indeed, the memory required to store the full set of matrix elements can rapidly exceed the RAM available on a single computer/node. To bypass this problem, the code can also share the matrix elements among several MPI processes as described in Sect. 5.4.

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References

1. J. Carlson, S. Gandolfi, F. Pederiva, S.C. Pieper, R. Schiavilla, K.E. Schmidt, R.B. Wiringa, Rev. Mod. Phys. 87, 1067 (2015). https://doi.org/10.1103/RevModPhys.87.1067
2. P. Ring, P. Schuck, The nuclear Many-Body problem (Springer-Verlag, New York, 1980)
3. A. Bohr, B.R. Mottelson, D. Pines, Phys. Rev. 110, 936 (1958). https://doi.org/10.1103/PhysRev.110.936
4. S.T. Belyaev, K. Dan, Vidensk. Selsk. Mat. Phys. Medd. 31, 11 (1958)
