In-medium $k$-body reduction of $n$-body operators

A flexible symmetry-conserving approach based on the sole one-body density matrix

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Abstract The computational cost of ab initio nuclear structure calculations is rendered particularly acute by the presence of (at least) three-nucleon interactions. This feature becomes especially critical now that many-body methods aim at extending their reach beyond mid-mass nuclei. Consequently, state-of-the-art ab initio calculations are typically performed while approximating three-nucleon interactions in terms of effective, i.e. system-dependent, zero-, one- and two-nucleon operators. While straightforward in doubly closed-shell nuclei, existing approximation methods based on normal-ordering techniques involve either two- and three-body density matrices or a symmetry-breaking one-body density matrix in open-shell systems. In order to avoid such complications, a simple, flexible, universal and accurate approximation method involving the convolution of the initial operator with a sole symmetry-invariant one-body matrix is presently formulated and tested numerically. Employed with a low-resolution Hamiltonian, the novel approximation method is shown to induce errors below 2–3% across a large range of nuclei, observables and many-body methods.

1 Introduction

Dealing fully with three-, possibly four-, nucleon interactions is non-trivial but tractable in a self-consistent mean-field Hartree-Fock (HF) or Hartree-Fock Bogoliubov (HFB) calculation. However, it becomes extremely cumbersome, if not impossible, beyond a certain nuclear mass when solving the $A$-body Schrödinger equation to good-enough accuracy beyond the mean field. Consequently, ab initio calculations of mid-mass nuclei are typically performed on the basis of the so-called normal-ordered two-body (NO2B) approximation that captures dominant effects of three-nucleon interactions while effectively working with two-nucleon operators [1,2]. In large-scale no-core shell-model calculations, the error induced by the NO2B approximation of the Hamiltonian was estimated to be of the order of 1–3% up to the oxygen region$^1$.

The NO2B approximation was originally designed by normal ordering the Hamiltonian with respect to a Slater determinant through standard Wick’s theorem [5]. The procedure involved the contraction of the three-body operator with the one-body density matrix of that product-state Slater determinant. In this context, the approximate NO2B Hamiltonian naturally displays the same symmetries as the original one. However, the naive extension of the NO2B approximation to methods applicable to open-shell nuclei expanding the exact solution with respect to a symmetry-conserving state represents a state whose associated one-body density matrix is symmetry-invariant, i.e. belongs to the trivial irreducible representation of the symmetry group of the Hamiltonian. While for the SU(2) group this condition is automatically satisfied for the normal one-body density matrix.

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$^1$For low-resolution Hamiltonians obtained via, e.g., the application of similarity renormalization group (SRG) transformations [3], the efficiency of the NO2B approximation can be understood on the basis of phase-space arguments in the calculation of homogeneous infinite nuclear matter [4]. In particular, the analysis of Ref. [4] makes clear that the quality of the approximation can only improve as the density (mass) of matter (nuclei) increases.

$^2$In the present work, a symmetry-conserving state represents a state whose associated one-body density matrix is symmetry-invariant, i.e. belongs to the trivial irreducible representation of the symmetry group of the Hamiltonian. While for the SU(2) group it makes necessary for the many-body state itself to be symmetry invariant, i.e. to be a $J=0^+$ state, for the U(1) group this condition is automatically satisfied for the normal one-body density matrix.
shell systems via the use of symmetry-breaking reference states poses a difficulty in that respect. Indeed, ignoring the normal-ordered three-body term delivers in such a situation an approximate operator that itself explicitly breaks the corresponding symmetry(ies) of the full Hamiltonian. This feature is unwelcome as it lacks the transparency of restricting the symmetry breaking to approximations of the many-body state, especially in view of the eventual restoration of the symmetry(ies).

Within the frame of many-body methods breaking U(1) symmetry associated with particle-number conservation [6–10] via the use of Bogoliubov reference states, a particle-number-conserving normal-ordered k-body (PNOkB) approximation of an arbitrary n-body operator was recently formulated and validated numerically [11]. Using the PNOkB approximation, ab initio calculations on singly open-shell nuclei based on U(1)-breaking and restored formalisms can thus be safely performed. As one currently becomes interested in methods (further) breaking SU(2) symmetry associated with angular-momentum conservation [12,13] to describe doubly open-shell nuclei, the symmetry-conserving NOkB approximation should be extended to this symmetry group, which happens to be neither easy nor transparent.

The difficulty is bypassed from the outset when describing open-shell systems through a so-called multi-reference method based on an explicitly correlated and symmetry-conserving reference state, e.g. in the multi-reference in-medium similarity renormalization group method [14,15]. In this context, it is natural to approximate the three-body interaction through its normal-ordering with respect to the correlated reference state on the basis of Kutzelnigg-Mukherjee’s Wick theorem [16]. The benefit however comes with the prize of having to contract the three-body operator not only with the one-body, but also with the two-body and three-body density matrices of the correlated state. A somewhat similar situation occurs within self-consistent Green’s function (SCGF) theory that can be formulated in terms of effective k-body vertices obtained by contracting initial n-body operators (n ≥ k) with fully correlated (n − k)-body density matrices [17].

In conclusion, several approaches exist to produce so-called effective, i.e. nucleus-dependent, interactions. The aim is to eventually discard the effective operator(s) of highest n-body character(s) whose contribution to, e.g., ground-state energies is (are) expected to be much smaller than for the original operator(s) carrying the same n-body character(s). Such a procedure always involves a contraction of the original operator(s) with a (set of) density matrix (matrices) reflecting (i) the symmetries and (ii) the correlations of the many-body state it (they) originates from and that is typically the reference state or the fully correlated state at play in the many-body method of interest.

In this context, the present work introduces a novel method to build a set of effective k-body interactions in view of approximating the initial Hamiltonian. While the Hamiltonian is indeed our primary target, the procedure can in principle be applied to any observable. Our goal is thus to formally justify and test numerically a novel approximation method that

1. only invokes contractions with a one-body density matrix,
2. uses a symmetry-invariant one-body density matrix,
3. is flexible regarding the many-body state used to compute that one-body density matrix,
4. re-expresses the approximate Hamiltonian in normal-ordered form with respect to the particle vacuum.

The benefits are that

1. the method does not involve l-body density matrices with l > 1,
2. the approximate Hamiltonian resulting from omitting certain effective k-body terms always possesses the same symmetry group as the original one,
3. the method does not necessarily have to employ the one-body density matrix associated with the many-body (reference) state at play in the method used to solve Schrödinger’s equation,
4. the resulting Hamiltonian is explicitly expressed in the original single-particle basis such that it can naturally be employed as the starting point of any many-body method.

Points (3) and (4) underline the fact that the approximation of the Hamiltonian and the resolution of the Schrödinger equation, although not unrelated, constitute two different problems and do not necessarily have to be dealt with on the basis of the same many-body scheme.

Per se, the method is applicable independently of the closed- or (doubly) open-shell character of the system as well as of the ground or excited nature of the targeted state. Still, point (2) implies that only one-body densities deriving from a J^π = 0^+ state can be employed in the approximation procedure, which obviously implies that the employed one-body density matrix does not necessarily derive from the targeted state/nucleus. With excited states of even-even nuclei in mind, one can most naturally approximate the Hamiltonian through the use of a one-body density matrix associated with the ground state. With odd-even or odd-odd systems in mind, one can employ the symmetry-invariant density matrix associated with a fake odd system described in terms of, e.g., a statistical mixture [18,19] in close spirit with the ensemble-normal ordering technique used in valence-space IMSRG.

Once again, this property can be justified for low-scale Hamiltonians on the basis of phase-space arguments [4].

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calculations of odd nuclei [20]. In the present paper, the focus is on even-even systems.

The paper is organized as follows. Section 2 is dedicated to the formulation of the method and its relation to existing ones. After explicating in Sect. 3 the hierarchy of one-body density matrices and many-body methods presently employed to test the approximation method, the corresponding numerical results are presented in Sect. 4. While conclusions are provided in Sect. 5, several appendices complement the paper with useful technical details.

2 Formalism

2.1 Definitions

2.1.1 Operators

An arbitrary particle-number-conserving operator $O$ can be written as

$$O \equiv \sum_{n=0}^{N} O^{nn},$$

where each $n$-body component reads in an arbitrary basis \{ $c_{a}^{\dagger}$, $c_{a}$ \} of the one-body Hilbert space $\mathcal{H}$ as

$$O^{nn} \equiv \frac{1}{n!} \frac{1}{n!} \sum_{a_{1} \ldots a_{n}} o_{a_{1} \ldots a_{n}}^{a_{1} \ldots a_{n}} A_{a_{1} \ldots a_{n}},$$

where

$$A_{a_{1} \ldots a_{n}}^{a_{1} \ldots a_{n}} \equiv c_{a_{1}}^{\dagger} \ldots c_{a_{n}}^{\dagger} c_{b_{n}} \ldots c_{b_{1}}$$

denotes a string of $n$ one-particle creation and $n$ one-particle annihilation operators such that $(A_{b_{1} \ldots b_{n}}^{a_{1} \ldots a_{n}})^{\dagger} = A_{b_{1} \ldots b_{n}}^{a_{1} \ldots a_{n}}$. This string is in normal order with respect to the particle vacuum $|0\rangle$, i.e.

$$N \left( A_{b_{1} \ldots b_{n}}^{a_{1} \ldots a_{n}} \right) = A_{b_{1} \ldots b_{n}}^{a_{1} \ldots a_{n}},$$

where $N(\ldots)$ denotes the normal ordering with respect to $|0\rangle$.

In Eq. (2), the $n$-body matrix elements $\{ o_{a_{1} \ldots a_{n}}^{a_{1} \ldots a_{n}} \}$ constitute a mode-2n tensor denoted as $o^{(n)}$, i.e. a data array carrying 2n indices associated with the $n$ ($n$) particle creation (annihilation) operators they multiply. The $n$-body matrix elements are fully anti-symmetric under the exchange of any pair of upper or lower indices, i.e.

$$o_{b_{1} \ldots b_{n}}^{a_{1} \ldots a_{n}} = \epsilon(\sigma_{n}) \epsilon(\sigma_{1}) o_{a_{n} \ldots a_{1}}^{a_{1} \ldots a_{n}},$$

where $\epsilon(\sigma_{n}) (\epsilon(\sigma_{1}))$ refers to the signature of the permutation $\sigma_{n}(\ldots) (\sigma_{1}(\ldots))$ of the $n$ upper (lower) indices.

2.1.2 Density matrices

The $l$-body density matrix associated with a many-body state $|\Theta\rangle$ constitutes a mode-2l tensor defined through

$$\left[ \rho^{(l)} \right]_{a_{1} \ldots a_{l}}^{b_{1} \ldots b_{l}} = \frac{\langle \Theta | A_{b_{1} \ldots b_{l}}^{a_{1} \ldots a_{l}} | \Theta \rangle}{\langle \Theta | \Theta \rangle}. \quad (6)$$

In the following, the superscripts $l$ and $\Theta$ are omitted for $l = 1$ and when dealing with a generic density matrix, respectively. The elements of $\rho^{(l)}$ inherit from $A_{b_{1} \ldots b_{l}}^{a_{1} \ldots a_{l}}$ a full anti-symmetry under the exchange of any pair of upper or lower indices along with a hermitian character, i.e.

$$\left[ \rho^{(l)} \right]_{a_{1} \ldots a_{l}}^{b_{1} \ldots b_{l}} = \left( \left[ \rho^{(l)} \right]_{a_{1} \ldots a_{l}}^{b_{1} \ldots b_{l}} \right)^{*}. \quad (7)$$

Given two density matrices $\rho^{(l)}$ and $\rho^{(k)}$, their tensor product

$$\rho^{(l)} \otimes \rho^{(k)} \equiv \rho^{(l)} \otimes \rho^{(k)}$$

defines a direct-product $(l+k)$-body density matrix through the mode-2$(l+k)$ tensor whose elements are given by

$$\left[ \rho^{(l)} \otimes \rho^{(k)} \right]_{a_{1} \ldots a_{l+k}}^{b_{1} \ldots b_{l+k}} = \rho^{(l)}_{a_{1} \ldots a_{l}} \rho^{(k)}_{b_{1} \ldots b_{k}}, \quad (9)$$

and display the hermitian property characterized in Eq. (7). Because of the direct-product character of $\rho^{(l)} \otimes \rho^{(k)}$, its elements are only partially anti-symmetrized, i.e. they are anti-symmetric under the exchange of any pair of the first $l$ (or last $k$) upper or lower indices.

In case one considers the $m$-fold tensor product of the same $l$-body density matrix $\rho^{(l)}$, the notation can be further simplified according to $\rho^{(m)} \equiv \rho^{(l)} \otimes \ldots \otimes \rho^{(l)}$. In particular, the $m$-fold tensor product of the generic one-body density matrix $\rho$ defines a mode-2$m$ tensor whose elements are

$$\left[ \rho^{(m)} \right]_{a_{1} \ldots a_{m}}^{b_{1} \ldots b_{m}} = \rho_{a_{1}} \cdots \rho_{a_{m}}^{b_{1}} \cdots \rho_{b_{m}}^{b_{m}}. \quad (10)$$

Because of its pure direct-product character, the elements of $\rho^{(m)}$ display no property under the exchange of any pair of upper or lower indices but inherit the hermitian property characterized by Eq. (7).

2.1.3 Distance

In the following, the extent to which two one-body density matrices $\rho$ and $\rho'$ deviate from one another will need to be

4 Conventionally, Eq. (6) is consistently extended to $l = 0$ via $\rho^{(0)} \equiv 1$. 
characterized. The distance
\[ d(\rho, \rho') \equiv \|\rho - \rho'\|, \]  
provides such a diagnostic, with \(\|\cdot\|\) the Frobenius norm reading for an arbitrary mode-\(n\) tensor \(T\) as
\[ \|T\| \equiv \sqrt{\sum_{l_1 \ldots l_n} T_{l_1 \ldots l_n} T_{l_1 \ldots l_n}^*}, \]  
where the superscript denotes elementwise complex conjugation.

2.1.4 Convolution

The convolution of the mode-\(2n\) tensor \(\rho^{(n)}\) associated with a \(n\)-body operator \(O^{mn}\) with the mode-\(2m\) tensor \((m \leq n)\) defining a \(m\)-body density matrix \(\rho^{(m)}\) generates the mode-
\(2(n-m)\) tensor \(\rho^{(n)} \cdot \rho^{(m)}\) with elements
\[ \left[\rho^{(n)} \cdot \rho^{(m)}\right]_{a_1 \ldots a_{n-m}, b_1 \ldots b_{n-m}} \equiv \sum_{a_{n-m+1} \ldots a_n} \rho^{(m)}_{a_{n-m+1} \ldots a_n} \rho^{(n)}_{b_1 \ldots b_{n-m}, a_{n-m+1} \ldots a_n}, \]  
The tensor \(\rho^{(n)} \cdot \rho^{(m)}\) is obviously a pure number whenever \(m = n\) and nothing but the initial tensor \(\rho^{(n)}\) whenever \(m = 0\).

Given two density matrices \(\rho^{(l)\Theta}\) and \(\rho^{(k)\Psi}\), it is straightforward to check that the convolution is such that the following identity holds
\[ \left(\rho^{(n)} \cdot \rho^{(m)\Theta}\right) \cdot \rho^{(l)\Psi} = \left(\rho^{(n)} \cdot \rho^{(l)\Psi}\right) \cdot \rho^{(m)\Theta} = \rho^{(n)} \cdot \left(\rho^{(m)\Theta} \otimes \rho^{(l)\Psi}\right). \]  

2.2 Standard NOkB approximation

2.2.1 Wick’s theorem

Let us consider a symmetry-conserving product state \(|\Phi\rangle\), i.e. a \(J^\Pi = 0^+\) Slater determinant. Standard Wick’s theorem [5] with respect to \(|\Phi\rangle\) entails four elementary contractions
\[ c_{a^\dagger b^\dagger}^\dagger c_{a b} : = 0, \]  
\[ c_{a^\dagger b}^\dagger c_{a^\dagger b^\dagger} = \rho^{\Phi_{ab}}, \]  
\[ c_{a b}^\dagger c_{a^\dagger b^\dagger} = \delta_{ab} - \rho^{\Phi_{a}}, \]  
\[ c_{a b}^\dagger c_{a b} : = 0, \]  
where \(\ldots\) denotes the normal ordering with respect to \(|\Phi\rangle\).

Applying Wick’s theorem, the operator \(O\) defined in Eq. (1) is rewritten as
\[ O = \sum_{k=0}^{N} O_{kk}^{\rho\Phi}, \]  
where \(O_{kk}^{\rho\Phi}\) is a \(k\)-body operator in normal-ordered form with respect to \(|\Phi\rangle\)
\[ O_{kk}^{\rho\Phi} = \sum_{a_1 \ldots a_k} \rho_{a_1 \ldots a_k}^{\Phi} A_{b_1 \ldots b_k}^{a_1 \ldots a_k}. \]  
Considering \(O^{mn}\) \((n \leq N)\) and \(k \leq n\), there are
\[ (n-k)\left(\begin{array}{c} n \\ n-k \end{array}\right) \]  
ways to perform \((n-k)\) non-zero contractions. Consequently, the matrix elements of \(O_{kk}^{\rho\Phi}\) are related to those defining the original contributions to \(O\) through
\[ e_{b_1 \ldots b_k}^{a_1 \ldots a_k} \rho_{a_1 \ldots a_k}^{\Phi} = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[\rho_{a_1 \ldots a_k}^{\Phi} \phi^{(n-k)\Theta}\right]_{b_1 \ldots b_k}^{a_1 \ldots a_k}. \]  

2.2.2 Approximation

The normal-ordered \(k\)-body (NOkB) approximation \(O_{NOkB}^{\rho\Phi}\) to the operator \(O\) proceeds by truncating the sum in Eq. (16) to the desired maximum value \(k\). While the original operator is obviously independent of \(\rho^{\Phi}\), \(O_{NOkB}^{\rho\Phi}\) does acquire such a dependence as soon as \(k < N\).

For example, the standard NO2B approximation consists of ignoring beyond normal-ordered 2-body terms to define the approximate Hamiltonian as [1,2]
\[ H_{NOkB}^{\rho\Phi} \equiv H^{00}_{\rho\Phi} + H^{11}_{\rho\Phi} + H^{22}_{\rho\Phi}. \]  

Generalizing the approach to a \(U(1)\)-breaking product state, i.e. a Bogoliubov reference state, standard Wick’s theorem gives rise to non-zero anomalous contractions (Eqs. (15a) and (15d)) such that the truncation procedure generates a particle-number-breaking operator. A different truncation scheme was thus formulated to design a particle-number conserving normal-ordered \(k\)-body (PNOkB) approximation in Ref. [11]. A similar problem arises when using a SU(2) non-invariant Slater determinant, i.e. whenever \(|\Phi\rangle\) is not a \(J^\Pi = 0^+\) state. Indeed, the standard NOkB approximation delivers an operator that is not rotationally invariant in such a case. Rather than extending the tedious approach designed in Ref. [11] for the \(U(1)\) case, a novel method is proposed in Sect. 2.3 that avoids such complications from the
outset by involving the one-body density matrix stemming from a symmetry-conserving many-body state.

2.2.3 Approximate operator in standard form

Starting from Eq. (16), it is interesting to re-express the operator back into a normal-ordered form with respect to the particle vacuum (Eq. 2). Doing so requires to apply Wick’s theorem backward, i.e. with respect to the particle vacuum. To do so, the only required non-zero contraction is given by

\[ (c^a \cdots c^b) :=-N((c^a \cdots c^b) :)=:c^a \cdots c^b =-\rho^b_a, \]  

which is nothing but the opposite of the elementary contraction at play in the first step. The original n-body part of \( O \) is obtained back in terms of the various contributions entering Eq. (16) such that the connection between their matrix elements is given by

\[ o_{b_1 \ldots b_n}^{a_1 \ldots a_n} = \sum_{l=n}^{N} (-1)^{l-n} \frac{1}{(l-n)!} \left[ o^{(l)}(\rho) \cdot \rho^{\otimes(l-n)} \right]_{b_1 \ldots b_n}^{a_1 \ldots a_n}, \]  

Truncating Eq. (16) according to the NOkB approximation and inserting the result into Eq. (22) delivers the matrix elements of the approximate n-body part of \( O \) in normal order with respect to the particle vacuum.

2.3 Generalized k-body approximation

The standard NOkB approximation relies on standard Wick’s theorem and is thus strictly defined with respect to a symmetry-conserving many-body state. Because this restriction is too severe in open-shell systems, a generalization of the procedure is now envisioned such that the involved one-body density matrix can originate from a more general many-body state.

2.3.1 Two-step procedure

Given the operator \( O \) and the one-body density matrix \( \rho \) associated with an arbitrary \( J^\Pi = 0^+ \) state, one first defines the set of anti-symmetrized matrix elements

\[ o_{b_1 \ldots b_n}^{a_1 \ldots a_k} (\rho) \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[ o^{(n)}(\rho) \cdot \rho^{\otimes(n-k)} \right]_{b_1 \ldots b_n}^{a_1 \ldots a_k}, \]  

in strict analogy with Eq. (19) but relaxing the necessity for the density matrix to originate from a Slater determinant.\(^6\)

The key point of the present development relates to the fact that, independently of the nature of \( \rho \), the inverse operation embodied by Eq. (22) remains valid in the present context and recovers the original operator’s matrix elements, i.e.

\[ o_{b_1 \ldots b_n}^{a_1 \ldots a_n} = \sum_{l=n}^{N} (-1)^{l-n} \frac{1}{(l-n)!} \left[ o^{(l)}(\rho) \cdot \rho^{\otimes(l-n)} \right]_{b_1 \ldots b_n}^{a_1 \ldots a_n}. \]  

This identity is proven in Appendix A. One can thus conclude that the combined operations embodied by Eqs. (19) and (22) are actually valid outside the reach of standard Wick’s theorem. Indeed, the two steps are utterly general operations, i.e. tensor products that are inverse from one another, holding independently of the nature of \( \rho \) (i.e. whether it stems from a Slater determinant or not). Standard Wick’s theorem is recovered as a particular case of the general tensor identities (23)–(24), namely when the one-body density matrix does originate from a Slater determinant.

Thus, the purpose of Eqs. (23) and (24) is to start from the set of tensors defining each n-body contribution to the original operator \( O \) in Eqs. (1)–(2) and to recover it after having gone through an intermediate set defined in strict analogy with the tensors generated via the single-reference normal ordering. While there is no benefit in applying the two-step procedure per se, it ensures that the original operator is exactly recovered when doing so. Based on this property, the method provides a useful way to produce nucleus-dependent approximations to the operator through the truncation of the intermediate set of tensors.

2.3.2 Approximation

In close analogy with the NOkB approximation, the k-body approximation of \( O \) is now introduced. First, the set of tensors defined through Eq. (23) is truncated according to

\[ \tilde{o}^{(l)}(\rho) \equiv o^{(l)}(\rho) \text{ for } l \leq k, \]  
\[ \tilde{o}^{(l)}(\rho) \equiv 0 \text{ for } l > k. \]  

Second, inserting Eq. (25) into Eq. (24) generates the set of tensors \( \tilde{o}^{(n)}(\rho) \) defining the k-body approximation of \( O \) in normal order with respect to the particle vacuum according to

\[ O^{kB}(\rho) \equiv \sum_{n=0}^{k} \tilde{o}^{(n)}(\rho), \]  

where the truncation of the sum naturally derives from Eq. (25). While the original operator \( O \) is independent of ordering involving the sole one-body density matrix. In this context, it becomes possible to associate an actual quasi-normal-ordered operator to the tensor \( \tilde{o}^{(k)}(\rho) \). However, given that such a quasi-normal-ordered operator is of no use in the present context, there is no need to invoke it.

\(^6\) The matrix elements introduced in Eq. (23) are not obtained through a set of algebraic operations on the original operator but via a straight convolution of tensors. Still, the present procedure could be formulated within the frame of the quasi-normal ordering of Ref. [21], which is itself an extension of Kutzelnigg and Mukherjee’s universal normal-
\( \rho, O^{kB}[\rho] \) does acquire such a dependence as a result of the truncation characterized by Eq. (25).

While \( O^{kB} \) can be built on the basis of an arbitrarily correlated (symmetry-conserving) state, it does not require the use of \( \rho^{(l)} \) with \( l > 1 \). As a result, the procedure is significantly simpler than the one associated with the application of Kutzelnigg-Mukherjee’s Wick theorem or the one at play in SCGF theory. The practicality of the approach also relates to the fact that the effective Hamiltonian is expressed in normal-ordered form with respect to the particle vacuum, i.e.,

\[ H^{\text{NO2B}} \]

\[ H^{\text{NO2B}} = \hat{\tilde{H}}^{(0)}[\rho] + \frac{1}{(1)^2} \sum_{a_1 b_1} \hat{\tilde{h}}_{a_1 b_1}^{(0)}[\rho] A_{a_1 b_1}^{(1)} + \frac{1}{(2)^2} \sum_{a_1 a_2 b_1 b_2} \hat{\tilde{h}}_{a_1 a_2 b_1 b_2}^{(1)}[\rho] A_{a_1 a_2 b_1 b_2}^{(2)} \cdot \cdot \cdot \]

where \( t_{b_1}^{a_1} \) denotes matrix elements of the kinetic energy whereas \( v_{b_1 b_2}^{a_1 a_2} \) and \( w_{b_1 b_2 b_3}^{a_1 a_2 a_3} \) denote anti-symmetric matrix elements of two- and three-body interactions, respectively.

Setting

\[ O^{00} \rightarrow 0, \]
\[ O^{11} \rightarrow T, \]
\[ O^{22} \rightarrow V, \]
\[ O^{33} \rightarrow W, \]

Eq. (25) gives for \( k = 2 \)

\[ \hat{\tilde{h}}_{a_1 b_1}^{(0)}[\rho] \equiv t^{(1)} \cdot \rho + \frac{1}{2!} v^{(2)} \cdot \rho^{(2)} + \frac{1}{3!} w^{(3)} \cdot \rho^{(3)}, \]
\[ \hat{\tilde{h}}_{a_1 a_2 b_1 b_2}^{(1)}[\rho] \equiv t^{(1)} \cdot v^{(2)} \cdot \rho + \frac{1}{2!} w^{(3)} \cdot \rho^{(2)}, \]
\[ \hat{\tilde{h}}_{a_1 a_2 a_3 b_1 b_2 b_3}^{(2)}[\rho] \equiv v^{(2)} \cdot w^{(3)} \cdot \rho, \]
\[ \hat{\tilde{h}}_{a_1 a_2 a_3 b_1 b_2 b_3}^{(3)}[\rho] \equiv 0. \]

Except for the key fact that \( \rho \) does not necessarily relate to a Slater determinant, Eq. (28) is formally identical to Eq. (20) defining \( H^{\text{NO2B}} \). Inserting Eq. (28) into Eq. (24), one eventually obtains the three tensors

\[ \hat{\tilde{h}}_{a_1 b_1}^{(0)}[\rho] \equiv \frac{1}{3!} w^{(3)} \cdot \rho^{(3)}, \]
\[ \hat{\tilde{h}}_{a_1 a_2 b_1 b_2}^{(1)}[\rho] \equiv t^{(1)} + \frac{1}{2!} w^{(3)} \cdot \rho^{(2)}, \]
\[ \hat{\tilde{h}}_{a_1 a_2 a_3 b_1 b_2 b_3}^{(2)}[\rho] \equiv v^{(2)} + w^{(3)} \cdot \rho, \]
\[ \hat{\tilde{h}}_{a_1 a_2 a_3 b_1 b_2 b_3}^{(3)}[\rho] \equiv 0. \]

In addition to the fact that, by construction, \( H^{\text{NO2B}}[\rho] \) does not contain a three-body operator, its structure differs from the original operator expressed in normal order with respect to the particle vacuum (Eq. (27)) by the fact that it incorporates the pure number \( \hat{\tilde{n}}^{(0)}[\rho] \).

### 3 Many-body methods and one-body density matrices

Equation (29) define a set of nucleus-dependent 0-, 1- and 2-body operators entering \( H^{\text{NO2B}}[\rho] \). As in the NO2B approximation, the inclusion of a large part of \( W \) into these effective operators, while treating \( T \) and \( V \) exactly, gives a clear argument that omitting \( h^{(3)}[\rho] \) leads to small, hopefully small enough, errors. Still, one is left with the question of the optimal character of the one-body density matrix to be employed for a given system and many-body approximation.

In the hypothesis that exact eigenstates of \( H \) in the \( A \)-body Hilbert space \( \mathcal{H}_A \) are known, one may expect that employing the one-body density matrix of the exact ground-state is optimal to reproduce the ground-state energy. In fact, this intuition is not correct.

From a formal viewpoint, it would be interesting to find the optimal one-body density matrix to be used in \( H^{\text{NO2B}}[\rho] \) to best reproduce, e.g., the energy associated with the (approximate) ground state \( |\Psi\rangle \) of the full Hamiltonian \( H \). This would

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however not be of practical use. Consequently, the numerical results displayed in Sect. 4 rely on testing a set of trial one-body density matrices while obtaining the solution to the A-body problem via various approximation methods. As will be concluded, the results are very robust with respect to the employed one-body density matrix as long as the latter respects a minimal set of properties.

3.1 Many-body methods

The many-body methods presently used to solve the A-body Schrödinger equation for a collection of doubly closed, singly open-shell and doubly open-shell even-even nuclei (to be specified later on) are

1. axially deformed Hartree-Fock-Bogoliubov (dHFB) theory [13,22],
2. the particle-number- and angular-momentum-projected HFB (PHFB) method [13,22,23] based on dHFB states,
3. the projected generator coordinate method (PGCM) [13,22] mixing PHFB states along the axial quadrupole moment of the underlying dHFB states,
4. quasi-particle random phase approximation for axially deformed and superfluid nuclei (dQRPA) in the finite amplitude method (FAM) formulation [24,25],
5. deformed Bogoliubov many-body perturbation theory at third order (dBMBPT(3)) [13,26–28].

Deformed HFB theory constitutes the mean-field baseline that can capture the bulk of static correlations in open-shell nuclei through the spontaneous breaking of U(1) and SU(2) symmetries. Based on it, PHFB, PGCM and dQRPA on the one hand and dBMBPT on the other hand, provide systematic beyond-mean-field extensions whose aim is to capture many-body correlations. While PHFB, PGCM and dQRPA do so via the addition of static correlations associated with the restoration of broken symmetries and the fluctuation of shapes, dBMBPT targets dynamical correlations through the resummation of elementary, i.e. quasi-particle, excitations. Former approaches access collective excited states whereas the latter naturally addresses absolute binding energies and associated ground-state observables.

The string of dHFB, PHFB, PGCM and dQRPA calculations can presently be performed with the full inclusion of three-body forces, i.e. employing a realistic nuclear Hamiltonian \( H \) without any form of approximation. Such ab initio calculations are the first of their kind [13,25] and allow us to benchmark the approximation of \( H \) by \( H^{2B}[\rho] \) on the basis of non-trivial many-body methods11. While it can be envisioned to do so in the future [27], BMBPT is however not implemented yet with full three-body interactions. Deformed BMBPT calculations are thus presently performed with \( H^{2B}[\rho] \) for various approximations to \( \rho \) and compared to those done earlier [9,10] on the basis of the PNO2B approximation [11].

3.2 Trial one-body density matrices

Employing the many-body schemes introduced above, the goal is to approximate \( H \) by \( H^{2B}[\rho] \) with \( \rho \) computed from various \( J^H = 0^+ \) trial states12, i.e.

1. spherical harmonic oscillator Slater determinant \( \rho^{sHOSD} \),
2. spherical HF(B) state \( \rho^{sHF(B)} \),
3. PHFB state \( \rho^{PHFB} \),
4. PGCM ground-state \( \rho^{PGCM} \),
5. standard spherical MBPT14 ground-state \( \rho^{sMBPT} \).

In the numerical results discussed in Sect. 4, \( \rho^{sHF(B)} \), \( \rho^{PHFB} \) and \( \rho^{PGCM} \) are extracted from the corresponding calculations performed with the full \( H \). Contrarily, \( \rho^{sMBPT} \) is obtained

9 Where BMBPT has already been applied quite systematically to semi-magic spherical nuclei [9,10], it is the first time it is performed on top of a deformed Boboliubov state [13] in view of describing doubly open-shell nuclei.

10 While helpful to discuss the performance of a many-body method, the distinction between dynamical and static correlation effects involves a fuzzy boundary, prominently displayed in the dQRPA case. Namely, the dQRPA equations can be derived within different frames, e.g. as a harmonic limit of the GCM equations [29] or via the linearization of time-dependent HFB equations [30,31]. Depending on these viewpoints, dQRPA either falls in the category of post-HFB extensions grasping static correlations (associated with fluctuation of shapes), or in the category of beyond-mean-field approaches aiming at capturing dynamical correlations (in terms of 2-quasi-particle excitations). In the present work, we make the arbitrary choice to categorize dQRPA among the former class of approaches.

11 PHFB and PGCM calculations based on realistic chiral Hamiltonians have been performed recently for the first time but at the price of approximating three-body operators [15,32]. The exact treatment of \( W \) in realistic PGCM calculations typically increases the CPU time by three orders of magnitude compared to using \( H^{2B}[\rho] \) [13].

12 Because correlations captured by QRPA do not feedback into the ground-state, there is no non-trivial one-body density matrix \( \rho^{sQRPA} \) associated with the spherical QRPA solution to be used in the construction of \( H^{2B}[\rho] \).

13 In open-shell nuclei, the invariant density matrix is obtained via the use of the equal filling approximation. This approach can be justified on the basis of a specific statistical mixture of sHO Slater determinants carrying the appropriate number of particles [19] or on the basis of a specific linear combination of sHO Slater determinants carrying different number of particles such that the linear combination has the correct number of particles on average [33].

14 Standard spherical MBPT denotes many-body perturbation theory based on a spherical Slater determinant reference state rather than on a particle-number-breaking Boboliubov reference state. The former is automatically obtained from the latter in closed-shell nuclei where the dHFB reference state reduces to the spherical HF Slater determinant.
from a calculation performed with the PNO2B approximation whereas $\rho^{\text{HOSD}}$ does not require any a priori calculation.

The two options $\rho^{\text{HFB}}$ and $\rho^{\text{BMBPT}}$ originate from symmetry-restricted HFB and BMBPT calculations, i.e. spherical HFB ensures the $J^{\Pi} = 0^+$ character of the state whereas standard spherical MBPT ensures particle-number conservation\(^{15}\). In the latter case, the restriction implies that the use of $\rho^{\text{SMBPT}}$ is limited to doubly closed-shell nuclei.

While the expression of $\rho^{\text{HFB(B)}}$ is textbook material [22], it is not the case for $\rho^{\text{PHFB}}$ and $\rho^{\text{PGCM}}$. Consequently, the derivation of the corresponding expressions are provided in Appendix B. For the sake of generality and future use [13], the derivation is actually performed for a more general quantity than presently needed, i.e. Appendix B provides the expressions for the transition one-body density matrix between two arbitrary initial $(J_i^{\Pi_i})$ and final $(J_f^{\Pi_f})$ PGCM states. The result of present interest is then obtained by setting $J_i^{\Pi_i} = J_f^{\Pi_f} = 0^+$. While the expression for $\rho^{\text{SMBPT}}$ is known material [34,35], the expression of $\rho^{\text{BMBPT}}$ it presently derives from is not. Consequently, the derivation of $\rho^{\text{BMBPT}}$ is provided in Appendix C for the sake of completeness and future use.

### 4 Results

#### 4.1 Studied nuclei

A set of properties (i.e. binding energies, matter radii, low-lying spectra as well as electromagnetic properties) are computed for a panel of representative nuclei using the many-body methods and the one-body density matrices introduced in Sect. 3. The panel ranges from light to medium-mass nuclei and contains

1. doubly closed-shell ($^{16}\text{O}$, $^{40}\text{Ca}$),
2. singly open-shell ($^{18}\text{O}$),
3. doubly open-shell ($^{20}\text{Ne}$, $^{30}\text{Ne}$, $^{24,40}\text{Mg}$, $^{42,48}\text{Ar}$),

systems. The goal is to cover oblate, spherical and prolate representatives among which some nuclei are soft and others are hard with respect to axial deformation\(^{16}\).

\(^{15}\) While it is not a problem to compute $\rho$ from a particle-number-breaking state carrying the correct particle number on average as in shFB, it happens that ensuring the correct average particle-number requires a non-trivial procedure in BMBPT beyond HFB [28]. For simplicity, we thus presently limit ourselves to nuclei for which dBMBPT automatically reduces to standard spherical MBPT.

\(^{16}\) Some of these nuclei, e.g. $^{24}\text{Mg}$, display a triaxial minimum if allowed to. Still, present calculations are restricted to axial symmetry.

#### 4.2 Numerical setting

The numerical solver allowing us to perform dHFB, PHFB, PGCM, dQRPA and dBMBPT calculations based on full two- and three-nucleon interactions will be detailed in two forthcoming publications [13,25]. For the present purpose, it is sufficient to specify that the one-body spherical harmonic oscillator basis is employed. The finite number of oscillator shells is set by the parameter $e_{\text{max}}$ such that $2n + l \leq e_{\text{max}}$, where $n$ and $\ell$ denote the principal quantum number and the orbital angular momentum of a given shell, respectively. The value of the harmonic oscillator frequency $\hbar\omega$ is further needed to fully characterize the working basis. Except if specified otherwise, all calculations are presently performed with $e_{\text{max}} = 8$ and $\hbar\omega = 20$ MeV. While these values do not permit to generate fully converged calculations of all the nuclei listed above, the conclusions drawn at the end of the paper are independent of them.

When representing a $n$-body operator, the natural truncation of the tensor-product basis of the $n$-body Hilbert space is set by $e_{\text{max}}$ and $n e_{\text{max}}$. One and two-body operators are thus represented using $e_{\text{max}} = 8$ and $e_{\text{max}} = 2 e_{\text{max}}$, respectively. However, $e_{\text{max}} = 8$, $10$, $12$ ($\ll 3 e_{\text{max}}$) is used to represent the three-nucleon interaction given that employing $3 e_{\text{max}}$ is largely beyond today’s capacities.\(^{17}\) This truncation will play a key role regarding the quality of the approximation associated with $H^{2B}[\rho]$ in medium-mass and/or neutron-rich nuclei.

The chiral effective field theory Hamiltonian $H$ presently employed combines a two-nucleon interaction at next-to-next-to-leading order (N3LO) [37,38] with a N2LO three-nucleon interaction [39]. It is then evolved to a lower momentum scale $\lambda_{\text{SRG}}$ via SRG transformations. While by default results obtained for $\lambda_{\text{SRG}} = 1.88$ fm\(^{-1}\) are discussed, $\lambda_{\text{SRG}} = 2.23$ fm\(^{-1}\) will also be used for comparison.

#### 4.3 Ground-state binding energy

##### 4.3.1 Deformed HFB

Let us first discuss the use of $H^{2B}[\rho]$ at the mean-field, i.e. dHFB, level. Figure 1 displays the error (in %) of the corresponding dHFB ground-state energies compared to the reference values obtained from the full $H$. Results are provided for $\rho = \rho^{\text{HOSD}}$ ( ), $\rho^{\text{HFB}}$ ( ), $\rho^{\text{PHFB}}$ ( ) and $\rho^{\text{PGCM}}$ ( ● ), as well as for $\rho = \rho^{\text{SMBPT}}$ ( ● ) whenever applicable, i.e. in doubly closed-shell nuclei.

One first observes that $H^{2B}[\rho]$ perform well for the five test one-body density matrices although a notable degradation is visible for $\rho = \rho^{\text{HOSD}}$. As can be inferred from

\(^{17}\) The largest value employed so far in actual calculations is $e_{\text{max}} = 24$ [36].
Fig. 1 Error (in %) of dHFB ground-state energies obtained with $H^{2B}[\rho]$ for the various test one-body density matrices. The error corresponding to the use of $\rho^{\text{HOSD}}$ for $^{40}\text{Mg}$ amounts to 2.6% and lies outside the figure. Calculations are performed with $e_{\text{max}} = 8$, $e_{3\text{max}} = 12$ and $\lambda_{\text{srg}} = 1.88$ fm$^{-1}$.

Table 1, the weaker performance of $\rho = \rho^{\text{HOSD}}$ is systematic but especially pronounced as the mass and/or the isospin-asymmetry of the system increases. While the same trend is at play for $\rho^{\text{sHF(B)}}$, $\rho^{\text{PHFB}}$ and $\rho^{\text{PGCM}}$, the error systematically remains below 0.2% for these three density matrices, with the exception of $^{40}\text{Mg}$ whose error lies around 0.7%. For $\rho^{\text{HOSD}}$, the average error over the set is significantly larger (1.2%) throughout the panel and peaks at about 2.6% in $^{40}\text{Mg}$ (not shown in the figure).

From a general standpoint, it is not surprising that the error due to the use of $H^{2B}[\rho]$ is small at the mean-field level. To best appreciate this feature, let us focus on doubly closed-shell $^{16}\text{O}$ and $^{40}\text{Ca}$ for which dHFB reduces to sHF. As shown in Table 1, the error is below 0.05% in these two nuclei for all test one-body density matrices but $\rho^{\text{HOSD}}$. As explained in Appendix E, the error would even be strictly zero in such a situation if $\rho$ were equated to the variational sHF one-body density matrix throughout the sHF iterations based on $H^{2B}[\rho]$. This procedure would be equivalent to working within the NO2B approximation, which is indeed exact at the sHF level, i.e. the NO2B approximation of the Hamiltonian only impacts post-sHF methods by construction. The fact that one rather takes $\rho$ to be a fixed, e.g. $\rho^{\text{HFB}}$ obtained from the full $H$, a priori determined one-body density matrix to build $H^{2B}[\rho]$ induces a marginal error in sHF calculations.

While the error remains below 0.05% in $^{16}\text{O}$ and $^{40}\text{Ca}$ for appropriate density matrices, the distinctly worse result obtained in $^{40}\text{Ca}$ for $\rho = \rho^{\text{HOSD}}$ underlines the fact that obtaining a very accurate description is not automatic even in this optimal situation, i.e. it is crucial that the test density matrix contains relevant physical information. Having said that, the results obtained with the other four test density matrices are so similar that no clear characteristic can be easily identified as far as the optimal choice is concerned. Neither the consistency with the employed many-body method nor the degree of correlations encoded in the one-body density matrix seem to constitute a decisive feature. For example, $\rho^{\text{sHFB}}$ performs as well as the more advanced $\rho^{\text{sMBPT}}$ that incorporates dynamical correlations beyond the mean field, as can be seen in Table 1. We will come back repeatedly to this question throughout the following sections.

While spherical doubly closed-shell nuclei are particularly amenable to a very accurate description, it is pertinent to investigate the dependence of the approximation on the axial quadrupole deformation of the HFB state. All nuclei in the set but $^{16,18}\text{O}$ and $^{40}\text{Ca}$ are doubly open-shell systems and thus spontaneously break rotational symmetry at the dHFB

Fig. 2 Upper panel: dHFB total energy curve of $^{20}\text{Ne}$ as a function of the axial quadrupole deformation computed with the full $H$. Lower panel: Error (in %) in the total energy curve when using $H^{2B}[\rho]$ with the various test one-body density matrices. Calculations are performed with $e_{\text{max}} = 8$, $e_{3\text{max}} = 10$ and $\lambda_{\text{srg}} = 1.88$ fm$^{-1}$.
Table 1 Average difference (in %) between ground-state dHFB energies computed with $H^{2B}[\rho]$ and $H$ for different sub-categories in the test panel and the various test one-body density matrices. The neutron-rich subcategory encompasses $^{30}$Ne, $^{40}$Mg and $^{48}$Ar. See Eq. (81a) for the definition of the cost function. Calculations are performed with $\varepsilon_{\text{max}} = 8, \varepsilon_{3\text{max}} = 12$ and $\lambda_{\text{arg}} = 1.88$ fm$^{-1}$.

|                | Closed shell | Open shell | Mass ≤ 30 | Mass > 30 | Neutron-rich | All   |
|----------------|--------------|------------|-----------|-----------|-------------|-------|
| $\rho_{\text{HOSD}}$ | 0.67         | 1.32       | 0.71      | 1.76      | 2.04        | 1.18  |
| $\rho_{\text{HFB}}$   | 0.04         | 0.20       | 0.10      | 0.25      | 0.29        | 0.17  |
| $\rho_{\text{PHFB}}$  | 0.04         | 0.21       | 0.09      | 0.28      | 0.33        | 0.17  |
| $\rho_{\text{PGCM}}$  | 0.05         | 0.23       | 0.09      | 0.30      | 0.37        | 0.18  |
| $\rho_{\text{MBPT}}$  | 0.04         |            |           |           |             |       |

level, $^{20}$Ne and $^{24}$Mg displaying the largest deformation of all.

The upper panel of Fig. 2 displays the dHFB total energy curve (TEC) calculated in $^{20}$Ne from the full $H$ as a function of the axial quadrupole deformation $\beta_{20}$. This nucleus is significantly deformed, the minimum of the TEC being located at $\beta_{20} = 0.45$. As visible from the lower panel, the error induced by $H^{2B}[\rho]$ is essentially zero at sphericity, except for $\rho = \rho_{\text{HOSD}}$ where it is equal to 0.3%, and grows only mildly with the deformation. The error remains below 1% up to a large deformation of $\beta_{20} = 0.8$ ($\beta_{20} = -0.4$) on the prolate (oblate) side for $\rho = \rho_{\text{HFB}}, \rho_{\text{PHFB}}$ or $\rho_{\text{PGCM}}$. For $\rho = \rho_{\text{HOSD}}$, the error is about twice as large along the TEC.

There exists a trend along the TEC, the results obtained with $\rho_{\text{HFB}}$ degrading slightly faster with the deformation than those obtained with $\rho_{\text{PGCM}}$ and $\rho_{\text{PHFB}}$. The trend is however not quantitatively significant as can be inferred from the systematic error over open-shell nuclei provided in Table 1. Eventually, it is remarkable that all three one-body density matrices give excellent and essentially equivalent results up to large deformations, especially given the fact that $\rho_{\text{HFB}}$ does not encode any information about deformation properties of $^{20}$Ne. This is a first indication of the robustness of the in-medium 2-body reduction method of 3-body interaction operators.

For orientation, it is interesting to analyze how the various components of $H^{2B}[\rho]$ (Eqs. 29–30) and $H$ (Eq. 27) contribute to the dHFB energy. Figure 3 decomposes the dHFB total energy accordingly in $^{16}$O and $^{20}$Ne. Results are provided for a schematic model space and $\rho = \rho_{\text{HFB}}$. Focusing first on $^{16}$O and making the hypothesis that the sHF density matrix is the same in both calculations, the inspection of Eq. (29) makes clear that (a) the 0-body part of $H^{2B}[\rho]$ is strictly equal to the sHF contribution originating from the three-body interaction in $H$ and that (b) the energy contribution associated with the 1- and 2-body parts of $H^{2B}[\rho]$
originating from the three-body interaction exactly cancel out. These features are indeed observed in the upper panel of Fig. 3 such that the total sHF energies are identical in both calculations. While this formal analysis does not hold for dHFB in general, the results displayed in the lower panel demonstrate that it remains valid in practice in a well-deformed nucleus such as $^{20}\text{Ne}$, which eventually elucidates the high-quality results obtained above over a large set of nuclei.

4.3.2 Deformed BMBPT

While it is satisfying that the error induced by $H^{2B}[\rho]$ is negligible at the mean-field, i.e. dHFB, level, it is to some extent expected and surely not sufficient to claim victory. The performance of $H^{2B}[\rho]$ must thus be tested in beyond mean-field methods where the accurate compensation observed above between the terms of $H$ and those of $H^{2B}[\rho]$ is not guaranteed to hold.

While such a test must be carried out for various ab initio methods, the present section focuses on ground-state energies obtained from dMBBPT that resums dynamical correlations in a perturbative fashion on top of a (possibly deformed and superfluid) HFB state. Present calculations are performed at the BMBPT(3) level that is known to reproduce essentially exact results based on SRG-evolved interactions to better than 2% in oxygen isotopes and those computed from non-perturbative expansion methods to better than 2% in semimagic nuclei up to the nickel region [9,10].

Although envisioned in the future, BMBPT calculations with explicit three-nucleon forces are not available yet. Consequently, calculations with $H^{2B}[\rho]$ are presently benchmarked against those obtained using the PNO2B approximation [11], which is the approximation employed so far in all published BMBPT calculations of semi-magic nuclei [9,10]. In doubly closed-shell nuclei, the PNO2B approximation reduces to NO2B that has itself being benchmarked against the use of full three-body interactions and shown to offer a typical 1 − 2% accuracy up to $^{16}\text{O}$ [1].

Deformed BMBPT(3) binding energy differences (in %) are displayed in Fig. 4. Results produced within both approximations agree to better than 0.3% over the whole set of considered nuclei, except for $\rho = \rho^{\text{HOSD}}$ where the difference increases up to 2%. Just as for the dHFB results discussed above, the use of a one-body density matrix encoding either static or dynamical correlations beyond the mean-field does not have a significant impact on the quality of $H^{2B}[\rho]$ such that the results are essentially equivalent to those obtained with $\rho = \rho^{\text{HFB(B)}}$. This can be confirmed quantitatively by inspecting the numbers reported in Table 2. Interestingly, the results also show that the average deviation is independent of the closed- or open-shell character of the nuclei under consideration whereas it slightly increases with the mass even though the deviation remains tiny in all cases.

These remarkable results indicate that the in-medium interaction and PNO2B approximation methods are equivalent as far as quantitative ab initio dMBBPT calculations of mid-mass nuclei are concerned. Given the earlier benchmarking of the NO2B in doubly-closed shell nuclei, the presently developed in-medium approximation method is well validated in fully-correlated binding energy calculations.

4.4 PHFB absolute energies and radii

In the following, we wish to go beyond ground-state energies and test the in-medium approximation method on spectroscopic properties. In order to do so, PHFB, PGC and dQRP calculations will be employed. While these techniques resum static correlations associated with the restoration of broken symmetries and the fluctuation of shapes, they do not account for dynamical correlations. As a result, whereas relative energies and spectroscopic quantities can be well converged and meaningful, absolute energies are not realistic, i.e. they are far from converged ab initio values. Still, it is useful to first investigate how these absolute energies differ when computed from $H$ and $H^{2B}[\rho]$.

In this section we thus analyse total (ground- and excited-state) energies obtained at the PHFB level. In addition, corresponding ground-state matter radii are presented. In doing so, the dependence of the results on numerical parameters such as $e_{3\text{max}}$, $e_{\text{max}}$ and $\lambda_{\text{stg}}$ is also investigated.
Table 2  Average difference (in %) of ground-state dBMBPT(3) energies obtained with $H^{2B}[\rho]$ and within the PNO2B approximation of $H$ for different sub-categories in the test panel and the various test one-body density matrices. The neutron-rich subcategory encompasses $^{30}$Ne, $^{40}$Mg and $^{48}$Ar. See Eq. (81c) for details on the cost function. Calculations are performed with $e_{\text{max}}=8$, $e_{3\text{max}}=12$ and $\lambda_{\text{arg}}=1.88$ fm$^{-1}$

|                  | Closed shell | Open shell | Mass $\leq 30$ | Mass $> 30$ | Neutron-rich | All      |
|------------------|--------------|------------|---------------|-------------|-------------|----------|
| $\rho^{\text{HOSD}}$ | 0.69         | 1.1        | 1.00          | 1.03        | 1.37        | 1.01     |
| $\rho^{\text{HFB(B)}}$ | 0.16         | 0.14       | 0.09          | 0.21        | 0.16        | 0.14     |
| $\rho^{\text{PHFB}}$     | 0.18         | 0.14       | 0.10          | 0.21        | 0.19        | 0.15     |
| $\rho^{\text{PGCM}}$     | 0.13         | 0.13       | 0.06          | 0.21        | 0.13        | 0.13     |
| $\rho^{\text{MBPT}}$     | 0.19         |            |               |             |             |          |

Fig. 5 Results of PHFB calculations with $H$ and $H^{2B}[\rho]$ for several test one-body density matrices $\rho$. Left and right panels display results obtained for $e_{3\text{max}}=8$ and 12, respectively, at fixed $e_{\text{max}}=8$. Upper panel: absolute energies of lowest $J^\Pi=0^+,2^+,4^+$ states to which the dHFB energy obtained from $H$ in each nucleus is subtracted. Lower panel: ground-state root-mean-square matter radii. Calculations are performed with $\lambda_{\text{arg}}=1.88$ fm$^{-1}$

4.4.1 Systematic analysis

Upper panels of Fig. 5 display binding energies of the lowest-lying $J^\Pi=0^+,2^+,4^+$ states obtained via PHFB calculations with $e_{3\text{max}}=8$ and 12 (at fixed $e_{\text{max}}=8$). The energy of each state obtained from $H$ (-----) is compared to those generated from $H^{2B}[\rho]$ with $\rho=\rho^{\text{HOSD}}$ (▲), $\rho^{\text{HFB(B)}}$ (●), $\rho^{\text{PHFB}}$ (×) and $\rho^{\text{PGCM}}$ (○), as well as with $\rho=\rho^{\text{MBPT}}$ (★) whenever applicable. Energies are shifted by the dHFB value obtained from the full $H$ for the corresponding system such that all nuclei can be displayed on the same figure.

Reference energies are well reproduced in light nuclei for all test one-body density matrices and both values of $e_{3\text{max}}$, i.e. absolute deviations remain below 1 MeV until $^{24}$Mg.
Increasing the mass and/or isospin asymmetry renders the approximation more and more sensitive to the value of $\epsilon_{3\text{max}}$. Given that ab initio calculations are known to be increasingly more sensitive to $\epsilon_{3\text{max}}$ with the mass and isospin-asymmetry of the system [40], it is not surprising that any approximation of the three-nucleon displays the same feature. Going from $\epsilon_{3\text{max}} = 8$, through $\epsilon_{3\text{max}} = 10$ (not shown) and to $\epsilon_{3\text{max}} = 12$, a clear convergence of the results is observed, although not quite yet for the heaviest and most neutron-rich nuclei of the panel. Eventually, converged results display a similar error in medium-mass nuclei to the one obtained in lighter systems, except for $\rho = \rho^{\text{HOSD}}$. Below, only results obtained for the largest reachable value of $\epsilon_{3\text{max}}$ (typically 12 but not always) are shown.

The lowest panels of Fig. 5 display ground-state root-mean-square matter radii (results are similar for excited-states radii). The conclusions are the same as for the energies. Eventually, radii are extremely well reproduced for all nuclei, states and test density matrices, with the exception of $\rho = \rho^{\text{HOSD}}$ for which a slight underestimation is visible in the heaviest systems.

Focusing on the right panels of Fig. 5, one does notice that the situation regarding the performance of the test one-body density matrices is qualitatively and quantitatively similar to the one encountered in dHFB and dBMBPT(3) calculations. As soon as the results are converged with respect to $\epsilon_{3\text{max}}$, PHFB energies and radii obtained with $H^{2B}[\rho]$ reproduce the reference results equally well with all employed one-body density matrices but $\rho^{\text{HOSD}}$, i.e. it seems necessary (compared to $\rho^{\text{HOSD}}$) and sufficient (compared to $\rho^{\text{PHFB}}$, $\rho^{\text{PGCM}}$ and $\rho^{\text{MBPT}}$) to employ a test one-body density matrix encoding the information of the spherical mean-field, i.e. $\rho^{\text{sHF(B)}}$.

The above analysis is put in more quantitative terms via the computation of systematic errors. Corresponding results are shown in Table 3. By construction, PHFB results are identical to sHF ones in doubly closed-shell nuclei given that the sole $0^+$ ground-state has been considered for these nuclei and given that the projections on particular number and angular momentum are superfluous for a sHF state. In the other nuclei where the projections typically add few MeV of correlations energy to the ground state, the average error over $J^H = 0^+, 2^+, 4^+, 6^+$ PHFB states is essentially the same as for dHFB ground-state energies, independently of the test one-body density matrix.

4.4.2 Dependence on $\epsilon_{\text{max}}$

Figure 6 probes the dependence of the results on the value of $\epsilon_{\text{max}}$ at fixed $\epsilon_{3\text{max}}$. First, one notices that radii are insensitive to $\epsilon_{\text{max}}$ and are perfectly reproduced. Second, no change is visible in the PHFB energies of $^{20}\text{Ne}$ when going from $\epsilon_{\text{max}} = 8$ to $\epsilon_{\text{max}} = 10$. In the more neutron-rich $^{30}\text{Ne}$ isotope, there exists a slight change of approximate PHFB energies. While the agreement with the reference results are still quantitatively good, the energies degrade slightly when going from $\epsilon_{\text{max}} = 8$ to $\epsilon_{\text{max}} = 10$. The slight evolution away from the reference results relates in fact to the lack of convergence of the results with respect to $\epsilon_{3\text{max}}$ discussed earlier. In the present case, $\epsilon_{3\text{max}}$ had to be set to 10 in order to be able to perform PHFB calculations with the explicit 3-body interaction at $\epsilon_{3\text{max}} = 10$.

While pushing the calculations to large values of $\epsilon_{3\text{max}}$ would probably improve the agreement further, the overall conclusion is that the high quality of $H^{2B}[\rho]$ depends only mildly on $\epsilon_{\text{max}}$ as long as the reference calculations themselves are converged enough. Although not shown, the same convergence behavior as a function of $\epsilon_{\text{max}}$ is at play in the BMBPT(3) ground-state energies reported on in Sect. 4.3.2.

4.4.3 Dependence on $\lambda_{\text{srg}}$

Figure 7 probes the dependence of the results on the smoothness of the Hamiltonian. The SRG Hamiltonian at $\lambda_{\text{srg}} = 2.23$ fm$^{-1}$ is less evolved than the one at $\lambda_{\text{srg}} = 1.88$ fm$^{-1}$ and produces spectra that are slightly less compressed. Still,
Table 3  Average error (in %) on absolute PHFB energies of low-lying $J^\pi = 0^+, 2^+, 4^+$ and $6^+$ states for different sub-categories in the test panel and the various test one-body density matrices. Calculations are performed with $\epsilon_{3\text{max}} = 8$, $\epsilon_{3\text{max}} = 12$ and $\lambda_{\text{arg}} = 1.88\text{ fm}^{-1}$. See Eq. (81b) for details on the cost function.

|                    | Closed-shell | Open shell | Mass $\leq 30$ | Mass $> 30$ | Neutron-rich | All   |
|--------------------|--------------|------------|----------------|-------------|--------------|-------|
| $\rho^\text{HOSD}$| 0.67         | 1.36       | 0.62           | 1.68        | 2.34         | 1.09  |
| $\rho^\text{HF(B)}$| 0.04         | 0.22       | 0.13           | 0.24        | 0.30         | 0.17  |
| $\rho^\text{PHFB}$ | 0.04         | 0.22       | 0.10           | 0.27        | 0.34         | 0.17  |
| $\rho^\text{PGCM}$| 0.05         | 0.24       | 0.11           | 0.29        | 0.38         | 0.19  |
| $\rho^\text{MBPT}$ | 0.04         |            |                |             |              |       |

![Fig. 7](image_url)  
Same as Fig. 6 but for two values of the SRG parameter $\lambda_{\text{arg}}$. Calculations are performed with $\epsilon_{\text{max}} = 8$, $\epsilon_{3\text{max}} = 12$ and $\lambda_{\text{arg}} = 1.88\text{ fm}^{-1}$.

![Fig. 8](image_url)  
Low-lying PHFB excitation spectra of doubly open-shell nuclei. Reference results calculated from $H$ are compared to those computed from $H^{2B}[\rho]$ using the various one-body test density matrices. Calculations are performed with $\epsilon_{\text{max}} = 8$, $\epsilon_{3\text{max}} = 12$ and $\lambda_{\text{arg}} = 1.88\text{ fm}^{-1}$.

4.5 Spectroscopy

Having analyzed absolute PHFB energies and radii, we are now in position to investigate spectroscopic observables.

4.5.1 PHFB

Low-lying PHFB excitation spectra of doubly open-shell nuclei computed from $H$ and $H^{2B}[\rho]$ are compared in Fig. 8. Being based on the minimum of the dHFB TEC, these spectra describe the low-lying part of the ground-state rotational band.

Reference results are well reproduced for all one-body test densities but $\rho^\text{HOSD}$ for which a degrading arises with increasing mass. Even in nuclei for which absolute PHFB energies were not converged yet with respect to $\epsilon_{3\text{max}}$ (e.g. $^{40}\text{Mg}$ and $^{20}\text{Ne}$), energy differences are fully consistent with the reference values.
Table 4  Average error (in %) on PHFB low-lying excitation energies computed from $H^2B[\rho]$ for various sub-categories of nuclei and test one-body density matrices. See Eq. (82) for details on the cost function. Calculations are performed with $\epsilon_{\text{max}} = 8$, $\epsilon_{3\text{max}} = 12$ and $\lambda_{\text{org}} = 1.88 \text{ fm}^{-1}$

|        | Mass $\leq 30$ | Mass $> 30$ | Neutron-rich | Total |
|--------|----------------|-------------|--------------|-------|
| $\rho_{\text{HOSD}}$ | 5.86           | 15.38       | 16.79        | 10.62 |
| $\rho_{\text{HFB(B)}}$ | 1.47           | 1.56        | 0.91         | 1.51  |
| $\rho_{\text{PHFB}}$  | 1.17           | 1.68        | 1.11         | 1.43  |
| $\rho_{\text{PGCM}}$  | 1.27           | 1.90        | 1.22         | 1.51  |

As for quantitative measures, systematic results are reported on in Table 4. Reference excitation energies are reproduced to better than 2% throughout the whole panel for $\rho_{\text{HFB(B)}}$, $\rho_{\text{PHFB}}$ and $\rho_{\text{PGCM}}$, which amounts to making errors of the order of a few tens of keVs. This is obviously negligible compared to other sources of uncertainties in state-of-the-art ab initio calculations. While this outcome further demonstrates the robustness of the approximation method, the 10% average error obtained for $\rho_{\text{HOSD}}$ underlines the fact that the employed one-body density matrix must be realistic enough to deliver high accuracy results. Given that the purpose of ab initio PHFB (and PGCM below) calculations is to access excitation energies and not absolute ones, one can be fully satisfied with the performances of $H^2B[\rho]$ in the present context.

4.5.2 PGCM

While PHFB calculations already provide a good test whenever the system is rigid with respect to collective variables, the PGCM opens the way to the wider class of so-called soft nuclei. More generally, it permits to include static correlations induced by shape fluctuations and to access associated vibrational excitations.

Presently, PGCM calculations of $^{20}\text{Ne}$ and $^{30}\text{Ne}$ along the axial quadrupole coordinate are performed. In order to obtain a first indication of the performance of $H^2B[\rho]$, Fig. 9 extends the study performed at the dHFB level in Sec. 4.3.1 by displaying the error obtained for the TEC of $J^\Pi = 0^+, 2^+, 4^+$ PHFB energies for the various test one-body density matrices. The $J^\Pi$ projected TEC constitutes the diagonal part of the Hamiltonian matrix at play in the Hill-Wheeler-Griffin secular equation of the PGCM calculation. The errors obtained along the projected TECs are strictly similar to those displayed in Fig. 2 at the dHFB level. This result gives confidence regarding the quality of the results that can be expected at the PGCM level.

Reference and approximate low-lying PGCM excitation energies of the ground-state rotational band and associated

Fig. 9  Same as the bottom panel of Fig. 2 for $J^\Pi = 0^+, 2^+, 4^+$ PHFB states

Fig. 10  Low-lying part of the PGCM ground-state rotational band of $^{20}\text{Ne}$. Reference results calculated from $H$ are compared to those computed from $H^2B[\rho]$ using various test one-body density matrices. Each energy level is displayed along with the magnetic dipole (below) and electric quadrupole (above) moments of the associated state. B(E2) transitions strengths are displayed using red arrows. Calculations are performed with $\epsilon_{\text{max}} = 8$, $\epsilon_{3\text{max}} = 10$ and $\lambda_{\text{org}} = 1.88 \text{ fm}^{-1}$
Table 5  Average error (in %) on PGCM excitation energies and spectroscopic observables computed from $H^{2B}[\rho]$ in $^{20}\text{Ne}$ and $^{30}\text{Ne}$ for various test one-body density matrices. See Eq. (81d) for details on the cost function. Calculations are performed with $e_{\text{max}}=8$, $e_{3\text{max}}=10$ and $\lambda_{\text{srg}}=1.88\text{ fm}^{-1}$.

| Nucleus | $^{20}\text{Ne}$ | $^{30}\text{Ne}$ |
|---------|-----------------|-----------------|
| Quantity | Spectrum | Observables | Spectrum | Observables |
| $\rho^\text{HOSD}$ | 2.95 | 1.43 | 4.53 | 2.85 |
| $\rho^\text{HFB(B)}$ | 1.46 | 0.71 | 2.60 | 2.57 |
| $\rho^\text{PHFB}$ | 0.36 | 0.55 | 2.59 |
| $\rho^\text{PGCM}$ | 0.26 | 0.48 | 2.98 | 2.85 |

Fig. 11  Same as Fig. 10 for $^{30}\text{Ne}$

electromagnetic observables are compared for $^{20}\text{Ne}$ and $^{30}\text{Ne}$ in Figs. 10 and 11, respectively. Due to numerical limitations, only three-body matrix elements up to $e_{3\text{max}}=10$ could be included in the full calculation, hence hindering the convergence in $^{30}\text{Ne}$. Still, building on the results reported in Fig. 9 an excellent agreement emerges in both nuclei for PGCM energies and electromagnetic observables, even more so in $^{20}\text{Ne}$ where sub-percent accuracy (see Table 5) is achieved. As before, a decent but less optimal reproduction of the reference results is obtained for $\rho = \rho^\text{HOSD}$. The excellent results obtained for electromagnetic observables testify the stability of the PGCM wave-functions themselves with respect to the in-medium approximation of the three-nucleon interaction.

4.5.3  dQRPA

QRPA is a method of choice to study excited states of both individual and collective characters, with energies ranging from a few MeV to tens of MeV. In this context, the performance of $H^{2B}[\rho]$ can be assessed by looking at, e.g., electromagnetic strength functions. Figures 12 and 13 display the electric isovector dipole ($E1$) strength computed with both $H$ and $H^{2B}[\rho^\text{HFB}]$, for $^{16}\text{O}$ and $^{20}\text{Ne}$ respectively. Similar results are obtained for the other test one-body density matrices and are reported in Table 6.

In $^{16}\text{O}$, where dQRPA reduces to sRPA built on top of a sHF Slater determinant, the difference between the strength functions are hardly noticeable. As in sHF calculations discussed earlier on, this relates to the fact that the sRPA error would actually be strictly zero if $\rho$ entering $H^{2B}[\rho]$ were taken as the variational sHF density matrix obtained from that approximate Hamiltonian. Because $\rho^\text{sHF}$ coming from
The above results validates the quality and robustness of $H^{2B}[\rho]$ in the dQRPA context. Although not shown for brevity, essentially identical results hold for other multipoles of the one-body transition operator. Furthermore, the dependence of the results on $e_{3\text{max}}$ is along the same line as the one discussed in Sect. 4.4.1.

4.6 Optimal one-body density matrix

The in-medium approximation of three-body interactions proposed in the present work appears to be very robust with respect to the employed symmetry-invariant one-body density matrix. All dHFB, dBMBPT, PHFB PGCM and dQRPA results presented above are of equal (excellent) quality for $\rho = \rho^{\text{sHFB}}$, $\rho^{\text{PHFB}}$ and $\rho^{\text{PGCM}}$ but are systematically deteriorated for the more simplistic choice $\rho = \rho^{\text{SHOSD}}$.

In this context, it is of interest to better assess this robustness and possibly characterize the optimal one-body density matrix to be used in the design of $H^{2B}[\rho]$. For this purpose, trial (symmetry-invariant) one-body density matrices $\{\rho^{\text{Rd}}\}$ are generated by means of the random sampling described in Appendix D. To evaluate the corresponding approximation $H^{2B}[\rho^{\text{Rd}}]$, the ground-state energy error

$$\Delta E_{\Psi}^{2B}[\rho] \equiv \frac{\langle \Psi | H^{2B}[\rho] | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

(31)

is considered; see Appendix D.1 for the working expression and a related discussion. The error function $\Delta E_{\Psi}^{2B}[\rho^{\text{Rd}}]$ computed for a large set of randomly generated matrices is shown in Fig. 14 as a function of the distance $\| \rho^{\text{Rd}} - \rho^{\Psi} \|$ between the trial one-body density matrix and the ground-state one $\rho^{\Psi}$ in the many-body calculation of interest. The data points corresponding to the physical one-body density matrices ($\rho^{\text{SHOSD}}$, $\rho^{\text{sHFB}}$, $\rho^{\text{PHFB}}$ and $\rho^{\text{PGCM}}$) are also displayed to better make sense of the results obtained so far. In addition to the distance to $\rho^{\Psi}$, each trial one-body density matrix is characterized by its von Neumann entropy

$$S[\rho] \equiv -\text{Tr} (\rho \ln \rho),$$

(32)

which, in the eigenbasis of $\rho$ with eigenvalues $\{r_a\}$ reads as Shannon’s entropy of information theory

$$S[\rho] \equiv -\sum_a r_a \ln r_a.$$

(33)

In the present context, the size of the entropy essentially characterizes how much the many-body state $\rho$ differs from a Slater determinant for which $S[\rho] = 0$, i.e. it is a measure of many-body correlations.

Results for $^{16}\text{O}$ computed in a small model space at the sHFB level are shown in the left panel of Fig. 14 while the right panel displays results for $^{20}\text{Ne}$ computed at the PHFB level. The sHFB calculation of $^{16}\text{O}$ illustrates the situation

\[ \text{Fig. 13 Same as Fig. 12 for } ^{20}\text{Ne} \]
Table 6  Average relative error (in %) on dQRPA excitation energies and on the total photo-emission cross section computed from $H^{2B}[\rho]$ in $^{16}$O and $^{20}$Ne for various test one-body density matrices. Calculations are performed with $\epsilon_{\text{max}} = 8$, $\epsilon_{3\text{max}} = 10$ and $\lambda_{\text{SG}} = 1.88 \text{ fm}^{-1}$

| Nucleus | Quantity | $^{16}$O | | $^{20}$Ne | |
|---------|---------|---------|----------|-------|----------|
| $\rho^{\text{HOSD}}$ | Excitation energy | 0.39 | Total photo-emission cross section | 0.04 | Excitation energy | 0.46 |
| $\rho^{\text{HFB}}$ | Total photo-emission cross section | 0.02 | | | Total photo-emission cross section | 0.63 |
| $\rho^{\text{PHFB}}$ | | 1.09 | | | 1.13 |
| $\rho^{\text{PGCM}}$ | | 1.13 | | | 0.44 |

Fig. 14  Ground-state energy error $\Delta E^{2B}_\Psi[\rho]$ associated with the use of $H^{2B}[\rho]$ as a function of the distance $\|\rho - \rho^\Psi\|$ between the test one-body density matrix $\rho$ and the actual ground-state one $\rho^\Psi$ in log-log scale. Left panel: sHF ($J^\Pi = 0^+$) solution for $^{16}$O. Right panel: PHFB ($J^\Pi = 0^+$) solution for $^{20}$Ne. Data points are for physical and randomly-sampled test one-body density matrices. For the latter, the color scale characterizes their von Neumann entropy. The dashed-dotted lines denote the cubic envelop extracted from the left panel and reported on the right panel. Calculations are performed for $\epsilon_{\text{max}} = 6$ and $\epsilon_{3\text{max}} = 6$

encountered for an uncorrelated state, i.e. the many-body solution $|\Psi\rangle$ is nothing but a symmetry-conserving Slater determinant. In this particular case, the ground-state energy error (see Eq. (74)) takes the simple form

$$\Delta E^{2B}_\Psi[\rho] = \frac{1}{3!} w^{(3)}(\rho - \rho^{\text{HFB}}) \otimes^{(3)}$$

and is thus minimal, actually null, for $\rho = \rho^{\text{HFB}}$. The fact that the optimal one-body density matrix is nothing but the one of the many-body state under scrutiny is confirmed numerically in the left panel of Fig. 14. In absence of genuine correlations, one expects from Eq. (34) that the sampled errors are bounded by a cubic envelope in the variable $\|\rho - \rho^{\text{HFB}}\|$, which indeed appears clearly in the numerical results. The coefficient (0.4) of that cubic envelope extracted from the data is a measure of the employed three-body interaction strength in the utilized model space.

Besides the null error delivered by $\rho = \rho^{\text{HFB}}$, the errors associated with the physical one-body density matrices $\rho^{\text{HOSD}}$ and $\rho^{\text{MBPT}}$ are provided on the figure. Compared to the full range of sampled one-body density matrices. Given that $\rho^{\text{HFB}}$ relates to a Slater determinant with 16 particles, the maximum distance is reached for densities associated with Slater determinants obtained by promoting the 16 particles from hole states.
\[ \rho^{\text{HOSD}} \] and \[ \rho^{\text{MBPT}} \] are rather close to \[ \rho^{\text{SHF}} \]. This is particularly true of \[ \rho^{\text{MBPT}} \], which is a sign of the weakly-correlated character of \[ 16 \text{O} \] when eventually going beyond the mean-field on the basis of a SRG-evolved Hamiltonian. Given the cubic upper-bound, such a proximity between the two density matrices implies a tiny error on the energy obtained for \[ \rho = \rho^{\text{MBPT}} \]. In spite of originating from a Slater determinant and thus sharing the same null entropy as \[ \rho^{\text{SHF}}, \rho^{\text{HOSD}} \] is about 3 times more distant from it than \[ \rho^{\text{MBPT}} \]. In agreement with the cubic law governing the error, plus being located closer to the envelope, the associated error is about 170 times larger. Given the softness of the employed three-body interaction, \[ \rho^{\text{HOSD}} \] still provides a small absolute error in the end. Eventually, the sampling provides a fair understanding that, as long as the test one-body density is not too distant from \[ \rho^{\text{SHF}}, \] its detailed properties do not matter much and the error is bound to be small.

Compared to the previous case, the right panel of Fig. 14 allows one to appreciate the qualitatively different situation encountered for a genuinely-correlated state. Indeed, the error \( \Delta E^{2B}_{\text{HFB}}[\rho] \) behaves now differently as a function of the distance\(^25\) \( \| \rho - \rho^{\text{PHFB}} \| \). As visible from Eq. (74), \( \Delta E^{2B}_{\text{PHFB}}[\rho] \) contains non-zero constant and linear terms in addition to the cubic term encountered in Eq. (34).

The constant term delivers the error \( \Delta E^{2B}_{\text{PHFB}}[\rho^{\text{PHFB}}] \) associated with the actual ground-state density, i.e. when setting \( \rho = \rho^{\text{PHFB}} \). The fact that this error is different from zero is a fingerprint of the fact the PHFB ground-state wave-function carries (at least) genuine three-body correlations. The value of the corresponding error additionally depends on the size of the three-body interaction convolved with the irreducible three-body density matrix (see Eq. (74)). As analyzed in Ref. [4] in connection with the NO2B approximation, a low-scale Hamiltonian makes the energy contribution from the residual three-body interaction small. For \( (\epsilon_{\text{max}} = 6; \epsilon_{\text{3max}} = 6) \) this error is \( \Delta E^{2B}_{\text{PHFB}}[\rho^{\text{PHFB}}] \approx 0.1 \text{MeV} \) whereas the better converged value obtained earlier on for \( (\epsilon_{\text{max}} = 8; \epsilon_{\text{3max}} = 12) \) is 0.5 MeV (0.4%); i.e. the error is small.

Increasing the distance from \( \rho = \rho^{\text{PHFB}} \), one can lower the error such that a minimum \( \min_{\rho} \Delta E^{2B}_{\text{PHFB}}[\rho] \) is found for \( \| \rho - \rho^{\text{PHFB}} \| = \text{few} \times 10^{-1} \) with a value several times smaller than \( \Delta E^{2B}_{\text{PHFB}}[\rho^{\text{PHFB}}] \). Passed the minimum the error typically increases and is eventually dominated by the cubic terms at large distances such that the cubic envelope extracted from the left panel becomes effective.

The physical density matrices \( \rho^{\text{HOSD}} \) and \( \rho^{\text{SHF}} \) are found right past the minimum such that their error is small and in fact similar to the one found at the origin. The profile of the error as a function of the distance \( \| \rho - \rho^{\text{PHFB}} \| \) rationalizes the fact that small errors can be found over a substantial range of density matrices to which the various physical one-body density matrices one may typically access all belong. This feature provides practitioners with a significant flexibility as far as the choice of the employed one-body density matrix is concerned. Beyond that appropriate interval the error rapidly increases with the distance, as testified by the use of \( \rho^{\text{HOSD}} \) sitting on the edge of it, such that one may not be too cavalier either regarding the choice of \( \rho \).

4.7 Lessons and perspectives

4.7.1 Main lessons

The above results demonstrate the usefulness of the proposed in-medium reduction method of three-body interaction operators in nuclear ab initio calculations. The fact that the method relies on the sole use of a one-body density matrix gives much credit to the simplicity of the method. Furthermore, the high-quality approximation was shown to be robust with respect to the employed one-body density matrix, which gives much credit to the flexibility of the method.

These conclusions have been validated for nuclei with closed and open-shell characters, i.e. displaying weak and strong correlations, for a large class of observables in light and mid-mass systems as well as for stable and exotic isotopes. While convincingly substantiated via the use of both perturbative and non-perturbative many-body methods, a further validation of the quality of the approximation on the basis of (non-perturbative) ab initio methods built on different paradigms is desirable in the future.

4.7.2 Algorithm

The independence of the results with respect to a large class of one-body density matrices is of prime importance for practical applications in the future, especially given that ab initio calculations aspire to move up the nuclear chart towards heavy, doubly open-shell nuclei. Specifically, the high-quality results obtained for \( \rho = \rho^{\text{SHF}} \) allow one to build \( H^{2B}[\rho] \) at the sole cost of running first a spherical HFB calculation with full three-body forces, thus bypassing the need to run any deformed HFB code followed by projections, which would already be too costly with explicit three-body forces in heavy nuclei requiring large values of \( \epsilon_{\text{3max}} \). Eventually, the envisioned working algorithm is

1. run a spherical HFB calculation with three-nucleon forces to extract \( \rho^{\text{SHF}} \),
2. build \( H^{2B}[\rho^{\text{SHF}}] \),
3. run the many-body method of interest with the two-body Hamiltonian $H^{2B}[\rho^{\text{HFB}}]$, such that even in (heavy) open-shell nuclei

- no two-body density matrix has to be extracted,
- no genuine open-shell calculation with an explicit three-nucleon operator has to be performed.

4.7.3 Odd-even and odd-odd nuclei

While the method presented in this article relies on the use of symmetry-invariant one-body densities, which can be generated only starting from $J^P = 0^+$ states (or a superposition of such states), it can also be easily used to construct effective $k$-body interactions for odd-even and odd-odd nuclei. For this purpose, one can employ the one-body density generated in a mean-field calculation of a spherical Bogoliubov vacuum constrained to have odd-even or odd-odd numbers of particles on average. In the case of odd-even systems, it was demonstrated in Ref. [18] that such a vacuum represents a good approximation to the true mean-field solution obtained with an odd number parity wave function.

Of course, the accuracy of the $k$-body interactions constructed in this way will have to be properly checked but there is no reason to believe that they would perform particularly worse than those generated to describe even-even nuclei.

4.7.4 Further perspectives

In the longer-term future, the in-medium reduction procedure proposed in the present work can be tested to deal with, e.g., four-body interactions [41–43] and/or three-body nuclear currents [44] at a reduced computational cost.

5 Conclusions

The present work introduced a novel method to approximate $n$-body operators in terms of $k$-body ones with $k < n$. This is highly pertinent to overcome the steep increase of the computational cost of many-body calculations due to the presence of three-nucleon interactions, especially as ab initio calculations aspire to move to heavier nuclei than presently possible.

The main advantages are that the method is accurate, universal, simple and flexible. The universality of the method not only relates to its applicability to all nuclei, independently of their closed or open-shell character, but also to its independence with respect to the many-body method eventually used to solve Schrödinger’s equation. The simplicity of the method relates to the fact that it requires the convolution of the, e.g., three-body operator with a sole symmetry-invariant one-body density matrix, even in open-shell nuclei. This it at variance with existing methods that either convolute the three-body operator with one-, two- and three-body density matrices in open-shell systems or with a symmetry-breaking one-body density matrix, thus leading to an approximate operator that explicitly breaks symmetries of the initial Hamiltonian. Eventually, the flexibility of the method relates to the possibility to use various one-body density matrices as an entry. As a matter of fact, the functional form of the error due to the use of the approximate Hamiltonian could be exploited to explain why accurate results can be obtained for a rather large class of one-body density matrices. Such a flexibility can be exploited to use a (not too) simple density matrix in practical calculations, e.g. the density matrix extracted from a spherical Hartree-Fock-Bogoliubov calculation.

Extensive numerical results have demonstrated the high accuracy of the approach over a wide range of nuclei and observables. The approximation method is thus ready to be employed in routine ab initio calculations in the future. Furthermore, the in-medium reduction procedure is ready to be tested on four-nucleon interactions and/or three-body nuclear currents in order to deal with them at a reduced computational cost.

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The third set of tensors is now shown to be the same as the initial one. Noting that

\[ \phi^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} = \sum_{k=1}^{N} \frac{1}{(k-l)!} \left( (\alpha^{(k)} \cdot \rho^{\otimes (k-l)}) \cdot \rho^{\otimes (l-n)} \right) \]

one obtains

\[ \hat{\phi}^{(n)}[\rho] = \sum_{l=n}^{N} \sum_{k=1}^{N} \frac{(-1)^{l-n}}{(l-n)! (k-l)!} \alpha^{(k)} \cdot \rho^{\otimes (l-n)} \]

\[ = \sum_{k=n}^{N} \left[ \sum_{l=n}^{k} \frac{(-1)^{l-n}}{(l-n)! (k-l)!} \right] \alpha^{(k)} \cdot \rho^{\otimes (k-n)} \]

\[ = \sum_{l=n}^{N} \left[ \sum_{k=n}^{l} (-1)^{l-n} \frac{1}{(l-n)! (k-l)!} \right] \alpha^{(k)} \cdot \rho^{\otimes (k-n)} \]

\[ = \sum_{k=n}^{N} \frac{\delta_{kn}}{(k-n)!} \alpha^{(k)} \cdot \rho^{\otimes (k-n)} \]

\[ = \phi^{(n)} \]

Equation (39) defines the unitary Bogoliubov transformation\(^{26}\) that is inverted according to

\[ c^{+}_{a} = \sum_{k} U^{ka}(q) \beta^{+}_{k} + V^{a}_{k}(q) \beta^{+}_{k} \] (40a)

\[ c_{a} = \sum_{k} U_{ka}(q) \beta_{k} + V^{a}_{k}(q) \beta^{+}_{k} \] (40b)

\section{PGCM transition density matrix}

A workable expression for the transition one-body density matrix between two PGCM states is obtained and eventually reduced to the particular case of present interest.

\subsection{B.1.1 Bogoliubov state}

The deformed Bogoliubov state \(|\Phi(q)\rangle\) characterized by the collective deformation \(q\) is a vacuum for the set of quasiparticle operators \([22]\)

\[ \beta^{+}_{k}(q) \equiv \sum_{a} U^{ka}(q) c^{+}_{a} + V^{a}_{k}(q) c_{a} \] (39a)

\[ \beta_{k}(q) \equiv \sum_{a} U^{a}_{ka}(q) c_{a} + V^{a}_{k}(q) c^{+}_{a} \] (39b)

B.1.2 PGCM state

Given a set of Bogoliubov states \(|\Phi(q)\rangle\) differing by the value of the collective deformation parameter \(q\), a PGCM state reads as

\[ |\Psi_{\mu}^{\sigma}\rangle \equiv \int dq f^{\sigma}_{\mu}(q) P^{\sigma}|\Phi(q)\rangle \]

While \(\mu\) denotes a principal quantum number, \(\sigma \equiv (JM JNZ)\) collects the set of symmetry quantum numbers labelling the many-body state, i.e. the angular momentum \(J\) and its projection \(M\), the parity \(\Pi = \pm 1\) as well as neutron \(N\) and proton \(Z\) numbers. The operator

\[ P^{\sigma} \equiv P^{J}_{M} P^{N} P^{Z} P^{\Pi} \]

collects the projectors on good symmetry quantum numbers

\[ P^{J}_{M} \equiv \sum_{K} g^{J}_{K}(q) P^{J}_{MK} \equiv \sum_{K} g^{J}_{K}(q) \frac{2J+1}{16\pi^{2}} \int_{[0,\pi] \times [0,2\pi]} d\Omega D^{J}_{MK}(\Omega) R_{J}(\Omega) \]

\[ P^{N} \equiv \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi_{N} e^{i\varphi_{N}} R_{N}(\varphi_{n}) \]

\[ P^{Z} \equiv \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi_{Z} e^{i\varphi_{Z}} R_{Z}(\varphi_{p}) \]

\[ P^{\Pi} \equiv \frac{1}{2} \sum_{\varphi_{n}=0,\pi} e^{\pm (1-\Pi)\varphi_{n}} \Pi(\varphi_{n}) \]

such that \(|\Psi_{\mu}^{\sigma}\rangle\) is an eigenstate of \(J^{2}, J_{z}, N, Z\) and \(\Pi(\pi)\), where the latter denotes the parity operator. The unknown coefficients \(f^{\sigma}_{\mu K} = f^{\sigma}_{\mu K}(q) g_{K}(q)\) are typically obtained by solving Hill-Wheeler-Griffin’s equation \([22]\). Note that, by definition, the coefficients \(f^{\sigma}_{\mu K}\) are presently defined such that the set of PGCM states \(|\Psi_{\mu}^{\sigma}\rangle; \mu = 1, 2, \ldots\) emerging from a calculation are ortho-normalized. In Eq. \((43)\), \(\Omega \equiv (\alpha, \beta, \gamma)\), \(\varphi_{n}\) and \(\varphi_{n}(\varphi_{p})\) denote Euler, parity and neutron-

\(^{26}\) The covariant indices notation used in this document is extended to \(U\) and \(V\) matrices, such that creator (annihilator) indices are lowered (raised) using complex conjugation, e.g. \(U^{*}_{ka}(q) = (U^{ka}(q))^{*}\).
(proton-) gauge angles, respectively. The rotation operators are given by

\[ R_J(\Omega) \equiv e^{-i\alpha J_x} e^{-i\beta J_y} e^{-i\gamma J_z}, \]
\[ R_N(\varphi_N) \equiv e^{-i\varphi_N N}, \]
\[ R_Z(\varphi_P) \equiv e^{-i\varphi_P Z}, \]
\[ \Pi(\varphi_\Pi) \equiv e^{-i\varphi_\Pi F}, \]

with the one-body operator

\[ F \equiv \sum_{ab} f_{ab} c^\dagger_a c_b \]

defined through its matrix elements \[45\]

\[ f_{ab} = \frac{1}{2} (1 - \pi_a) \delta_{ab}, \]

where \(\pi_a\) denotes the parity of one-body basis states that are presently assumed to carry a good parity. Last but not least, \(D_{MK}^J(\Omega) \equiv \langle JM|R_J(\Omega)|JK\rangle\) defines Wigner D-matrices, where \(|JM\rangle\) denotes a generic eigenstate of \(J^2\) and \(J_z\).

B.1.3 Off-diagonal one-body density matrix

Given a state \(|\Phi(q)\rangle\) defined through the Bogoliubov transformation \((U(q), V(q))\) and the common index

\[ \theta \equiv (\Omega, \varphi_n, \varphi_p, \varphi_\Pi) \]

encompassing all rotation angles, the state obtained through multiple rotations

\[ |\Phi(q, \theta)\rangle \equiv R_J(\Omega) R_N(\varphi_N) R_Z(\varphi_P) \Pi(\varphi_\Pi) |\Phi(q)\rangle, \]

is also a Bogoliubov state whose Bogoliubov transformation \((U(q, \theta), V(q, \theta))\) can be obtained from \((U(q), V(q))\) and from the characteristics of the rotation operators \[22,46\].

A crucial quantity in terms of which the final results will be expressed is the so-called off-diagonal one-body density matrix

\[ \rho(q', q, \theta)_{ab} \equiv \frac{\langle \Phi(q')|c^\dagger_a c_b|\Phi(q, \theta)\rangle}{\langle \Phi(q')|\Phi(q, \theta)\rangle}, \]

which involves two different Bogoliubov states and, as such, can be computed explicitly from the sole knowledge of \((U(q'), V(q'))\) and \((U(q, \theta), V(q, \theta))\) \[22,46\].

B.2 Definition

Considering two PGCM states, the one-body transition density matrix can now be defined through\(^{27}\)

\[ \rho_{\mu_f \mu_i \sigma_i}^{\sigma_f \sigma_i} \equiv \langle \rho_{\mu_f \mu_i} | c^\dagger_a c_b | \psi_{\sigma_i} \rangle \]

\[ = \int dq_f dq_i f_{\mu_f}^{\sigma_f} (q_f) f_{\mu_i}^{\sigma_i} (q_i) \]

\[ \times \langle \Phi(q_f)| P_{\mu_f}^{JM} c^\dagger_a c_b | \Pi(\Omega) | \Phi(q_i) \rangle, \]

\[ = \int dq_f dq_i \sum_{K_f K_i} f_{\mu_f}^{\sigma_f} (q_f) f_{\mu_i}^{\sigma_i} \delta_{\Omega, \Omega'(\pi_a \pi_b)} \Pi_i \]

\[ \times \delta N_f N_i \delta Z_f Z_i \frac{1}{2} J_{\mu_f \mu_i}^J \rho_{q_f q_i} a', \]

where

\[ \rho_{q_f q_i} a' \equiv \langle \Phi(q_f)| P^{JM} c^\dagger_a c_b | \Pi(\Omega) | \Phi(q_i) \rangle, \]

and where the action of \(P^{JM} c^\dagger_a c_b \Pi \) was easily resolved.

B.3 Simplified expressions

B.3.1 Expanding the projectors

In order to evaluate this matrix element, the left angular-momentum projector is expanded according to Eq. (43a) such that Eq. (51) is rewritten as

\[ \rho_{q_f q_i} a' \equiv \langle \Phi(q_f)| P^{JM} c^\dagger_a c_b | \Pi(\Omega) | \Phi(q_i) \rangle, \]

\[ = \int d\Omega \sum_{M'} D_{MK_f}^{J_f} (\Omega) D_{MK_i}^{J_i} (\Omega) \]

\[ \times \langle \Phi(q_f)| c^\dagger_a | \Omega' \rangle c_b | \Omega \rangle \frac{1}{2} J_{\mu_f \mu_i}^J \rho_{q_f q_i} a', \]

where the rotated creation and annihilation operators are defined as

\[ c^\dagger_a | \Omega \rangle \equiv R_J(\Omega) c^\dagger_a R_J(\Omega), \]

\[ c_b | \Omega \rangle \equiv R_J(\Omega) c_b R_J(\Omega), \]

and where the identity

\[ R_J(\Omega)^\dagger P_{MK_i}^{J_i} = \sum_{M'} D_{MK_i}^{J_i} (\Omega) R_J(\Omega)^\dagger P_{MK_i}^{J_i}, \]

has been used.

\(^{27\,}\) In the present derivation, the density matrix is restricted to be diagonal in the isospin quantum number, i.e. single-particle states \(a\) and \(b\) carry the same isospin projection quantum number.
B.3.2 Spherical one-body basis

In case one-body basis states carry spherical indices \((a \equiv n_a, j_a, m_a, \pi_a, q_a \equiv a_u, j_u, m_u)\), the operators \(c_{a \alpha j am}^\dagger\) and \((-1)^{m_a-j_a}c_{a \alpha j am}\) transform like the \(m_a^{th}\) component of a rank-\(j_a\) spherical tensor under the action of \(SU(2)\), which leads to

\[
\begin{align*}
c_{a \alpha j am}^\dagger [\Omega] & \equiv \sum_m D_{mab}^*(\Omega)c_{a \alpha j am}^\dagger, \\
c_{a \alpha j am} [\Omega] & \equiv \sum_m D_{mam}^*(\Omega)c_{a \alpha j am}.
\end{align*}
\]  

(55a)

(55b)

Consequently, the transition density matrix can be simplified as

\[
\rho_{q f q i}^{J_f J_i K_f, K_i, \sigma_i, \sigma_f, b} = \frac{2J_f + 1}{16\pi^2} \sum_{m m'} \sum_{M M'} \sum_{\lambda\psi}\lambda
\begin{align*}
&\times \left( \int d\Omega D_{M J_f M J_i}^{J_f}(\Omega) D_{m m'}^{J_i}(\Omega) D_{m m'}^{J_i}(\Omega) \right) \\
&\times \langle \Phi(q_f)|c_{a \alpha j am}^\dagger c_{a \alpha j am} p_{M K_i} \rho_{N K_i}^N \rho_{Z K_i}^Z |\Phi(q_i)\rangle.
\end{align*}
\]  

(56)

The integral over Wigner-D matrices is performed analytically and generates a sum over Clebsch-Gordan coefficients and \(3j\)-symbols according to

\[
\begin{align*}
&\frac{1}{16\pi^2} \int d\Omega D_{M J_f M J_i}^{J_f}(\Omega) D_{m m'}^{J_i}(\Omega) D_{m m'}^{J_i}(\Omega) \\
&= \sum_{\lambda\psi}\lambda\psi
\begin{align*}
&\times \left( \sum_{M} \int d\Omega D_{M J_f M J_i}^{J_f}(\Omega) D_{m m'}^{J_i}(\Omega) D_{m m'}^{J_i}(\Omega) \right) \\
&\times \langle \Phi(q_f)|c_{a \alpha j am}^\dagger c_{a \alpha j am} p_{M K_i} \rho_{N K_i}^N \rho_{Z K_i}^Z |\Phi(q_i)\rangle.
\end{align*}
\]  

(57)

The remaining matrix element in Eq. (56) is easily obtained in terms of the off-diagonal one-body density matrix defined through Eq. (49)

\[
\langle \Phi(q_f)|c_{a \alpha j am}^\dagger c_{a \alpha j am} p_{M K_i} \rho_{N K_i}^N \rho_{Z K_i}^Z |\Phi(q_i)\rangle = \frac{2J_i + 1}{16\pi^2} \left( \frac{1}{2\pi} \right)^2 \int d\theta D_{M K_i}^{J_i}(\Omega) e^{i\theta_{N K_i}^N} e^{i\psi_{Z K_i}^Z} \langle \Phi(q_f)\rangle \langle \Phi(q_i)|.,
\]

(58)

knowing that the overlap \(\langle \Phi(q_f)|\Phi(q_i, \theta)\rangle\) between two arbitrary non-orthogonal Bogoliubov states can be computed in several ways [47,48].

B.3.3 Special case of present interest

One is presently interested in the one-body density matrix of a \(J^a = 0^+\) state. In the above set of equations, it corresponds to setting \(J_f = J_i = 0, M_f = M_i = 0\) and \(I_\perp = +1\). In this case, the triangular inequalities encoded in the \(3j\)-symbols impose that

\[
\begin{align*}
\lambda &= 0, \\
m_a &= m_b, \\
j_a &= j_b, \\
m &= m',
\end{align*}
\]  

(59a)

(59b)

(59c)

(59d)

such that Eq. (57) becomes

\[
\begin{align*}
&\frac{1}{16\pi^2} \int d\Omega D_{M J_f M J_i}^{J_f}(\Omega) D_{m m'}^{J_i}(\Omega) D_{m m'}^{J_i}(\Omega) \\
&= \delta_{m a m b} \delta_{j a j b} \delta_{m m'} \frac{1}{2J_a + 1}.
\end{align*}
\]  

(60)

The fact that the initial and final states are the same and thus carry the same particle further requires that \(\pi_a = \pi_b\). Eventually, Eq. (56) reduces to

\[
\begin{align*}
&\rho_{q f q i}^{J_f J_i K_f, K_i, \sigma_i, \sigma_f, b} = \delta_{j a j b} \delta_{m a m b} \delta_{\pi a \pi b} \left( \frac{1}{16\pi^2} \right)^2 \left( \frac{1}{2\pi} \right)^2 \left( \frac{1}{2\pi} \right)^2 \\
&\times \left( \sum_{M} \int d\theta e^{i\theta_{N K_i}^N} e^{i\psi_{Z K_i}^Z} \langle \Phi(q_f)\rangle \langle \Phi(q_i, \theta)|.,
\end{align*}
\]  

(61)

The diagonal character of the one-body density matrix in \((j, m)\) and its independence on \(m\) is made clear in Eq. (61) and ends the derivation.

C BMBPT transition density matrix

The BMBPT(2) transition one-body density matrix is presently derived within the frame of a so-called \textit{expectation-value} many-body scheme rather than within a \textit{projective} one, i.e. it is computed directly through Eq. (6) for \(I = 1\) and \(|\theta\rangle \equiv |\psi_{\text{BMBPT}(2)}\rangle\). The derivation can actually be performed within the larger frame of the Bogoliubov configuration-interaction (BCI) formalism such that BCI-like expansion coefficients are eventually obtained within the frame of BMBPT(2) [49].

The present applications are eventually limited to standard MBPT, i.e. calculations are restricted to doubly closed-shell nuclei for which BMBPT reduces to MBPT on top of a \(J^a = 0^+\) Slater determinant.
C.1 Bogoliubov algebra

In methods based on a Bogoliubov vacuum $|\Phi(q)\rangle$, the grand potential\(^{28}\),

$$\Omega \equiv H - \mu A,$$

must be used rather than the Hamiltonian to control the average particle-number in the system. The many-body algebra is more conveniently worked out by normal-ordering all operators with respect to $|\Phi(q)\rangle$ and by expressing them in terms of quasi-particle operators. Limiting oneself to two-body operators\(^{29}\), the grand potential is thus written as

$$\Omega = \Omega^{00}(q) + \Omega^{20}(q) + \Omega^{11}(q) + \Omega^{02}(q)$$

$$+ \Omega^{31}(q) + \Omega^{22}(q) + \Omega^{13}(q) + \Omega^{04}(q),$$

where $\Omega^{ij}(q)$ denotes the normal-ordered component involving $i$ ($j$) quasi-particle creation (annihilation) operators, e.g.,

$$\Omega^{31}(q) \equiv \frac{1}{3!} \sum_{k_1,k_2,k_3,k_4} \Omega_{k_1k_2k_3k_4}(q) \beta_{i,k_1}(q) \beta_{i,k_2}(q) \beta_{i,k_3}(q) \beta_{i,k_4}(q),$$

where the matrix elements are anti-symmetric with respect to the exchange of any pair of upper or lower indices. For more details about the normal ordering procedure, see Refs. [9, 10, 13, 26–28].

C.2 BCI state

In BCI, many-body states are written as a CI-like expansion on top of the (deformed) Bogoliubov vacuum. Presently truncated to single and double excitations, the BCISD ansatz reads as

$$|\Psi(q)\rangle \equiv \left(1 + \sum_{k_1,k_2} C^{k_1,k_2}(q) \beta_{i,k_1}(q) \beta_{i,k_2}(q)ight)$$

$$+ \sum_{k_1,k_2,k_3,k_4} C^{k_1,k_2,k_3,k_4}(q) \beta_{i,k_1}(q) \beta_{i,k_2}(q) \beta_{i,k_3}(q) \beta_{i,k_4}(q)$$

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

where the unknown coefficients, anti-symmetric with respect to the exchange of any pair of upper indices, can be obtained by diagonalization of $\Omega$ or via BMBPT.

\(^{28}\) In practice two separate Lagrange multipliers $\mu_N$ and $\mu_Z$ are introduced to account for neutron and proton chemical potentials, such that the average neutron and proton numbers are conserved individually.

\(^{29}\) This is the case when working with two-body forces only or within the PNO2B or the presently developed 2B approximation.

C.3 Expression in quasi-particle space

C.3.1 Definition

Considering two different BCISD states $|\Psi^i(q)\rangle$ and $|\Psi^j(q)\rangle$, the four transition one-body density matrices defined in terms of quasi-particle operators are given by

$$\rho_{ij}^{k_1k_2}(q) \equiv \frac{\langle \Psi^i(q)|\beta_{i,k_1}(q)\beta_{i,k_2}(q)|\Psi^j(q)\rangle}{\sqrt{\langle \Psi^i(q)|\Psi^i(q)\rangle \langle \Psi^j(q)|\Psi^j(q)\rangle}},$$

$$\kappa_{ij}^{k_1k_2}(q) \equiv \frac{\langle \Psi^i(q)|\beta_{i,k_1}(q)\beta_{i,k_2}(q)|\Psi^j(q)\rangle}{\sqrt{\langle \Psi^i(q)|\Psi^j(q)\rangle \langle \Psi^j(q)|\Psi^i(q)\rangle}},$$

$$\sigma_{ij}^{k_1k_2}(q) \equiv \frac{\langle \Psi^i(q)|\beta_{i,k_1}(q)\beta_{i,k_2}(q)|\Psi^j(q)\rangle}{\sqrt{\langle \Psi^i(q)|\Psi^i(q)\rangle \langle \Psi^j(q)|\Psi^j(q)\rangle}},$$

among which the relations

$$\kappa_{ij}^{k_1k_2}(q) = (\kappa_{ji}^{k_2k_1}(q))^*,$$

$$\sigma_{ij}^{k_1k_2}(q) = (\rho_{ij}^{k_2k_1}(q))^* - 1,$$

hold.

C.3.2 Matrix elements

Starting from Eqs. (63)-(64) and applying Wick’s theorem, one obtains

$$\rho_{ij}^{k_1k_2}(q) = \frac{1}{\sqrt{\langle \Psi^i(q)|\Psi^i(q)\rangle \langle \Psi^j(q)|\Psi^j(q)\rangle}}$$

$$\times \left[\frac{1}{2} \sum_{k_3} C^{f_*}_{k_1k_3}(q) C^{i}_{k_2k_3}(q)\right]$$

$$+ \frac{1}{2} \sum_{k_3,k_4,k_5} C^{f_*}_{k_1k_3k_4k_5}(q) C^{i}_{k_2k_3k_4k_5}(q),$$

and

$$\kappa_{ij}^{k_1k_2}(q) = \frac{1}{\sqrt{\langle \Psi^i(q)|\Psi^i(q)\rangle \langle \Psi^j(q)|\Psi^j(q)\rangle}}$$

$$\times \left[\frac{1}{2} C^{f}_{k_1k_2}(q)\right]$$

$$+ \frac{1}{2} \sum_{k_3,k_4,k_5} C^{f_*}_{k_1k_3k_4k_5}(q) C^{i}_{k_2k_3k_4k_5}(q).$$
The expressions of $k^{fi}$ and $a^{*fi}$ are then deduced via Eq. (65) whereas the norm entering the denominators of the transition one-body density matrices reads, e.g., as
\[ \langle \Psi^{f}(q)|\Psi^{i}(q) \rangle \equiv 1 + \sum_{k_{1}k_{2}} C^{i}_{k_{1}k_{2}}(q) C^{f}_{k_{1}k_{2}}(q) \]
+ \sum_{k_{1}k_{2}k_{3}k_{4}} C^{i}_{k_{1}k_{2}k_{3}k_{4}}(q) C^{f}_{k_{1}k_{2}k_{3}k_{4}}(q).

C.4 Expression in one-particle space

Inserting the inverse Bogoliubov transformation (Eq. 40), the normal one-body density matrix expressed in terms of particle operators is obtained under the form
\[ \rho^{fi}_{a}(q) \equiv \frac{\langle \Psi^{f}(q)|c_{a}^{\dagger}c_{b}|\Psi^{i}(q) \rangle}{\sqrt{\langle \Psi^{f}(q)|\Psi^{f}(q) \rangle \langle \Psi^{i}(q)|\Psi^{i}(q) \rangle}} \]
= \sum_{k_{1}k_{2}} \left[ U^{k_{2}}_{k_{1}}(q) \rho^{fi}_{k_{1}k_{2}}(q) U^{*}_{k_{1}a}(q) \right.
- V^{fi}_{k_{2}}(q) \sigma^{fi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \\
- V^{fi}_{k_{2}}(q) \kappa^{fi}_{k_{1}k_{2}}(q) U^{*}_{k_{1}a}(q) + U^{k_{2}}_{k_{1}}(q) \kappa^{fi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right]. \tag{66}

C.5 One-body density matrix

In the present work, one is interested in the case where $|\Psi^{i}(q)\rangle = |\Psi^{f}(q)\rangle \equiv |\Psi(q)\rangle$ such that Eq. (66) reduces to
\[ \rho^{\Psi}_{a}(q) = \sum_{k_{1}k_{2}} \left[ V^{k_{2}}_{k_{1}}(q) V^{k_{1}}_{k_{1}a}(q) \right.
+ U^{k_{2}}_{k_{1}}(q) \rho^{\Psi}_{k_{1}k_{2}}(q) U^{*}_{k_{1}a}(q) \\
- \left( V^{k_{2}}_{k_{1}}(q) \rho^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right)^{*} \right.
- \left( V^{k_{2}}_{k_{1}}(q) \kappa^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right)^{*} \\
+ U^{k_{2}}_{k_{1}}(q) \kappa^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right]. \tag{67}

When time-reversal symmetry is preserved, the one-body density matrix can be chosen to be real such that the final expression reads as
\[ \rho^{\Psi}_{a}(q) = \rho^{\Psi}_{a}(q) \]
+ \sum_{k_{1}k_{2}} \left[ U^{k_{2}}_{k_{1}}(q) \rho^{\Psi}_{k_{1}k_{2}}(q) U^{*}_{k_{1}a}(q) \\
- V^{k_{2}}_{k_{1}}(q) \rho^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right.
- V^{k_{2}}_{k_{1}}(q) \kappa^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \\
+ U^{k_{2}}_{k_{1}}(q) \kappa^{\Psi}_{k_{1}k_{2}}(q) V^{k_{1}}_{k_{1}a}(q) \right], \tag{68}

where $\rho^{\Phi}_{a}(q)$ denotes the one-body density matrix of the reference state $|\Phi(q)\rangle$ such that the additional terms relate to BCISD corrections on top of it.

C.6 BMBPT coefficients

The coefficients of the BCISD state obtained at first- and second-order in BMBPT are now explicitly provided [49]. Given that the present application is limited to a $J^{{\pi}} = 0^+$ Slater determinant reference state $|\Phi(q)\rangle$, the resulting one-body density matrix $\rho^{\Psi}_{a}(q)$ is actually proportional to $\delta_{ij}$ and relates to a many-body state that is an eigenvector of the particle-number operator.

C.6.1 Partitioning

To formulate BMBPT with respect to the Bogoliubov reference state $|\Phi(q)\rangle$, the grand potential is split into an unperturbed term $\Omega_{0}$ and a residual part $\Omega_{1}$ [9, 26, 27]
\[ \Omega_{0}(q) = \Omega_{0}^{00}(q) + \tilde{\Omega}_{11}^{11}(q) \]
\[ \Omega_{1}(q) = \Omega_{20}(q) + \tilde{\Omega}_{11}^{11}(q) + \Omega_{02}(q) + \Omega_{00}(q) \]
+ $\Omega_{40}(q) + \Omega_{31}(q) + \Omega_{22}(q) + \Omega_{13}(q) + \Omega_{04}(q)$, with $\tilde{\Omega}_{11}^{11}(q) \equiv \Omega_{11}^{11}(q) - \tilde{\Omega}_{11}^{11}(q)$ and where the normal-ordered one-body part of $\Omega_{0}(q)$ is diagonal, i.e.,
\[ \tilde{\Omega}_{11}^{11}(q) \equiv \sum_{k} E_{k}(q) \beta_{k}^{\dagger}(q) \beta_{k}(q) , \]
with $E_{k}(q) > 0$ for all $k$.

C.6.2 First-order correction

At first order in BMBPT, singles and doubles BCI-like coefficients read as
\[ C^{(1)k_{1}k_{2}}(q) \equiv - \frac{\Omega^{k_{1}k_{2}}(q)}{E_{k_{1}k_{2}}(q)} , \tag{70a} \]
\[ C^{(1)k_{1}k_{2}k_{3}k_{4}}(q) \equiv - \frac{\Omega^{k_{1}k_{2}k_{3}k_{4}}(q)}{E_{k_{1}k_{2}k_{3}k_{4}}(q)} , \tag{70b} \]
where $E_{k_{1}k_{2}...}(q) \equiv E_{k_{1}}(q) + E_{k_{2}}(q) + \ldots$. 

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C.6.3 Second-order correction

At second order in MBPT, singles and doubles BCI-like coefficients read

\[
C^{(2)k_1k_2}(q) = \frac{1}{6} P(k_1/k_2) \sum_{k_3k_4} C^{(1)k_1k_2k_3}(q) \Omega_{k_1k_2k_3}^{k_4}(q) \\
+ \frac{1}{2} \sum_{k_3k_4} C^{(1)k_2k_3k_4}(q) \Omega_{k_2k_3k_4}^{k_1}(q) \\
+ \frac{1}{2} \sum_{k_3k_4} C^{(1)k_3k_4k_1}(q) \Omega_{k_3k_4k_1}^{k_2}(q) \\
+ P(k_1/k_2) \sum_{k_3} C^{(1)k_1k_3}(q) \Omega_{k_1k_3}^{k_2}(q),
\]

(71a)

\[
C^{(2)k_2k_3k_4}(q) \equiv \frac{1}{2} P(k_1/k_2/k_3k_4) \sum_{k_5k_6} C^{(1)k_2k_3k_4}(q) \Omega_{k_2k_3k_4}^{k_5k_6}(q) \\
+ P(k_4/k_1k_2k_3) \sum_{k_5} C^{(1)k_1k_2k_3}(q) \Omega_{k_1k_2k_3}^{k_4}(q) \\
+ P(k_1/k_2k_3k_4) \sum_{k_5} C^{(1)k_3k_4k_1}(q) \Omega_{k_3k_4k_1}^{k_2}(q) \\
+ P(k_1/k_2k_3k_4) \left[ C^{(1)k_2}(q) C^{(1)k_3}(q) \right],
\]

(71b)

where anti-symmetrizing operators \( P(\cdots / \cdots) \) are expressed in terms of the of the permutation operator as

\[
P(k_1/k_2) \equiv 1 - P_{k_1k_2},
\]

(72a)

\[
P(k_1/k_2k_3k_4) \equiv 1 - P_{k_1k_2} - P_{k_1k_3} - P_{k_1k_4}.
\]

(72b)

\[
P(k_1/k_2k_3k_4) \equiv 1 - P_{k_1k_2} - P_{k_1k_3} - P_{k_1k_4} + P_{k_1k_3k_4}.
\]

(72c)

D Error-function sampling

D.1 Error function

The error function introduced in Eq. (31) can be interpreted as the first-order correction to the energy due to the perturbation \( \delta H[\rho] \equiv H_{2B}[\rho] - H \). Knowing that for a generic \( n \)-body operator \( O^{(nn)} \)

\[
\left\langle \Psi \left| O^{(nn)} \right| \Psi \right\rangle = \frac{1}{n!} \sum_{n_1 \cdots n_n} \left\langle \Psi \left| A_{b_1 \cdots b_n}^{a_1 \cdots a_n} \right| \Psi \right\rangle \\
= \left( \frac{1}{n!} \right)^2 \rho^{(n)} \cdot W^{(n)}.
\]

(73)

Eq. (31) can be written as

\[
\Delta E_{2B}^{2B}[\rho] = - \left( \frac{1}{3!} \right)^2 w^{(3)} \cdot (\rho^{(3)}) \Psi \\
+ \left( \frac{1}{2!} \right)^2 \left( w^{(3)} \cdot (\rho^{(2)}) \Psi \right) \cdot \rho \\
- \frac{1}{2!} \left( w^{(3)} \cdot (\rho \cdot \rho^{(2)}) \Psi \right) \\
+ \frac{1}{3!} w^{(3)} \cdot (\rho \cdot \rho \cdot \rho \Psi) \\
= - \left( \frac{1}{3!} \right)^2 \lambda^{(3)} \Psi \\
+ \left( \frac{1}{2!} \right)^2 \left( (w^{(3)} \lambda^{(2)} \Psi) \cdot (\rho - \rho \Psi) \right) \\
+ \frac{1}{3!} w^{(3)} \cdot (\rho - \rho \Psi \cdot \rho \Psi) \Xi(3)
\]

(74)

where \( \lambda^{(n)} \Psi \) denotes the irreducible \( n \)-body density matrix (or cumulants) [50,51] that, for \( n \geq 2 \), encodes genuine \( n \)-body correlations in \( |\Psi\rangle \). Whenever \( |\Psi\rangle \) reduces to a Slater determinant, one has \( \lambda^{(n)} \Psi = 0 \) for \( n \geq 2 \). Inspecting Eq. (74), one observes that the error

1. only depends on the three-nucleon interaction and involves up to the 3-body (irreducible) density matrix of \( |\Psi\rangle \),
2. can be written as a cubic polynomial in the variable \( \rho - \rho \Psi \) whenever involving irreducible density matrices of \( |\Psi\rangle \),
3. is zero (and thus minimal in absolute value) for \( \rho = \rho \Psi \) whenever \( |\Psi\rangle \) contains at most genuine 2-body correlations, which is notably the case whenever \( |\Psi\rangle \) reduces to a Slater determinant,
4. is in general non-zero for \( \rho = \rho \Psi \) and measures in that case genuine 3-body correlations encoded into \( \chi^{(3)} \Psi \). While the error does not minimize for \( \rho = \rho \Psi \) in general, the fact that \( \rho = \rho \Psi \) is the optimal solution whenever \( |\Psi\rangle \) contains at most genuine 2-body correlations indicates that the optimal \( \rho \) cannot be very different from \( \rho \Psi \) whenever \( |\Psi\rangle \) is a weakly correlated \( J^\Pi = 0^+ \) state.

D.2 Random one-body density matrices

The goal is to sample the error function \( \Delta E_{2B}^{2B}[\rho] \) within the space of one-body density matrices \( \{\rho\} \) associated with \( J^\Pi = 0^+ \) states\(^{30}\). Thus, a large set of density matrices

\(^{30}\) Strictly speaking, and as the procedure detailed in Sect. 2.3 makes clear, the one-body density matrix employed in the construction of \( H_{2B}[\rho] \) does not have to be actually related to a many-body state, i.e. it does not have to be \( N \)-representable. It is at least mandatory to use trial one-body density matrices carrying the fingerprints of the symmetry constraints associated with a true state in order for \( H_{2B}[\rho] \) to
\( \{ \rho^{Rd} \} \) is randomly generated in the sHO basis \(|a\rangle; a \equiv a_d j_a m_a \) under the constraints that

\[
\rho_b^a = (\rho_a^b)^* , \tag{75a}
\]

\[
\rho_a^b \equiv \delta_{j_a j_b} \delta_{m_a m_b} \delta_{\pi_a \pi_b} e^{\delta \rho_{a b}} , \tag{75b}
\]

\[\text{Tr} \rho = 1 \langle 1 \rangle, \rho = A, \tag{75c}\]

\[0 \leq \text{diag}(\rho) \leq 1, \forall b, \tag{75d}\]

where \( \langle 1 \rangle \) denotes the identity operator on \( \mathcal{H}_1 \) and where diag(\( \rho \)) gathers the eigenvalues. More specifically, the procedure works as follows

1. choice of a reference one-body density matrix \( \rho^{ref} \),

2. diagonalization of \( \rho^{ref} \)

\[
\rho^{ref} \equiv L^T \text{diag}(\rho) L, \tag{76}\]

where \( L \) denotes an orthogonal matrix.

3. choice of two coefficients \( a_d, \ a_o \) characterizing the amplitude of the random perturbation to be performed next.

4. sampling of a random perturbation \( \delta r \) of the diagonal matrix elements of \( r \) verifying

\[
\sum_a \delta r_a = 0, \tag{77a}\]

\[r_a + \delta r_a \in [0, 1], \forall a, \tag{77b}\]

\[|\delta r_a| \leq a_d, \forall a. \tag{77c}\]

5. sampling of a random skew-symmetric matrix \( \delta l \) with all upper-diagonal coefficients chosen via a normal distribution \( \mathcal{N}(0, 1) \).

6. exponentiation of \( \delta l \) to obtain an orthogonal matrix

\[\delta L \equiv \exp[\alpha_o \delta l]. \tag{78}\]

7. computation of the random neighbour of \( \rho^{ref} \)

\[\rho^{Rd} \equiv (L \delta L)^T \text{diag}(r + \delta r) L \delta L. \tag{79}\]

Although the sampling is not uniform, all densities with the required properties can in principle be obtained via this method.

\[\text{E Spherical Hartree-Fock field}\]

Given a test one-body density matrix \( \rho \) and considering that the many-body state of interest \( |\Psi\rangle \) is a Slater determinant, the one-body Hamiltonian at play in the HF minimization problem based on \( H^{2B}[\rho] \) is, given Eq. (74),

\[
\begin{align*}
\left[ h^{HF(2B)}_{\rho} |\rho^{\Psi}; \rho \right]_b &= \frac{\delta \langle \psi | H^{2B}[\rho] | \psi \rangle}{\delta [\rho^{\Psi}]}_b \\
&= \frac{\delta \langle \psi | H \rho^{\Psi} \rangle}{\delta [\rho^{\Psi}]}_b + \frac{\delta \Delta E^{2B}_\Psi}{\delta [\rho^{\Psi}]}_b \\
&= [h^{HF}[\rho^{\Psi}]^a - \frac{1}{2} \left\langle w^{(3)} | (\rho - \rho^{\Psi})^{(2)} \right\rangle^a]_b. \tag{80}
\end{align*}
\]

In Eq. (80), \( h^{HF}[\rho^{\Psi}] \) denotes the one-body HF Hamiltonian obtained from the full \( H \) whose associated solution is \( \rho^{\Psi} \). Equation (80) allows one to appreciate the implications of using \( H^{2B}[\rho] \) at the sHF level, i.e. in the mean-field calculation of a doubly closed-shell nucleus such as \( ^{16}\text{O} \) and \( ^{40}\text{Ca} \).

One observes that

- in general, the use of \( H^{2B}[\rho] \) generates an additional term on top of \( h^{HF}[\rho^{\Psi}] \), eventually leading to \( \rho^{\Psi} \neq \rho^{\Psi} \) and \( \Delta E^{2B}_\Psi \neq 0 \) at convergence,

- even when using \( H^{2B}[\rho^{\Psi}] \), the additional term differs from zero such that \( \rho^{\Psi} \neq \rho^{\Psi} \) and \( \Delta E^{2B}_\Psi \neq 0 \) at convergence,

- only if one were to set \( \rho = \rho^{\Psi} \) in \( H^{2B}[\rho] \) throughout the iterative procedure, thus modifying the approximate Hamiltonian along the way, would the correction term vanish in Eq. (80) at convergence and the sHF solution based on \( H^{2B}[\rho] \) be the same as the one obtained from \( H \). This particular case is equivalent to constructing \( H^{2B}[\rho] \) through Wick’s theorem with respect to the self-consistent sHF Slater determinant itself and is thus identical to the NO2B procedure, which indeed does not lead to any approximation at the HF level.

\[\text{F Measure of the systematic deviations}\]

In order to assess quantitatively the errors induced by the approximation and compare the different effective interactions, measures of the average deviation between the results obtained with \( H^{2B}[\rho] \) and \( H \) are introduced for each method, i.e.

\[
\begin{align*}
\rho^{ref}_{HF} &\equiv \frac{1}{n_{\text{data}}} \sum_{n_{\text{nucle}}} \left| \frac{E_{HF}^{\Psi}[\rho] - E_{HF}^{\Psi}}{E_{HF}^{\Psi}} \right| , \tag{81a} \\
\rho^{ref}_{PHFB} &\equiv \frac{1}{n_{\text{data}}} \sum_{n_{\text{nucle}}} \sum_f \left| \frac{E_{PHFB}^{\Psi}[\rho] - E_{PHFB}^{\Psi}}{E_{PHFB}^{\Psi}} \right|. \tag{81b}
\end{align*}
\]
where in practice states up to $J = 6$ are taken into account when applicable and where $O$ denotes any observable computed within the PGCM formalism (energy, electric and magnetic moments, transitions and radii). In each case, $n_{\text{data}}$ denotes the number of terms in the sum(s).

The deviation on PHFB excitation energies is given by the formula

$$r_{\text{PHFB-S}} \equiv 1 \frac{1}{n_{\text{data}}} \sum_{n_{\text{nuclei}}} \sum_{J} \left| \frac{\delta E_{\text{PHFB}}(\rho) - \delta E_{\text{PHFB}}^{J}}{\delta E_{\text{PHFB}}} \right|.$$  

(82)

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