Effect of pairing correlations on the isospin-mixing parameter in deformed $N = Z$ even-even nuclei

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Within the particle-number conserving highly truncated diagonalization approach (amounting to a severely truncated shell model built on self-consistent mean-field single-particle states), we investigate the isospin mixing in the ground state of axially deformed even-even $N = Z$ nuclei with $A < 80$. The Skyrme interaction in its SIII parametrization is used to generate the self-consistent mean-field solution, whereas the effective residual interaction is approximated by density-independent δ interactions in the $T = 0$ and $T = 1$ isospin channels. In the correlated ground state of the considered nuclei, the obtained values of the isospin-mixing parameter range from a few tens of a percent to a couple of percents. The pairing correlations in both isospin channels are found to increase a little the isospin-mixing parameter with respect to the Hartree-Fock value by two competing mechanisms. In the $T = 0$ channel, isospin mixing is brought mostly by neutron-proton one-pair excitations, whereas in the $T = 1$ channel it is essentially generated by the difference between neutron-neutron and proton-proton one-pair excitations.

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I. INTRODUCTION

One of the most striking aspects of the structure of atomic nuclei is the very small violation of the isospin invariance. This is so even for heavy nuclei where the Coulomb interaction is thought *a priori* to act in a nonperturbative manner. As pointed out, for instance, in Ref. [1], this is attributable to the weak variation of the symmetry-breaking Coulomb field over the nuclear volume. It has also been suggested from phenomenological and fundamental (at the level of quarks having different masses) points of view that genuine isospin nonconserving parts of the strong interaction should be considered [2]. They should, however, be rather small as compared to their conserving counterparts.

As a consequence, a nuclear ground state $|\Psi\rangle$ may be thought as being composed of mostly a $T_0 = |T_z|$ component, where $T_z = (N - Z)/2$, with a small $T_0 + 1$ admixture, namely, omitting other degrees of freedom for simplicity,

$$|\Psi\rangle \approx c_0\,|T_0\,T_z\rangle + c_1\,|T_0 + 1\,T_z\rangle, \tag{1}$$

with $|c_0|^2 + |c_1|^2 = 1$, all above kets being normalized. The isospin-mixing parameter is then simply given by $\alpha = |c_1|^2$.

Even though in most cases the isospin invariance may be flatly assumed, there are phenomena where a specific knowledge of the isospin mixing is needed. This is the case whenever some observed transition or reaction would be forbidden, should this invariance be exactly fulfilled.

It has also been noticed (see the seminal paper by MacDonald [3], as well as Ref. [4] as an example of further studies) that the amount of isospin mixing of the T_0 and $T_0 + 1$ isospin components in the ground state could be related with RPA-like correlations associated with the isovector monopole mode. Interesting cases where the isospin mixing has to be considered are also related with β-decay properties (see, e.g., the review of Ref. [5]). Of particular importance in that respect are the studies of superallowed $0^+ \to 0^+$ nuclear β decays in the context of the tests of the *conserved-vector-current* hypothesis (see, e.g., Ref. [6]) through ft-value measurements. Hence, a specific determination of the effect of the isospin mixing is required to correct the value yielded by the crude isospin-multiplet approximation. This yields the so-called δ_C correction term (see, e.g., Ref. [7]).

Before entering in a subsequent study into a detailed assessment of the transition matrix element involved in such particular decays, we consider it interesting to evaluate first the actual importance of the isospin mixing, as measured, for instance, by α. This is the subject of the present paper.

Presently available theoretical estimates of the isospin mixing fall into three different categories.

(i) First, one has to quote the hydrodynamical approach of Bohr, Damgård, and Mottelson [8], which consists of quantifying the normal modes associated with the polarization effect of the Coulomb field on a spherically symmetrical isovector density. In $N = Z$ nuclei this approach yields the probability α of the $T = 1$ component, in sole addition to the dominating $T = 0$ component, which is given by

$$\alpha = 3.5 \times 10^{-7} Z^2 A^{2/3}. \tag{2}$$

It therefore amounts, for example, for the ^{40}Ca nucleus to about 0.16%. In nuclei having a neutron excess, α (meaning now the probability of the $|T_z| + 1$ component over the dominating $|T_z|$ component) is estimated to be equal to the value given by Eq. (2) divided by $|T_z| + 1$. This reduction, which is expressed in terms of a factor being merely the square of a Clebsch-Gordan coefficient, had been first advocated by Lane and

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Soper [9]. It yields, for example, for the ^{48}Ca nucleus, a value of α of about 0.04%.

(ii) The second class of approaches is based on shell-model calculations. Their success is contingent, as usual within such an approach, upon the relevance of the matrix elements in use. For the description of isospin mixing, an accurate determination of Coulomb matrix elements is, of course, of paramount importance (see, for instance, the discussion of Coulomb energy differences in $A = 47$ and $A = 49$ mirror pairs [10]). This constitutes an *a priori* necessary condition to provide valuable answers to the question left open on the real importance of isospin nonconserving forces as studied, for example, to explain the isobaric multiplet yrast energies in Ref. [11]. Other concerns are related to a good description of radial single-particle wave functions as in, for example, Ref. [12] to describe asymmetry factors in parity-violating electron scattering. One definite difficulty of shell-model calculations is attributable to the fact that they do not take into account any core isospin mixing, except, of course, for the no-core shell model calculations limited to very light nuclei (see, for instance, Ref. [13]).

(iii) One might then be inclined to think that microscopic calculations making use of phenomenological nucleon-nucleon forces should be able to describe the polarization effects of the Coulomb interaction, at least at the mean-field level, in a satisfactory way. Indeed, as opposed to shell-model calculations, mean-field calculations are expected to provide rather elaborate single-particle wave functions and they do not rely on any inert-core approximation. However, apart from possible consequences of well-known symmetry violations inherent to the mean-field approximation requiring isospin projection, as done by Caurier [14] and Satuła [15], they require as a next very important step to account accurately for the correlations. This may be done without serious problems for RPA-type correlations, as performed, for instance, in Refs. [16,17]. In Ref. [16], it is shown that the hydrodynamical ansatz of Ref. [8] underestimates the isospin mixing by a factor of 2 to 4 (see Fig. 3 of Ref. [16]).

Calculations within the RPA for the isovector monopole mode of Ref. [4] provide upper limits for α, for example, about 1.45% in ^{40}Ca as calculated with the Skyrme SIII effective force [18]. It is important to note that the latter approaches do not include pairing correlations. There are good practical reasons for such an omission. The usual handling of pairing correlations within a kind of Bogoliubov quasiparticle vacuum approximation as in the BCS or Hartree-Fock-Bogoliubov theory is totally unfit for the isospin-mixing problem. Indeed, such an ansatz yields spurious components in the particle numbers of both charge states, giving rise, in turn, to a spurious mixing of T_z components. This invalidates *a priori* any attempt to extract out of these solutions any meaningful T-mixing properties.

This is why we make use of the highly truncated diagonalization approach (HTDA), which can be interpreted as a strongly truncated shell model built on a self-consistent Hartree-Fock-BCS solution [19–25]. Moreover, we focus on the role of $T = 1$ and $T = 0$ pairing correlations, leaving for a future work the inclusion on an equal footing of RPA correlations in the HTDA framework as in Ref. [24]. Because we are interested in the isospin-symmetry-breaking mechanisms at the many-body level, we choose the SIII parametrization of the Skyrme energy-density functional to generate the self-consistent mean field as a representative parametrization. To describe the pairing correlations we use zero-range density-independent residual interactions in both isospin channels. The use of more recent Skyrme parametrizations or finite-range residual interactions would not alter the generality of our conclusions.

In this paper we focus on even-even $N = Z$ nuclei because they exhibit stronger isospin mixing than other even-even nuclei. Moreover, the Hartree-Fock approximation applied to these nuclei does not spuriously break the isospin symmetry in the absence of isospin nonconserving interactions (in our work the Coulomb interaction only), as numerically checked in Ref. [15]. For the mean-field approach to hold, we need to restrict to rigid nuclei, that is, nuclei exhibiting a stiff potential energy surface in the deformation space around the ground-state minimum. To keep contact with available experimental data, we limit ourselves to light- and medium-mass nuclei ($A < 80$). Moreover, we consider only axially symmetric ground-state shapes. According to the calculations of Refs. [26,27], the nuclei to retain are thus ^{28}Si, ^{48}Cr, ^{68}Se (oblate and prolate solutions responsible for a shape coexistence [28]), and ^{76}Sr.

In this work we study the mechanisms by which the $T = 0$ and $T = 1$ pairing correlations bring isospin mixing into the HTDA ground state of well-deformed $N = Z$ even-even nuclei. In addition, we test the quality of the usual approximation (1) consisting of neglecting the $T \geqslant 2$ components in the expansion of the nuclear ground state onto eigenstates of the $\hat{\mathbf{T}}^2$ operator and analyze the sensitivity of the isospin admixture to the treatment of the Coulomb interaction.

The paper is organized as follows. In Sec. II we present the HTDA formalism and the algebraic approach to isospin projection after variation to extract the isospin-mixing parameter. We also discuss the properties of the approximate good-isospin basis, made of the same eigenvectors of $\hat{\mathbf{T}}^2$ as those obtained in the limit where the Coulomb interaction is vanishing. Then in Secs. III to V we present and discuss successively the results about the isospin-mixing in the mean-field solutions and the structure of the pair-correlated ground-state solutions and their isospin mixing. Concluding remarks and perspectives are given in Sec. VI.

II. THEORETICAL FRAMEWORK

A. The highly truncated diagonalization approach

In self-consistent mean-field-plus-pairing approaches making use of a phenomenological density-dependent effective interaction, such as the Skyrme-Hartree-Fock-BCS or the Gogny-Hartree-Fock-Bogoliubov approximations, the ground state is a quasiparticle vacuum taking the form of a linear

combination of Slater determinants corresponding to different particle numbers (for neutrons and protons). It is obtained by a variational procedure leading to a self-consistent one-body eigenvalue problem.

In contrast, the HTDA framework explicitly preserves the particle-number symmetry through the expansion of the ground state in a basis of Slater determinants corresponding to the same number of neutrons and protons. The ground-state solution is determined by diagonalizing the Hamiltonian in a basis relevant to the type of correlations to be described (here pairing correlations). In this way, the HTDA approach can be viewed as a kind of intrinsic-state shell model. However, instead of using an underlying harmonic-oscillator one-body potential, we use the one-body potential issuing from a Skyrme-Hartree-Fock-BCS calculation. We thus expect that, owing to the self-consistency of the thus obtained mean-field solution, the many-body basis can be chosen much smaller than in the standard shell-model approach.

More precisely, the HTDA Hamiltonian is a phenomenological effective Hamiltonian based on the following steps. We begin with a Hamiltonian written as the sum of the kinetic energy $\hat{K}$, the nuclear interaction $\hat{V}_{NN}$ (assumed here to be a two-body operator), and the Coulomb interaction $\hat{V}_C$ (between pointlike protons):

$$\hat{H} = \hat{K} + \hat{V}_{NN} + \hat{V}_C. \tag{3}$$

The total interaction between the nucleons, $\hat{V}_{NN} + \hat{V}_C$, is denoted by $\hat{V}$. Then we consider an attractive one-body potential $\hat{U}$, obtained in this work by a Skyrme-Hartree-Fock-BCS calculation, and the associated one-body Hamiltonian $\hat{H}_0$ defined by

$$\hat{H}_0 = \hat{K} + \hat{U}, \tag{4}$$

whose single-particle eigenstates $|k\rangle$, corresponding to the eigenvalues e_k, are assumed to form an orthonormal basis of the one-body space (including position, spin, and isospin degrees of freedom). The lowest eigenstate of $\hat{H}_0$ is a quasiparticle vacuum of particle-hole type, in other words, a Slater determinant, denoted by $|\Phi_0\rangle$. In the following this state is called merely quasivacuum and serves as a reference state in the definition of all normal products. We can express the Hamiltonian $\hat{H}$ as the sum of a one-body Hamiltonian, which we refer to as the *independent quasiparticle Hamiltonian* $\hat{H}_{\rm iqp}$, a residual-interaction operator $\hat{V}_{\rm res}$ and a constant depending on $|\Phi_0\rangle$,

$$\hat{H} = \hat{H}_{\rm iqp} + \hat{V}_{\rm res} + \langle\Phi_0|\hat{H}|\Phi_0\rangle. \tag{5}$$

The independent quasiparticle Hamiltonian $\hat{H}_{\rm iqp}$ is the normal-product form of $\hat{H}_0$,

$$\hat{H}_{\rm iqp} =: \hat{H}_0 := \hat{H}_0 - \langle\Phi_0|\hat{H}_0|\Phi_0\rangle. \tag{6}$$

In the single-particle basis associated with $\hat{H}_0$, $\hat{H}_{\rm iqp}$ takes, in second quantization, the form

$$\hat{H}_{\rm iqp} = \sum_k e_k \ :\hat{a}_k^\dagger \hat{a}_k:, \tag{7}$$

where the operator $\hat{a}_k^\dagger$ creates a nucleon in a state $|k\rangle$ whose isospin is implicitly specified in the label k, whereas a_k annihilates a nucleon in the state $|k\rangle$. The residual interaction $\hat{V}_{\rm res}$ is defined by

$$\hat{V}_{\rm res} =: \hat{V} : + : \overline{V} - \hat{U} :, \tag{8}$$

where $\overline{V}$ denotes the one-body reduction of $\hat{V}$ for $|\Phi_0\rangle$ and $\hat{V} =: \hat{V} : + : \overline{V} : + \langle\Phi_0|V|\Phi_0\rangle$ according to the Wick theorem applied to the two-body operator $\hat{V}$, so that $: \hat{V} : = \hat{V} - \overline{V} + \langle\Phi_0|V|\Phi_0\rangle$. Because the potential $\hat{U}$ comes from a Hartree-Fock-BCS calculation, it is expected to slightly differ from $\overline{V}$ when the solution to the BCS equations corresponds to nonvanishing pairing gaps. In the HTDA framework we neglect the contribution $: \overline{V} - \hat{U} :$ to the residual interaction $\hat{V}_{\rm res}$.

A proper account of pairing correlations beyond $|\Phi_0\rangle$ requires one to use in $\hat{V}_{\rm res}$ a nucleon-nucleon interaction $\hat{V}_{NN}$ having satisfactory particle-particle matrix elements. Very few Skyrme parametrizations provide a good description of mean-field and pairing properties simultaneously. Those that do (such as, e.g., the SkP parametrization [29]) are unfortunately not fitted to reproduce pairing properties in $N = Z$ nuclei. Therefore, we resort to replacing the nuclear two-body interaction $\hat{V}_{NN}$ in $\hat{V}_{\rm res}$ with a contact interaction in the form of a density-independent δ interaction $\hat{V}_\delta$. The nuclear part $\hat{V}_{NN,\rm res}$ of the residual interaction is thus written as

$$\hat{V}_{NN,\rm res} \approx : \hat{V}_\delta : . \tag{9}$$

In this way, the expectation value of $\hat{V}_{NN,\rm res}$ in the quasivacuum $|\Phi_0\rangle$ vanishes.

Then one has to ensure that the δ interaction acts on states of well-defined spin and isospin. One therefore writes $\hat{V}_\delta$ in the form

$$\hat{V}_\delta = \hat{V}_\delta^{(T=0)} + \hat{V}_\delta^{(T=1)}, \tag{10}$$

with [22]

$$\hat{V}_\delta^{(T)} = V_0^{(T)}\, \delta(\mathbf{r}_1 - \mathbf{r}_2)\, \hat{\Pi}_S\, \hat{\Pi}_T, \tag{11}$$

where $\hat{\Pi}_S$ ($\hat{\Pi}_T$) is the spin (isospin) projection operator in the two-body subspace of the Fock space. Because of the space-symmetric character of the δ interaction, specific combinations of $\hat{\Pi}_S$ and $\hat{\Pi}_T$ operators are imposed when acting on an antisymmetrized two-body state, namely ($S = 0$, $T = 1$) and ($S = 1$, $T = 0$). The strength of $\hat{V}_\delta$ in the $T = 0$ channel is usually expressed as a fraction x of the strength in the $T = 1$ channel,

$$V_0^{(T=0)} = x\, V_0^{(T=1)}. \tag{12}$$

The calculation of the two-body matrix elements of $\hat{V}_\delta$ is presented in Appendix A.

In practical HTDA applications, as in any shell-model calculation, the many-body basis in which the Hamiltonian is diagonalized has to be truncated. Here we consider a model space including single-pair (SP), double-pair (DP), and triple-pair (TP) excitations—with respect to the quasivacuum $|\Phi_0\rangle$—whose particle-hole excitation energy does not exceed a given cutoff energy $E_{\rm cut}$. We choose $E_{\rm cut}$ as three times the empirical intershell energy $\hbar\omega(A) = 41\, A^{-1/3}$ (in MeV). Because the correlations considered in this work are of pairing type in both $T = 1$ and $T = 0$ channels, all combinations of nn, np, and pp pairs in the excited configurations are taken into account.

B. Treatment of the Coulomb interaction

As mentioned at the beginning of the previous section, the finite size of nucleons is not taken into account in the present work. Therefore, the Coulomb interaction $\hat{V}_C$ acts between pointlike protons only. Moreover, given the partitioning (5) of the Hamiltonian $\hat{H}$, it contributes to the mean-field channel through a term $\hat{U}_C$ in the one-body potential $\hat{U}$ as well as to the residual interaction $\hat{V}_{\rm res}$ through a term $\hat{V}_{C,\rm res}$ approximated by

$$\hat{V}_{C,\rm res} \approx : \hat{V}_C :, \tag{13}$$

because we consistently neglect the term $: \overline{V}_C - \hat{U}_C :$ in Eq. (8). Therefore, the residual interaction used in this work can be written as

$$\hat{V}_{\rm res} \approx : \hat{V}_\delta : + : \hat{V}_C : . \tag{14}$$

For an accurate description of isospin mixing, we evaluate $\hat{U}_C$ exactly instead of using the Slater approximation [30]. To do so, we calculate the two-body matrix elements of $\hat{V}_C$ in the axially deformed harmonic-oscillator basis as discussed in Refs. [31,32] and recalled in Appendix B to keep this paper self-contained. These matrix elements are also used to evaluate exactly $: \hat{V}_C :$ in the many-body basis.

C. Approximate isospin distribution

From a general point of view, any many-body state $|\Psi\rangle$ of a (N, Z) nucleus can be expanded on good-isospin states,

$$|\Psi\rangle = \sum_{T=T_0}^{T_0+n} \sum_{\xi} a^{(n)}_{T,\xi} |\xi\ T\ T_z\rangle, \tag{15}$$

where ξ denotes all degrees of freedom other than isospin, $T_z = (N-Z)/2$, $A = N+Z$, and n is the number of T values beyond T_0 that are included. The maximal T value $T = A/2$ results from angular-momentum coupling rules. However, this expansion is known to rapidly converge with T for the ground state of an even-N–even-Z nucleus and can be truncated at $T_0 + n \ll A/2$. The resulting isospin probability distribution of $|\Psi\rangle$ is thus defined by

$$P^{(n)}_\Psi(T) = \sum_{\xi} \left| a^{(n)}_{T,\xi} \right|^2 \quad (T_0 \leqslant T \leqslant T_0 + n) \tag{16}$$

and is the solution to the linear system of equations

$$\langle\Psi|\Psi\rangle = \sum_{T=T_0}^{T_0+n} P^{(n)}_\Psi(T), \tag{17}$$

$$\langle\Psi|\hat{\mathbf{T}}^2|\Psi\rangle = \sum_{T=T_0}^{T_0+n} T(T+1)\, P^{(n)}_\Psi(T), \tag{18}$$

$$\langle\Psi|\hat{\mathbf{T}}^4|\Psi\rangle = \sum_{T=T_0}^{T_0+n} T^2(T+1)^2\, P^{(n)}_\Psi(T), \tag{19}$$

$$\vdots$$

$$\langle\Psi|\hat{\mathbf{T}}^{2n}|\Psi\rangle = \sum_{T=T_0}^{T_0+n} T^n(T+1)^n\, P^{(n)}_\Psi(T). \tag{20}$$

Setting $\tau_i = (T_0+i)(T_0+i+1)$ for i ranging from 0 to n, one can bring this system to the matrix form:

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ \tau_0 & \tau_1 & \tau_2 & \cdots & \tau_n \\ \tau_0^2 & \tau_1^2 & \tau_2^2 & \cdots & \tau_n^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \tau_0^n & \tau_1^n & \tau_2^n & \cdots & \tau_n^n \end{pmatrix}}_{\mathcal{V}} \begin{pmatrix} P^{(n)}_\Psi(T_0) \\ P^{(n)}_\Psi(T_0+1) \\ P^{(n)}_\Psi(T_0+2) \\ \vdots \\ P^{(n)}_\Psi(T_0+n) \end{pmatrix} = \begin{pmatrix} \langle\Psi|\Psi\rangle \\ \langle\Psi|\hat{\mathbf{T}}^2|\Psi\rangle \\ \langle\Psi|\hat{\mathbf{T}}^4|\Psi\rangle \\ \vdots \\ \langle\Psi|\hat{\mathbf{T}}^{2n}|\Psi\rangle \end{pmatrix}. \tag{21}$$

One can recognize a Vandermonde linear system of order $n+1$ with a nonvanishing determinant

$$\det \mathcal{V} = \prod_{0 \leqslant i < j \leqslant n} (\tau_j - \tau_i). \tag{22}$$

The Vandermonde matrix $\mathcal{V}$ can be analytically inverted to yield the following expression of the isospin distribution [33]:

$$P^{(n)}_\Psi(T) = \delta_{TT_0} + \sum_{j=1}^{n} \Gamma^{(n)}_{T-T_0\,j}\, \mathcal{T}_{2j}(T_0), \tag{23}$$

with

$$\Gamma^{(n)}_{ij} = (-)^{i+j}\, \frac{\sigma_{n-j}(\tau_0, \ldots, \tau_{i-1}, \tau_{i+1}, \ldots, \tau_n)}{\prod_{k=0}^{i-1}(\tau_i - \tau_k) \prod_{k=i+1}^{n}(\tau_k - \tau_i)}, \tag{24}$$

and

$$\mathcal{T}_{2k}(T) = \langle\Psi|\hat{\mathbf{T}}^{2k}|\Psi\rangle - T^k(T+1)^k, \quad k \in \mathbb{N}. \tag{25}$$

In the coefficients $\Gamma^{(n)}_{ij}$, $\sigma_k(X_1, X_2, \ldots, X_{\mathcal{N}})$ is the elementary symmetric polynomial of degree k whose general expression is

$$\sigma_k(X_1, \ldots, X_{\mathcal{N}}) = \sum_{1 \leqslant n_1 \leqslant \cdots \leqslant n_k \leqslant \mathcal{N}} X_{n_1} X_{n_2} \cdots X_{n_k}$$

and satisfying the identity (for any parameter λ)

$$\prod_{\ell=1}^{\mathcal{N}} (\lambda - X_\ell) = \sum_{k=0}^{\mathcal{N}} (-)^k \lambda^{\mathcal{N}-k} \sigma_k(X_1, \ldots, X_{\mathcal{N}}).$$

The isospin-mixing parameter for a nuclear state having a dominant isospin contribution T_d is defined by

$$\alpha = 1 - P^{(n)}_\Psi(T_d). \tag{26}$$

In the ground state of even-even $N = Z$ nuclei (i.e., $T_d = T_0 = 0$) we thus have for $n = 1$

$$\alpha = \tfrac{1}{2} \langle\Psi|\hat{\mathbf{T}}^2|\Psi\rangle, \tag{27}$$

that is the well-known expression $\alpha = \frac{1}{2}\langle\Psi|\hat{T}_-\hat{T}_+|\Psi\rangle$, and for $n = 2$ we obtain

$$\alpha = \tfrac{2}{3}\langle\Psi|\hat{\mathbf{T}}^2|\Psi\rangle - \tfrac{1}{12}\langle\Psi|\hat{\mathbf{T}}^4|\Psi\rangle. \quad (28)$$

The calculation of the matrix elements of the $\hat{\mathbf{T}}^4$ operator is presented in detail in Appendix C.

D. Approximate good-isospin basis

To analyze the isospin content of the pair-correlated ground state of an even-even $N = Z$ nucleus, the relevant many-body basis is built from the above-described Slater-determinant basis using a (real) unitary transformation which corresponds to the diagonalization of $\hat{\mathbf{T}}^2$ in the space spanned by the many-body basis in the limit where the Coulomb interaction is switched off. In this limit the Slater-determinant many-body basis can be partitioned in subsets of pair excitations of given orders that are separately invariant under $\hat{\mathbf{T}}^2$.

In each category mentioned above, an additional partitioning of the many-body basis is possible to obtain small groups (called *cluster* in the following) which are individually invariant under $\hat{\mathbf{T}}^2$. This partitioning comes from a general mechanism. Let us illustrate it within the subset of SP configurations.

A single-particle excitation involves one hole level and one particle level (fourfold degenerate because of the time-reversal and isospin symmetries). For a given hole level ℓ and a given particle level λ, four different SP excitations can occur, one *nn*-pair, one *pp*-pair, and two *np*-pair excitations. Such a set of levels thus defines a *cluster* of four many-body states. Let us call $\bar{\ell}$ ($\bar{\lambda}$) the time-reversal conjugate state of ℓ (λ), $n^\dagger_\lambda$ ($p^\dagger_\lambda$) the creation operator of a neutron (proton) in the state $|\lambda\rangle$, and n_ℓ (p_ℓ) the annihilation operator of a neutron (proton) in the state $|\ell\rangle$. With this notation, the like-nucleon pair excitations are defined, for a given cluster, by

$$|\Phi_{20}\rangle = n^\dagger_\lambda n^\dagger_{\bar{\lambda}} n_{\bar{\ell}} n_\ell|\Phi_0\rangle, \quad (29)$$

$$|\Phi_{02}\rangle = p^\dagger_\lambda p^\dagger_{\bar{\lambda}} p_{\bar{\ell}} p_\ell|\Phi_0\rangle, \quad (30)$$

whereas the two possible *np* pair excitations are

$$|\Phi_{11}\rangle = n^\dagger_\lambda p^\dagger_{\bar{\lambda}} p_{\bar{\ell}} n_\ell|\Phi_0\rangle, \quad (31)$$

$$|\Phi'_{11}\rangle = n^\dagger_\lambda p^\dagger_{\bar{\lambda}} p_\ell n_{\bar{\ell}}|\Phi_0\rangle. \quad (32)$$

The time-reversal symmetric expressions of the *np* pair excitations are

$$|\widetilde{\Phi}_{11}\rangle = \frac{1}{\sqrt{2}}\big(|\Phi_{11}\rangle + |\overline{\Phi}_{11}\rangle\big), \quad (33)$$

$$|\widetilde{\Phi}'_{11}\rangle = \frac{1}{\sqrt{2}}\big(|\Phi'_{11}\rangle + |\overline{\Phi}'_{11}\rangle\big). \quad (34)$$

Such a cluster is decoupled, according to $\hat{\mathbf{T}}^2$, from the other clusters defined by different sets of hole and particle levels (let us say m and μ with $m \neq \ell$ or $\mu \neq \lambda$ or both). All clusters are composed by the same type of SP excitations described above.

Thus, one can diagonalize the $\hat{\mathbf{T}}^2$ operator applying the same unitary transformation for each cluster whatever the size of the many-body basis. In terms of the proton-proton pair excitation $|\Phi_{02}\rangle$, neutron-neutron pair excitation $|\Phi_{20}\rangle$, and time-reversed symmetrized neutron-proton pair excitations $|\widetilde{\Phi}_{11}\rangle$ and $|\widetilde{\Phi}'_{11}\rangle$ created on the quasivacuum $|\Phi_0\rangle$, the eigenstates of $\hat{\mathbf{T}}^2$ are given, for a given cluster, by

$$|\Psi_{01}\rangle = \frac{1}{\sqrt{2}}(|\widetilde{\Phi}_{11}\rangle + |\widetilde{\Phi}'_{11}\rangle), \quad (35)$$

$$|\Psi_{02}\rangle = \frac{1}{\sqrt{3}}(|\Phi_{02}\rangle + |\Phi_{20}\rangle) + \frac{1}{\sqrt{6}}(|\widetilde{\Phi}_{11}\rangle - |\widetilde{\Phi}'_{11}\rangle), \quad (36)$$

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|\Phi_{02}\rangle - |\Phi_{20}\rangle), \quad (37)$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{6}}(|\Phi_{02}\rangle + |\Phi_{20}\rangle) - \frac{1}{\sqrt{3}}(|\widetilde{\Phi}_{11}\rangle - |\widetilde{\Phi}'_{11}\rangle). \quad (38)$$

The same idea exposed here for the SP excitation can be applied for the DPs and TPs but with a new aspect that generalizes what we have seen up to now.

Indeed, the number of levels (hole and particle) involved in a DP or a TP excitation is not unique. One has various *classes* of clusters according to the number of levels involved in a given cluster of excitations. The case of DP excitations is presented as an example in Table I. The possible classes of DP excitations with the corresponding value of the isospin T are listed in this table. A similar, but necessarily more complex table can be drawn for TP excitations.

TABLE I. Description of the possible classes of clusters within the DP-type excitations.

No. of levels (Hole, Particle)	Size of clusters	Isospin	
		T value	Degeneracy
(1, 1)	1	0	1
(1, 2) or (2, 1)	4	0	2
		1	1
		2	1
(2, 2)	38	0	10
		1	12
		2	12
		3	3
		4	1

In the presence of the Coulomb interaction, of much smaller strength (and longer range) than the nuclear force, the states (35)–(38) are generally expected to remain to a good approximation eigenstates of $\hat{\mathbf{T}}^2$ and the diagonal matrix elements of $\hat{\mathbf{T}}^2$ in these states to only slightly differ from the integer values $T(T+1)$. For this reason we call them *quasi-eigenstates* of $\hat{\mathbf{T}}^2$ associated with the nearest corresponding integer value of T. The same holds in the subsets of states beyond one-pair excitations but the expressions of the quasi-eigenstates become less transparent and are not given here. Altogether they form an approximate good-isospin basis.

The approximate eigenstate character for $\hat{\mathbf{T}}^2$ of the states of this basis constitutes what we call the *decoupled-cluster approximation* (DCA), an approximation checked numerically in Sec. V B below.

For practical calculations of the isospin admixtures in the dominantly $T = 0$ correlated ground state of an even-even

$N = Z$ nucleus, the DCA has an important consequence, which will become obvious when writing the pair-correlated ground-state solution $|\Psi\rangle$ as

$$|\Psi\rangle = a_0\,|\Phi_0\rangle + |\Psi_{\rm SP}\rangle + |\Psi_{\rm DP}\rangle + |\Psi_{\rm TP}\rangle, \tag{39}$$

where $|\Psi_{\rm SP}\rangle$, $|\Psi_{\rm DP}\rangle$, and $|\Psi_{\rm TP}\rangle$ contain, respectively, all the SP, DP, and TP pair excitations. For each category of multiple-pair excitations generically noted MP, we can then decompose the corresponding contribution $|\Psi_{\rm MP}\rangle$ to $|\Psi\rangle$ into the clusters k of approximate good-isospin basis states $|\Psi^{(k)}_{{\rm MP},T,i}\rangle$ (where i labels the different quasi-eigenstates associated with the same isospin T) in the following way:

$$|\Psi_{\rm MP}\rangle = \sum_{k,T,i} a^{(k)}_{{\rm MP},T,i}\,\big|\Psi^{(k)}_{{\rm MP},T,i}\big\rangle, \tag{40}$$

where the normalized state $|\Psi^{(k)}_{{\rm MP},T,i}\rangle$ is an approximate eigenstate of $\hat{\mathbf{T}}^2$ such that

$$\hat{\mathbf{T}}^2\big|\Psi^{(k)}_{{\rm MP},T,i}\big\rangle \approx \lambda^{(k)}_{{\rm MP},T,i}\big|\Psi^{(k)}_{{\rm MP},T,i}\big\rangle, \tag{41}$$

with $\lambda^{(k)}_{{\rm MP},T,i} \approx T(T+1)$. It then follows that each subset MP of pair excitations of a given order is approximately globally invariant under the action of the $\hat{\mathbf{T}}^2$ operator. Furthermore, the expectation value of the $\hat{\mathbf{T}}^2$ operator in the state $|\Psi_{\rm MP}\rangle$ can be approximated by a sum of *diagonal* matrix elements only,

$$\langle\Psi_{\rm MP}|\hat{\mathbf{T}}^2|\Psi_{\rm MP}\rangle \approx \sum_{k,T,i} \big|a^{(k)}_{{\rm MP},T,i}\big|^2 \lambda^{(k)}_{{\rm MP},T,i}. \tag{42}$$

The isospin-mixing parameter of $|\Psi\rangle$ can be split into the contribution α_0 of the quasivacuum $|\Phi_0\rangle$ and a contribution $C_{\rm corr}$ from the pairing correlations

$$\alpha = \alpha_0 + C_{\rm corr}, \tag{43}$$

As derived in Appendix D, the latter contribution takes the following form in the DCA

$$C_{\rm corr} \approx \sum_{\rm MP} C_{\rm MP}, \tag{44}$$

where the contribution $C_{\rm MP}$ from the MP excitations is defined by

$$C_{\rm MP} = \sum_{T,i} |a_{{\rm MP},T,i}|^2\big(P_{\Phi_0}(0) - P_{{\rm MP},T,i}(0)\big). \tag{45}$$

Separating out the $T = 0$ terms and introducing the isospin-mixing parameter $\alpha_{{\rm MP},0,i} = 1 - P_{{\rm MP},0,i}(0)$ of the quasi-eigenstate $|\Psi_{{\rm MP},0,i}\rangle$, we can write the contribution to α from the MP excitations as

$$C_{\rm MP} = \sum_i |a_{{\rm MP},0,i}|^2(\alpha_{{\rm MP},0,i} - \alpha_0) + \sum_{T\geqslant 1,i} |a_{{\rm MP},T,i}|^2\big(P_{\Phi_0}(0) - P_{{\rm MP},T,i}(0)\big). \tag{46}$$

Whereas the second term of $C_{\rm MP}$ in Eq. (46) is always positive, the first term can be negative if some states $|\Psi_{{\rm MP},0,i}\rangle$ contain a smaller isospin mixing than $|\Phi_0\rangle$. Therefore, $C_{\rm MP}$ is not necessarily positive.

Equation (46) reveals the two competing mechanisms by which the pairing correlations bring isospin impurity in the state $|\Psi\rangle$. A combination $|\Psi_{{\rm MP},T,i}\rangle$ of MP excitations alters the isospin mixing with respect to that of $|\Phi_0\rangle$ when the product of its weight $|a_{{\rm MP},T,i}|^2$ by the probability difference $\Delta P_{{\rm MP},T,i}(0) = P_{\Phi_0}(0) - P_{{\rm MP},T,i}(0)$ is large in absolute value. This condition distinguishes two categories of states which can contribute to the value of α: Those corresponding to $T = 0$ and contributing to the first term of $C_{\rm MP}$ and those corresponding to other values of T which contribute to the second term of $C_{\rm MP}$. On the one hand, the contributing states $|\Psi_{{\rm MP},0,i}\rangle$, which are characterized by a small value of $|\alpha_{{\rm MP},0,i} - \alpha_0|$, are those appearing with a large weight in the correlated state $|\Psi\rangle$. On the other hand, the states $|\Psi_{{\rm MP},T,i}\rangle$ with $T \geqslant 1$, for which $\Delta P_{{\rm MP},T,i}(0)$ is close to 1, can play a role in the isospin mixing of $|\Psi\rangle$ provided their weight $|a_{{\rm MP},T,i}|^2$ is at least of the order of a typical value of $|\alpha_{{\rm MP},0,i} - \alpha_0|$, which is a rather small quantity. We can thus expect that the major contribution to α will be brought by the SP quasi-eigenstates with $T = 0$ and $T = 1$.

III. ISOSPIN MIXING IN THE MEAN-FIELD SOLUTIONS

A. Conditions of the calculations

As mentioned above, our study is devoted to even-even $N = Z$ nuclei whose ground-state shapes calculated in the HF + BCS approach are axially symmetric. Between $A = 20$ and $A = 100$ only five nuclei satisfy these conditions (regardless of the Skyrme parametrization used): ^{28}Si (oblate ground state), ^{48}Cr (prolate ground state), ^{68}Se (oblate and prolate minima), and ^{76}Sr (prolate ground state). At this first stage, the one-body effect of pairing correlations is taken into account in the BCS approximation so as to generate a single-particle spectrum as realistic as possible. As mentioned in Sec. II B, the exchange Coulomb potential is treated exactly in the HF + BCS calculations. In these calculations the SIII parametrization [18] of the Skyrme force is used and the single-particle wave functions are expanded in the axially deformed harmonic oscillator basis including 11 oscillator major shells ($N_0 = 10$ in the notation of Ref. [34]). The oscillator parameters ω_z and $\omega_\perp$ are optimized for each nucleus using the Slater approximation to the exchange Coulomb potential because this adjustment is not significantly sensitive to the treatment of the exchange Coulomb potential. The BCS equations are self-consistently solved in a single-particle window going from the lowest-energy state up to 6 MeV above the Fermi level. To do so we use the seniority force of Ref. [23] whose strengths are defined by $g_\tau = G_0/(11 + N_\tau)$, where $N_\tau = \{N, Z\}$ and $G_0 = -17.7$ MeV. This force is supplemented by a smooth cutoff characterized by the width parameter $\mu = 0.2$ MeV in the notation of Ref. [23].

B. Calculation of the isospin-mixing parameter

In Fig. 1 we display the variation of the isospin-mixing parameter of the quasivacuum Slater determinant $|\Phi_0\rangle$—called

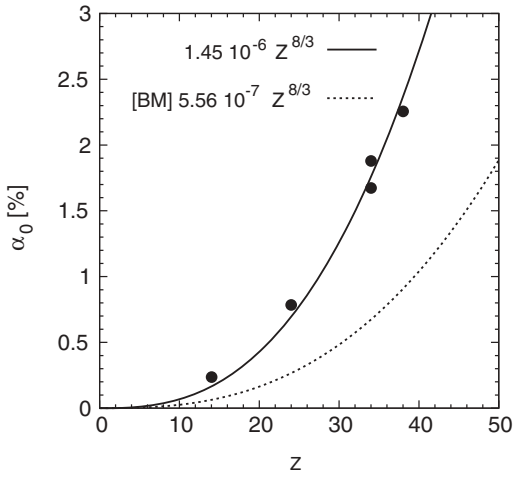

FIG. 1. Isospin-mixing parameter α_0 in the particle-hole quasivacuum $|\Phi_0\rangle$ for deformed even-even nuclei along the $N = Z$ line as a function of Z. The prediction of Bohr and Mottelson [1] is plotted in a dotted line for comparison.

mean-field solution—as a function of Z for the above four deformed even-even $N = Z$ nuclei (including both local minima in ^{68}Se). They follow the Bohr and Mottelson $Z^{8/3}$ trend of Eq. (2) but with a coefficient 2.6 times larger (see Introduction and Ref. [16]).

We have tested the role of the treatment of the exchange Coulomb potential in the mean-field solution by performing calculations of the isospin-mixing parameter in $|\Phi_0\rangle$ for the five considered solutions. As can be deduced from Table II the relative error is very small and does not exceed 3.5%.

It can be easily shown that the isospin mixing parameter in the quasivacuum $|\Phi_0\rangle$ of a $N = Z$ nucleus can be expressed as

$$\alpha_0 = -\sum_{j=1}^{n} \Gamma_{0j}^{(n)} \langle \Phi_0 | \hat{T}_-^j \hat{T}_+^j | \Phi_0 \rangle. \quad (47)$$

One finds that each of the expectation values in Eq. (47) depends only on partial overlaps of spin-space wave functions of the occupied neutron and proton states in $|\Phi_0\rangle$. Let us show this, as an example, for the lowest order (i.e., $n = 1$),

$$\alpha_0 \approx \frac{\langle \Phi_0 | \hat{T}_- \hat{T}_+ | \Phi_0 \rangle}{2} \approx \frac{1}{2} \left(Z - \sum_{\nu,\pi \in |\Phi_0\rangle} |\langle\langle \nu | \pi \rangle\rangle|^2 \right), \quad (48)$$

where ν and π denote the neutron and proton states occupied in $|\Phi_0\rangle$ and $\langle\langle \nu | \pi \rangle\rangle$ their spin-space overlap.

The remarkably weak difference between the values of α_0 listed in Table II seems to indicate that the different treatments of Coulomb terms (namely exact versus Slater approximation) induce a very small difference in the overlap of neutron and proton states. From this a very small difference between neutron and proton spin-space wave functions in both treatments can be inferred.

However, in a previous paper [32] (see also the references quoted therein) we have shown that the treatment of the Coulomb exchange potential at the mean-field level is of noticeable consequence on the proton single-particle energies. Even if this effect does not imply a difference in the isospin-mixing parameter α_0 for $|\Phi_0\rangle$, it will be very important, as we see in Sec. V C, when we treat pairing correlations within the HTDA approach.

TABLE II. Isospin-mixing parameter α_0 (expressed in %) in the particle-hole quasivacuum $|\Phi_0\rangle$ with the exchange Coulomb potential treated exactly and in the Slater approximation.

Nucleus	α_0	
	Exact	Slater
^{28}Si (oblate)	0.235	0.239
^{48}Cr (prolate)	0.784	0.785
^{68}Se (oblate)	1.880	1.815
^{68}Se (prolate)	1.673	1.635
^{76}Sr (prolate)	2.255	2.227

IV. STRUCTURE OF THE PAIR-CORRELATED GROUND STATES

To interpret the results of isospin-mixing calculations presented in the next section, in particular the role of pairing correlations, we need first to study the structure of the pair-correlated ground states calculated in the HTDA framework.

As is well known, in HF + BCS or HTDA pairing calculations in even-even nuclei away from the $N = Z$ line, the ground state is dominated by the HF solution and $T_z = \pm 1$ (nn and pp) pair excitations of a relatively low order. In the studied $N = Z$ nuclei we expect, in contrast, the np-pair excitations to play an important role in the correlated GS wave function. This is why our residual interaction includes the neutron-proton contribution in the $T = 0$ channel (characterized by the strength parameter $V_0^{(T=0)}$ of $\hat{V}_\delta$) in addition to the full $T = 1$ channel (i.e., including the $T_z = 0$ component) with the strength parameter $V_0^{(T=1)}$.

A. Convergence of the correlated wave functions

First, we investigate the convergence of the GS wave function as a function of the maximum pair-excitation order in three different truncation schemes: SP excited configurations beyond the quasivacuum (noted $|\Phi_0\rangle + \text{SP}$), SP and DP excitations (noted $|\Phi_0\rangle + \text{SP} + \text{DP}$), and all pair excitations up to three pairs (noted $|\Phi_0\rangle + \text{SP} + \text{DP} + \text{TP}$). In Fig. 2, the weights of the quasivacuum a_0^2, SP excitations $\langle \Psi_{\text{SP}} | \Psi_{\text{SP}} \rangle$ and DP excitations $\langle \Psi_{\text{DP}} | \Psi_{\text{DP}} \rangle$, obtained in the three truncation schemes, are displayed as functions of $V_0^{(T=1)}$ (left column) and, for a fixed value of $V_0^{(T=1)} = -200$ MeV fm^3, as functions of x (right column) in the representative ^{48}Cr nucleus. As can be seen the contribution of the SP configurations to the GS wave function is very well converged in the $|\Phi_0\rangle + \text{SP} + \text{DP}$

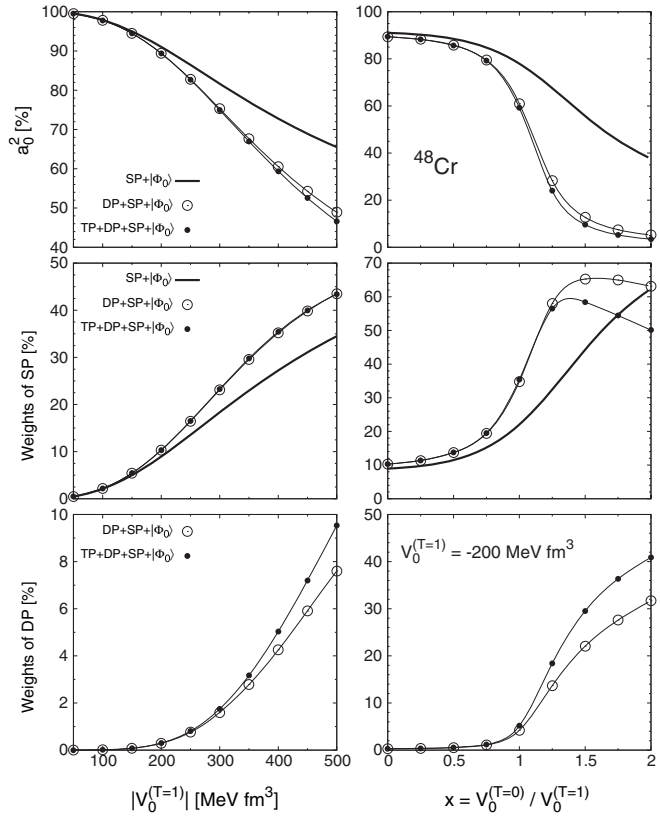

FIG. 2. Convergence of the ground-state structure as a function of the number of pair-excitations in the ^{48}Cr nucleus. The weights of the components of the correlated wave function (up to the DP excitations) are plotted as a function of $V_0^{(T=1)}$ (left panels) and as a function of x (right panels) for $V_0^{(T=1)} = -200$ MeV fm^3.

truncation scheme for all considered values of $V_0^{(T=1)}$ and for all values of x in the (physically most relevant) range $0 \leqslant x \leqslant 1.25$. In this truncation scheme, the weight of DP excitations is converged to within about 1% for all considered values of $V_0^{(T=1)}$ and in the range $0 \leqslant x \leqslant 1$. However, the role of TP excitations ceases to be negligible for $x \gtrsim 1.25$. Because these configurations can be included at a reasonable price in computation time, we choose the $|\Phi_0\rangle + \mathrm{SP} + \mathrm{DP} + \mathrm{TP}$ truncation scheme in all subsequent calculations.

B. Structure of the correlated wave functions in the particle-hole excitation basis

In Fig. 3 we show for all the nuclei under study the variation of the weights of SP, DP, and TP excitations in the correlated ground state as functions of $|V_0^{(T=1)}|$ (left column) and as functions of x for $V_0^{(T=1)} = -300$ MeV fm^3 (right column). As an overall trend we observe that the SP, DP, and TP contributions are increasing functions of $|V_0^{(T=1)}|$ and x as expected. For $x = 0$, the TP contribution is negligible over the considered range of $V_0^{(T=1)}$ in all the studied nuclei, and the weight of DP excitations is about one order of magnitude smaller than the SP contribution. This hierarchy among the MP configurations is preserved as a function of x up to $x \sim 0.75$.

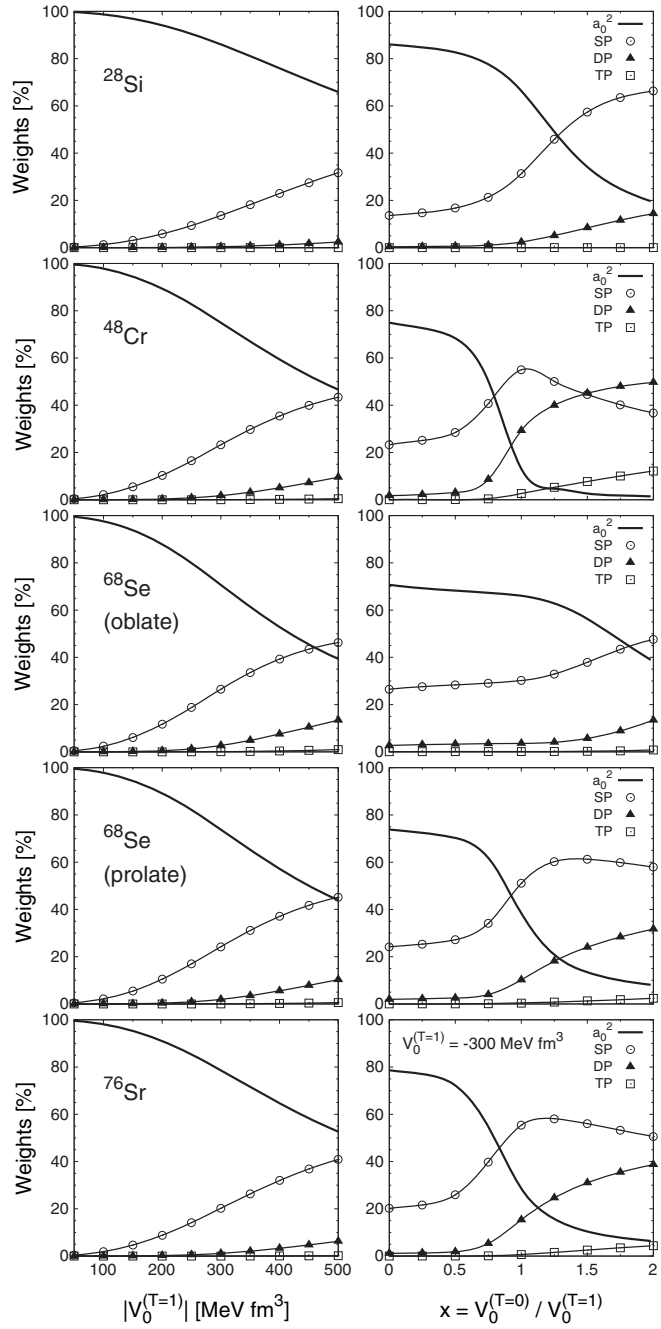

FIG. 3. Contributions of the quasivacuum (thick solid lines), SP (thin solid lines with open circles), DP (thin solid lines with solid triangles), and TP (thin solid lines with open squares) excitations to the correlated ground state for the four selected $N = Z$ deformed even-even nuclei [^{28}Si, ^{48}Cr, ^{68}Se (oblate and prolate solutions), and ^{76}Sr from top to bottom], as functions of $|V_0^{(T=1)}|$ (left panels) and as functions of x for $V_0^{(T=1)} = -300$ MeV fm^3 (right panels).

For larger values of x, the contribution of SP excitations tends to saturate and decrease in conjunction with a sharp rise of the DP contribution. The TP contribution are also negligible over the considered range of x except for the ^{48}Cr where these excitations start to play a sizable role for $x \gtrsim 1$.

C. Structure of the correlated wave functions in the approximate good-isospin basis

Before turning to the isospin mixing in the correlated ground state $|\Psi\rangle$, let us analyze the structure of $|\Psi\rangle$ in the approximate good-isospin basis, $\mathcal{B}_T$, spanned by the states $|\Psi_{\mathrm{MP},T,i}\rangle$, as a function of the strengths $V_0^{(T)}$. Because the isospin symmetry is weakly broken in nuclear states, we expect the ground state $|\Psi\rangle$ of an even-even $N = Z$ nucleus to have an isospin content easier to analyze in the $\mathcal{B}_T$ basis than in the basis spanned by $|\Phi_0\rangle$ and its MP excitations. We postpone to the next section the test of the DCA which will establish the approximate good-isospin character of the $\mathcal{B}_T$ basis.

As discussed above, the pairing correlations are driven by the SP configurations as long as the $T = 0$ channel does not dominate over the $T = 1$ channel, even though the DP excitations are essential to obtain the correct weight of SP excitations. We thus focus on the SP subset of the $\mathcal{B}_T$ basis. Figure 4 presents the total weights of the four different types of SP states defined by Eqs. (35) to (38) for the representative ^{48}Cr nucleus. As clearly shown by the logarithmic scale, the SP excitations are, in the absence of the $T = 0$ residual interaction, largely dominated by the $|\Psi_{02}^{(k)}\rangle$ states. Interestingly, one observes that the contribution from $T = 1$ quasi-eigenstates of $\hat{\mathbf{T}}^2$ is about one order of magnitude larger than the contribution from $|\Psi_{01}^{(k)}\rangle$ states. When the $T = 0$ channel is included, one progressively evolves from a regime driven by the $|\Psi_{02}^{(k)}\rangle$ states ($x \leqslant 1$ region) to a regime where the $|\Psi_{01}^{(k)}\rangle$ states dominate ($x \gtrsim 1$ region). Moreover, the total weight of the $|\Psi_1^{(k)}\rangle$ states generally drops when x becomes close to 1. Over the considered ranges of $V_0^{(T=1)}$ and $V_0^{(T=0)}$, the $|\Psi_2^{(k)}\rangle$ states contribute so little that their total weight is not visible even on the logarithmic scale of Fig. 4.

The variations of these weights with the two channels of the residual interaction can be qualitatively understood from a perturbative argument. Let us expand the SP component of the correlated ground-state solution $|\Psi\rangle$ to first order of *many-body perturbation theory* (MBPT) in $\hat{V}_{\mathrm{res}}$ around the quasivacuum $|\Phi_0\rangle$. The resulting correction $|\delta\Psi_{\mathrm{SP}}\rangle$ can be written as

$$|\delta\Psi_{\mathrm{SP}}\rangle = \sum_k |\delta\Psi_{\mathrm{SP}}^{(k)}\rangle, \tag{49}$$

where the un-normalized contribution $|\delta\Psi_{\mathrm{SP}}^{(k)}\rangle$ from the cluster k is given by

$$\begin{aligned}|\delta\Psi_{\mathrm{SP}}^{(k)}\rangle = x_0|\Psi_{01}^{(k)}\rangle + \frac{1}{\sqrt{3}}\left[\left(\frac{1+\varepsilon\lambda}{1-\varepsilon^2}+\frac{1+\mu_1}{2}\right)x_1+\mu_0 x_0\right]\\ \times|\Psi_{02}^{(k)}\rangle - \frac{1}{\sqrt{2}}\frac{\varepsilon+\lambda}{1-\varepsilon^2}x_1|\Psi_1^{(k)}\rangle\\ +\frac{1}{\sqrt{6}}\left[\left(\frac{\varepsilon(\varepsilon+\lambda)}{1-\varepsilon^2}-\mu_1\right)x_1-2\mu_0 x_0\right]|\Psi_2^{(k)}\rangle.\end{aligned} \tag{50}$$

The dimensionless quantities ε, λ, μ_T, and x_T (with $T = 0$ or 1) appearing in Eq. (50) depend on the cluster label k. However, to simplify the notation we do not carry this index along. These quantities are defined by

$$\varepsilon = \frac{\Delta e_p^{(k)} - \Delta e_n^{(k)}}{\Delta e_p^{(k)} + \Delta e_n^{(k)}}, \tag{51}$$

$$x_1 = \frac{\langle\Phi_{20}^{(k)}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle + \langle\Phi_{02}^{(k)}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle}{\Delta e_p^{(k)} + \Delta e_n^{(k)}}, \tag{52}$$

$$\lambda = \frac{\langle\Phi_{20}^{(k)}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle - \langle\Phi_{02}^{(k)}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle}{x_1\left(\Delta e_p^{(k)} + \Delta e_n^{(k)}\right)}, \tag{53}$$

$$x_0 = \frac{\langle\widetilde{\Phi}_{11}^{(k)}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle + \langle\widetilde{\Phi}'^{(k)}_{11}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle}{\sqrt{2}\left(\Delta e_p^{(k)} + \Delta e_n^{(k)}\right)}, \tag{54}$$

$$\mu_0 = \frac{\langle\widetilde{\Phi}_{11}^{(k)}|\hat{V}_{\mathrm{res}}^{(T=0)}|\Phi_0\rangle - \langle\widetilde{\Phi}'^{(k)}_{11}|\hat{V}_{\mathrm{res}}^{(T=0)}|\Phi_0\rangle}{\sqrt{2}x_0\left(\Delta e_p^{(k)} + \Delta e_n^{(k)}\right)}, \tag{55}$$

$$\mu_1 = \sqrt{2}\,\frac{\langle\widetilde{\Phi}_{11}^{(k)}|\hat{V}_{\mathrm{res}}^{(T=1)}|\Phi_0\rangle - \langle\widetilde{\Phi}'^{(k)}_{11}|\hat{V}_{\mathrm{res}}^{(T=1)}|\Phi_0\rangle}{x_1\left(\Delta e_p^{(k)} + \Delta e_n^{(k)}\right)} - 1, \tag{56}$$

where $\Delta e_n^{(k)}$ ($\Delta e_p^{(k)}$) is the difference between the energies of the particle and hole levels for neutrons (protons). These six quantities vanish in the limit of exact isospin symmetry. The $T = 1$ channel of $\hat{V}_{\mathrm{res}}$ is the only one contributing to x_1 and λ, whereas only the $T = 0$ channel contributes to x_0. Because both channels can contribute to the difference $\langle\widetilde{\Phi}_{11}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle - \langle\widetilde{\Phi}'_{11}|\hat{V}_{\mathrm{res}}|\Phi_0\rangle$, a superscript is added to $\hat{V}_{\mathrm{res}}$ to specify the isospin channel.

Because the isospin symmetry is weakly broken, all the quantities λ, ε, and μ_T are very small in each SP cluster. Therefore, the hierarchy of the terms contributing to the total weight of SP excitations, observed in Fig. 4, emerges

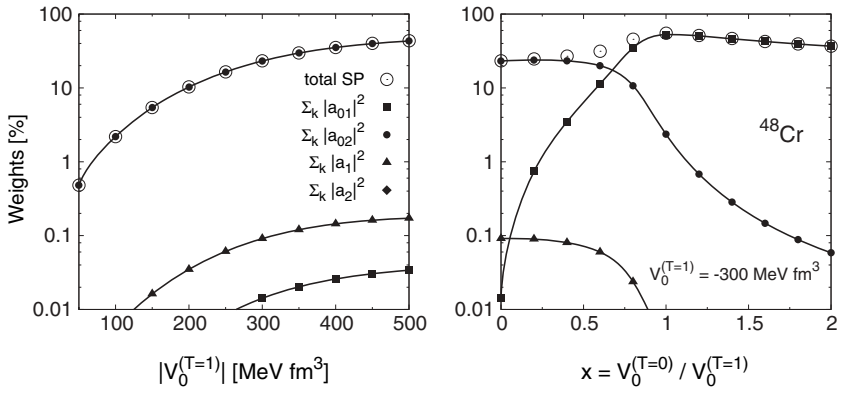

FIG. 4. Weights of SP quasi-eigenstates of $\hat{\mathbf{T}}^2$ in the $|\Psi_{\mathrm{SP}}\rangle$ contribution to the HTDA solution $|\Psi\rangle$ as functions of $|V_0^{(T=1)}|$ (left panel) and as functions of x (right panel). Solid squares, circles, triangles, and diamonds correspond to the sums over clusters of the weights of $|\Psi_{01}^{(k)}\rangle$, $|\Psi_{02}^{(k)}\rangle$, $|\Psi_1^{(k)}\rangle$, and $|\Psi_2^{(k)}\rangle$ states, respectively. The latter contribution is not visible with the chosen scales.

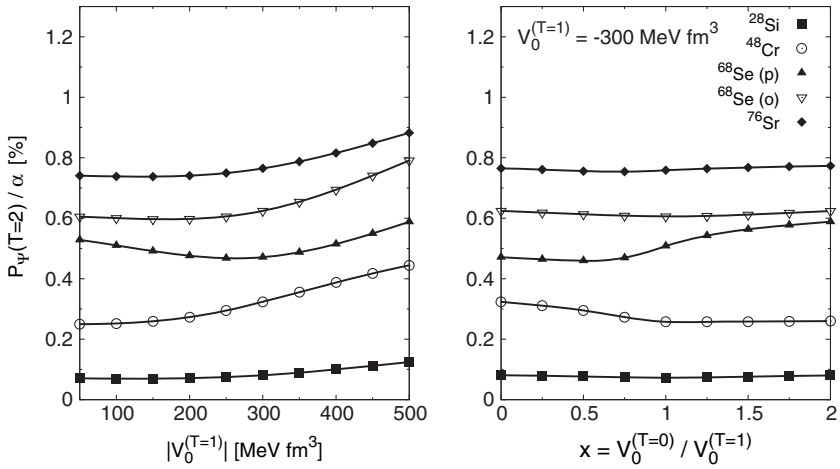

FIG. 5. Variation of the relative $T = 2$ contribution to the isospin-mixing parameter with the strength $V_0^{(T=1)}$ of the residual interaction in the $T = 1$ channel (left panel) and with x (right panel) for the four selected $N = Z$ deformed even-even nuclei [^{28}Si, ^{48}Cr, ^{68}Se (oblate and prolate solutions), and ^{76}Sr].

from Eq. (50). By decreasing order of importance, the $T = 1$ channel, governed by the dimensionless strength x_1, populates essentially the $|\Psi_{02}^{(k)}\rangle$ quasi-eigenstates, then the $|\Psi_1^{(k)}\rangle$ terms (proportional to ε) and with a negligible contribution the $|\Psi_2^{(k)}\rangle$ terms (proportional to ε^2). The $|\Psi_{01}^{(k)}\rangle$ contribution does not appear in the $T = 1$ channel at order 1 of the MBPT. On the contrary, the $T = 0$ channel strongly favors the $|\Psi_{01}^{(k)}\rangle$ states and to a much lesser extent the other quasi-eigenstates. The $|\Psi_1^{(k)}\rangle$ states do not, in particular, contribute to $|\Psi\rangle$ at first order of MBPT in the presence of the $T = 0$ channel alone.

V. ISOSPIN MIXING IN THE CORRELATED GROUND STATES

We now calculate the isospin-mixing parameter α in the correlated ground-state solutions of the previous section.

A. Role of the $T = 2$ component

First we investigate the influence of the truncation order n introduced in Sec. II C by comparing the isospin-mixing parameters given by Eq. (27) when truncating at $n = 1$ and by Eq. (28) when the truncation order is $n = 2$.

The relative deviation between the different evaluations of the isospin-mixing parameter is driven by the relative contribution of the $T = 2$ component to $\alpha^{(n=2)}$:

$$\frac{\alpha^{(n=2)} - \alpha^{(n=1)}}{\alpha^{(n=2)}} = -2\,\frac{P_\Psi^{(2)}(T=2)}{\alpha^{(n=2)}}. \tag{57}$$

The ratio $P_\Psi^{(2)}(T = 2)/\alpha^{(n=2)}$ is displayed for each nucleus in Fig. 5. As expected, this quantity is very small, one or two orders of magnitude smaller than the $P_\Psi^{(2)}(1)$ contribution. This holds for all studied nuclei and regardless of the strength of the residual interaction in each isospin channel. The relative contribution of $P_\Psi^{(2)}(2)$ to the isospin admixture increases with Z but never exceeds 1% in the considered nuclei. In the following, we therefore neglect the $T = 2$ contribution to α which is then calculated from the expectation value of $\hat{\mathbf{T}}^2$ only according to Eq. (27).

B. Contribution of pairing correlations to α

Let us now discuss the amount of isospin mixing brought by the $T = 1$ and $T = 0$ pairing correlations. In Fig. 6 the relative contribution to α from correlations, namely $C_{\rm corr}/\alpha = (\alpha - \alpha_0)/\alpha$, is plotted for the five studied HTDA solutions as a function of $|V_0^{(T=1)}|$ (left column) for $x = 0$ and as a function of x for the typical strength $V_0^{(T=1)} = -300$ MeV fm^3 (right column). Manifestly, the response of the isospin-mixing parameter to the residual interaction strongly depends on the isospin channel. Whereas $C_{\rm corr}/\alpha$ increases significantly with $|V_0^{(T=1)}|$ for all HTDA ground-state solutions, it varies with a

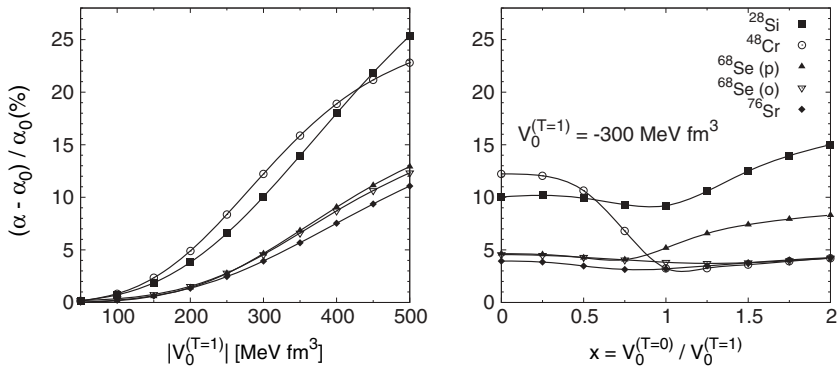

FIG. 6. Variation of the correlation contribution to the isospin-mixing parameter (calculated without the $T = 2$ component) with the strength $V_0^{(T=1)}$ of the residual interaction in the $T = 1$ channel (left panel) and with x (right panel) for the four selected $N = Z$ deformed even-even nuclei [^{28}Si, ^{48}Cr, ^{68}Se (oblate and prolate solutions), and ^{76}Sr].

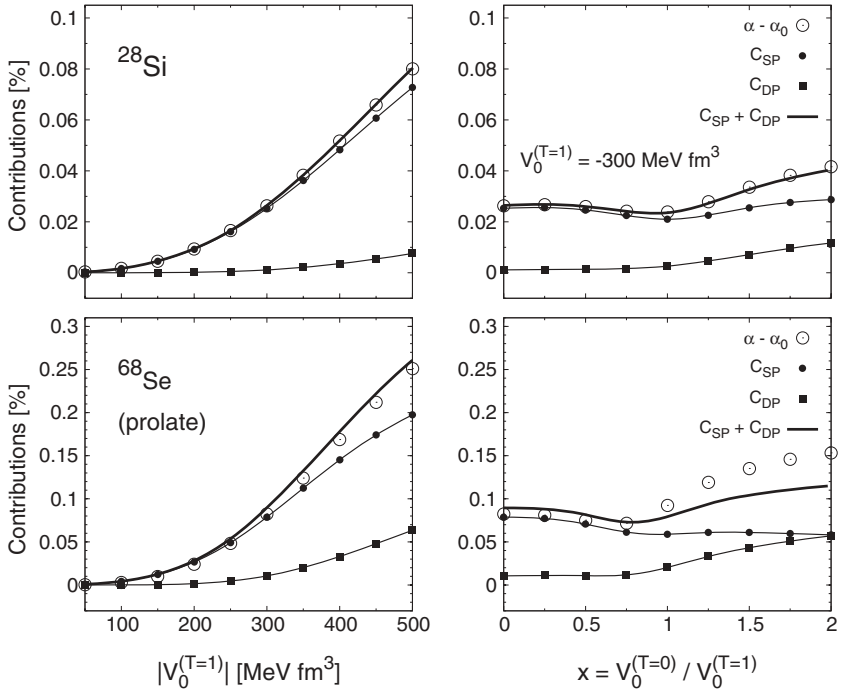

FIG. 7. Decomposition of the correlation contribution to the isospin-mixing parameter (calculated without the $T = 2$ component) according to Eq. (44) resulting from the DCA including the SP ($C_{\rm SP}$) and DP ($C_{\rm DP}$) contributions only. (Left) Variation with $V_0^{(T=1)}$ and $x = 0$. (Right) Variation with x for $V_0^{(T=1)} = -300$ MeV fm^3.

much smaller amplitude as a function of $V_0^{(T=0)}$ and depends significantly on the considered nucleus.

To explain in simple terms the behavior of α with the strength of the residual interaction, we need to rely on the DCA presented in Sec. II D. Let us first assess the quality of this approximation.

Figure 7 presents the analysis of the isospin-mixing parameter in the framework of the DCA with SP and DP contributions for two typical examples, the ^{28}Si ground state and the prolate solution of the ^{68}Se nucleus. The left column shows the variations of the SP and DP contributions to $C_{\rm corr}$ as functions of $|V_0^{(T=1)}|$ and the right column corresponds to their variations with x. The roles of TP configurations and cross terms beyond the DCA appear, by definition, as the difference between the value of $C_{\rm corr}$ (represented by the open circles) and the DCA value up to DP excitations $C_{\rm SP} + C_{\rm DP}$ (shown by the thick solid line). The latter value is referred to as the DCA(SP + DP) value in the following. Overall, in the considered ranges of $T = 1$ and $T = 0$ strengths, the SP contribution largely dominates and the terms beyond DCA(SP + DP) are negligible for all the HTDA solutions (with one exception in the prolate solution of ^{68}Se for $x \geqslant 1$). More precisely, an excellent agreement between the full α value and the DCA(SP + DP) approximation is systematically obtained for all considered nuclei in the absence of $T = 0$ pairing correlations. This shows at the same time that the TP excitations and the cross terms play a negligible role. As a result, matrix elements of the forms $\langle\Phi_0|\hat{\mathbf{T}}^2|\Psi_{\rm SP}\rangle$, $\langle\Psi_{\rm SP}|\hat{\mathbf{T}}^2|\Psi_{\rm DP}\rangle$, and $\langle\Psi_{\rm DP}|\hat{\mathbf{T}}^2|\Psi_{\rm TP}\rangle$ can be neglected. Because they depend only on the single-particle states associated with the quasivacuum $|\Phi_0\rangle$, the cross terms are also negligible in the presence of $T = 0$ pairing. This validates the DCA and the expression (44) of the correlation contribution to α. Therefore, any visible deviation of the DCA(SP + DP) results from the full calculation of α can be attributed to the missing TP contribution in the DCA result. It is then interesting to note that an overestimation by the DCA(SP + DP) calculation occur in some cases. As discussed at the end of Sec. II, this means that the TP excitations responsible for this deviation have, overall, a purer isospin content than the SP and DP configurations.

We can now investigate the mechanisms by which the $T = 1$ and $T = 0$ pairing correlations bring isospin mixing into the correlated ground state.

In Fig. 8 the $C_{\rm SP}$ and $C_{\rm DP}$ contributions to α in ^{76}Sr, chosen here as a typical example, are plotted with open circles as functions of $|V_0^{(T=1)}|$ with $x = 0$ (left column) and as functions of x with $V_0^{(T=1)} = -300$ MeV fm^3 (right column). They are decomposed into additive contributions from quasi-eigenstates of $\hat{\mathbf{T}}^2$ with different T values, as in Eq. (45). The SP and DP excitations bring isospin mixing into the correlated ground-state solution through the same mechanisms.

In the absence of a $T = 0$ residual interaction, the isospin mixing is essentially brought by the $T = 1$ quasi-eigenstates and to a much lesser extent by the $T = 0$ quasi-eigenstates. According to Eq. (46), this means that the two mechanisms predicted at the end of Sec. II D are simultaneously at work but the one involving the $T = 1$ quasi-eigenstates dominates. In particular for the SP contribution, the $|\Psi_1^{(k)}\rangle$ states, despite their small weights, introduce $T \approx 1$ impurities in $|\Psi_{\rm SP}\rangle$ in a more efficient way than do the $T = 0$ quasi-eigenstates.

When the $T = 0$ channel comes into play, a change of regime operates around $x = 1$. While the contributions from the $T = 1$ quasi-eigenstates to $C_{\rm SP}$ and $C_{\rm DP}$ decrease with increasing x and vanish between $x = 1$ and $x = 2$, the role of the $T = 0$ quasi-eigenstates (actually $|\Psi_{01}^{(k)}\rangle$ states for SP contributions, corresponding to np pairs only) becomes more and more important as x increases.

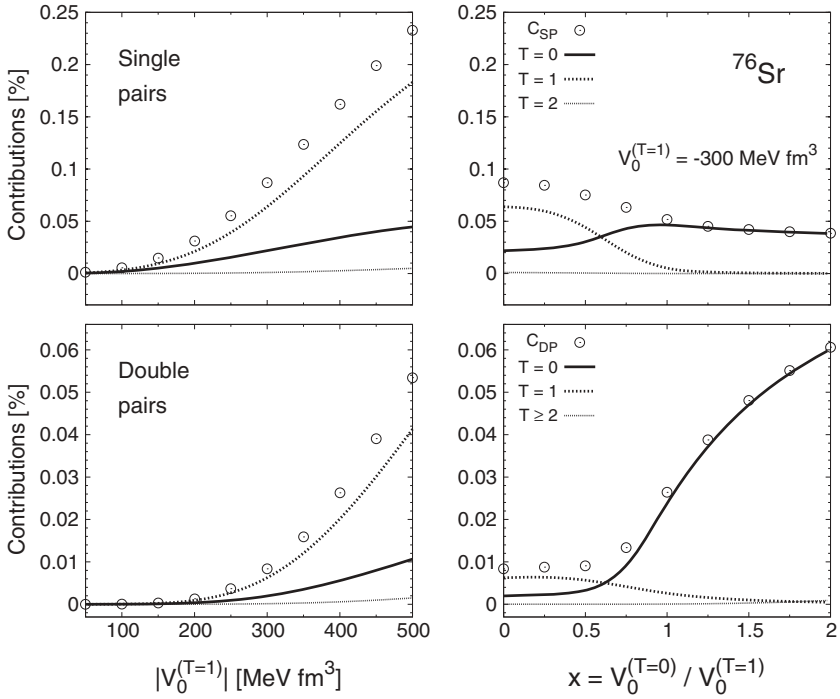

FIG. 8. DCA analysis by T values of the SP (top row) and DP (bottom row) contributions to α in ^{76}Sr. (Left column) Variations with $V_0^{(T=1)}$ and $x = 0$; (right column) variations with x for $V_0^{(T=1)} = -300$ MeV fm^3.

As expected from the negligible contribution of $P(2)$ to α, the $T \geqslant 2$ quasi-eigenstates never contribute in a sizable way over the whole considered range of strengths.

C. Influence of the treatment of the Coulomb interaction

Finally, we investigate the effects of the treatment of the Coulomb interaction on the isospin admixture of the correlated ground states.

On the one hand, we have calculated α in the HTDA solutions with the Slater approximation to the exchange terms of the mean-field potential. For the ^{76}Sr nucleus, Fig. 9 compares the resulting isospin admixtures (thin solid lines with open circles) with those calculated with an exact treatment of exchange Coulomb terms (thick solid lines), as functions of $|V_0^{(T=1)}|$ with $x = 0$ in the left panel and as functions of x with $V_0^{(T=1)} = -300$ MeV fm^3 in the right panel.

Overall, the Slater approximation leads to smaller isospin impurities. Using the results of Ref. [32], this can be explained by an underestimation of proton particle-hole excitation energies within the Slater approximation, the neutron particle-hole excitation energies being virtually unaffected. This translates into smaller values of the quantities ε and, according to Eq. (50), to smaller contributions of the $|\Psi_1^{(k)}\rangle$ quasi-eigenstates to C_{SP}. It is thus no surprise to observe that the difference between the isospin admixtures obtained using the Slater approximation and the exact Coulomb exchange terms increases with $|V_0^{(T=1)}|$. However, it decreases with the strength in the $T = 0$ channel. This can be understood from the fact that, when the $T = 0$ channel dominates in the residual interaction, the contributions to α from the $|\Psi_1^{(k)}\rangle$ states practically vanish in both calculations, whereas the contribution from the $|\Psi_{01}^{(k)}\rangle$ states, insensitive to ε according to Eq. (50), becomes dominant in $|\Psi_{SP}\rangle$.

However, we have studied the effect on α of the Coulomb contribution to the residual interaction as defined in Eq. (14). In addition to the δ interaction, we use the bare Coulomb interaction. In Fig. 9 we present also the variation of α with the two channels of the δ residual interaction calculated without (thick solid lines) and with (thin solid lines with open squares)

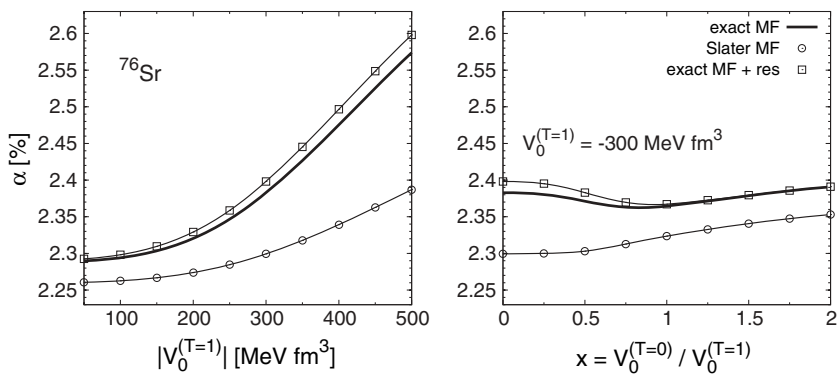

FIG. 9. Isospin-mixing parameter α of the HTDA ground state obtained in three different calculations: with exact exchange terms in the Coulomb mean field and without residual Coulomb interaction (thick solid line, labeled "exact MF"), with the Slater approximation to the exchange Coulomb mean field and without residual Coulomb interaction (thin solid line with open circles, labeled "Slater MF") and with an exact treatment of the full Coulomb interaction (thin solid line with open squares, labeled "exact MF + res"). (Left) Variation with $V_0^{(T=1)}$; (right) variation with x for $V_0^{(T=1)} = -300$ MeV fm^3.

the Coulomb contribution to $\hat{V}_{\rm res}$ for the ^{76}Sr nucleus. In both cases the exact Coulomb interaction is included in the mean field. In general, the full treatment of the Coulomb interaction produces additional isospin mixing, a trend that is found to increase with the proton number.

The difference between the α values calculated with and without the residual Coulomb interaction increases, as expected, when the $T = 1$ channel becomes stronger, but decreases to zero when the $T = 0$ channel dominates over the $T = 1$ channel. The DCA analysis of the SP contribution to α offers a simple explanation. When the $T = 0$ pairing correlations dominate, the weights of $|\Psi_{02}^{(k)}\rangle$ and $|\Psi_{1}^{(k)}\rangle$ states vanish (see Fig. 4). Therefore, the SP contribution is driven by the $|\Psi_{01}^{(k)}\rangle$ states which appear in the perturbed expression (50) with a coefficient independent of λ and ε. In this regime dominated by the $T = 0$ pairing, the Coulomb residual interaction is thus unable to induce isospin mixing in the pair-correlated wave function.

Before concluding, it is worth keeping in mind that the above-discussed residual Coulomb interaction is not renormalized to the HTDA model space. In this context one can expect that using the bare Coulomb interaction in the HTDA calculations underestimates the effect of the residual contribution to the isospin-mixing parameter. However, assuming that renormalizing the Coulomb interaction in the residual channel amounts to a mere multiplying factor in the coupling strength, which would not exceed an order of magnitude, one would still obtain a weak impact of $\hat{V}_{C,\rm res}$ on α.

VI. CONCLUSION AND PERSPECTIVES

In this work we have performed HTDA calculations of the isospin-mixing parameter α in the ground states of ^{28}Si, ^{48}Cr, and ^{76}Sr (all prolate deformed), as well as in the oblate and prolate local minima of ^{68}Se. We have used the Skyrme SIII effective interaction in the mean-field channel and a density-independent δ interaction in the pairing channel. At the mean-field level, we have calculated exactly the exchange Coulomb contribution to the Hartree-Fock Hamiltonian and in the HTDA Hamiltonian we have included the Coulomb contribution to the residual interaction.

First we have studied in details the influence of both isospin channels of the pairing residual interaction $\hat{V}_{\rm res}$ on the structure of the HTDA ground state. As an overall trend the amount of pairing correlations increases as a function of the strength of the $T = 1$ channel through an increasing weight of the one-pair excitations, slightly renormalized by the presence of higher-order pair excitations. This is also the case with the $T = 0$ channel up to a threshold $|V_0^{(T=0)}| \sim |V_0^{(T=1)}|$ beyond which the one-pair excitations saturate and hand over to the DP excitations.

Then we have calculated explicitly the $T = 2$ contribution to the isospin-mixing parameter α. It has been found rapidly increasing as a function of Z but always negligible (less than 1% of α) as already known.

Moreover, we have shown that the unitary transformation which diagonalizes the $\hat{\mathbf{T}}^2$ operator in the absence of the Coulomb interaction keeps this property to a good approximation even in the presence of the Coulomb interaction. This transformation assumes a simple block-diagonal form in clusters of the multipair excitations of given order, characterized by a set of hole and particle levels, and makes it possible to easily express the correlation contribution to the isospin-mixing parameter as the sum of the difference between the isospin admixtures of the quasivacuum and the approximate good-T states. In this approach, which call the DCA, we have found that the pairing correlations bring isospin mixing in the ground state through a competition of approximate good-T states with $T = 1$ for the residual interaction in the $T = 1$ channel and $T = 0$ for the $T = 0$ channel. More precisely, the approximate good-T states contributing the most to α involve neutron-proton one-pair excitations for $T = 0$ and the difference between neutron-neutron and proton-proton one-pair excitations for $T = 1$.

Finally, we have shown that the Slater approximation significantly underestimates the α parameter and that the Coulomb contribution to the residual interaction has a negligible impact on α (of the same order of magnitude as the contribution of the $T = 2$ component). In quantitative studies of isospin mixing, the Coulomb interaction should thus be treated exactly at the mean-field level but can be omitted in the residual interaction within the HTDA framework.

In the light of the present work we expect that the observables sensitive to isospin-symmetry breaking—essentially along the $N = Z$ line—require a good treatment of $T = 1$ as well as $T = 0$ pairing correlations. This is substantiated by our recent studies of superallowed $0^+ \to 0^+$ Fermi transitions [35] and magnetic moments in odd-mass nuclei near the $N = Z$ line [36]. We shall investigate further the impact of pairing correlations on these quantities in future papers.

In addition to the pairing correlations, we expect the vibrational correlations to play a role in the structure of the correlated ground state, especially in spherical nuclei, and to bring an additional contribution to the ground-state isospin mixing. These correlations can be described on the same footing as the pairing correlations in the HTDA framework [24]. In the future it remains to design a realistic and tractable residual interaction to describe simultaneously both kinds of correlations in the HTDA framework. As a first step a finite-range residual interaction of a Gaussian form (as the central Gogny interaction) would be straightforward to implement given that the matrix elements of the Coulomb interaction have been calculated analytically through a Gaussian expansion of the $1/r$ function. In a longer term a more consistent way to treat those correlations in HTDA would be to perform a self-consistent calculation allowing us to take into account the effect of the correlations into the mean field as it has been proposed in Ref. [21].

ACKNOWLEDGMENTS

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APPENDIX A: MATRIX ELEMENTS OF THE δ RESIDUAL INTERACTION

If we denote the space-spin-isospin basis by $\{|\mathbf{r}\sigma\tau\rangle, \mathbf{r} \in \mathbb{R}^3, \sigma, \tau = \pm\frac{1}{2}\}$ ($\tau = \frac{1}{2}$ for a neutron state, $\tau = -\frac{1}{2}$ for a proton state), we can write the single-particle state $|k\rangle$, which is an eigenstate of $\hat{T}_z$ with the eigenvalue τ_k, as

$$|k\rangle = \int d^3\mathbf{r} \sum_\sigma \varphi_k^{(\sigma)}(\mathbf{r})|\mathbf{r}\sigma\tau_k\rangle. \tag{A1}$$

With the assumption of axial symmetry, $|k\rangle$ is, in addition, an eigenstate of the third component $\hat{J}_z$ of the angular momentum operator, with the eigenvalue $\Omega_k\hbar$, and can be expanded in the cylindrical harmonic-oscillator basis $\{|Nn_z\Lambda\sigma\tau\rangle\}$, with the notation of Ref. [34] to which we add the isospin quantum number, as

$$|k\rangle = \sum_{N,n_z,\sigma} C^{(k)}_{Nn_z\Lambda_k^{(\sigma)}\sigma\tau_k} \left|Nn_z\Lambda_k^{(\sigma)}\sigma\tau_k\right\rangle, \tag{A2}$$

where $\Lambda_k^{(\sigma)} = \Omega_k - \sigma$ ($\sigma = \pm 1/2$). The action of the time-reversal operator $\hat{\mathcal{T}}$ on $|\sigma\rangle$ implies that

$$\hat{\mathcal{T}}|\sigma\rangle = (-1)^{\frac{1}{2}-\sigma}|-\sigma\rangle, \tag{A3}$$

and the wave function of the time-reversed state $|\bar{k}\rangle$ is therefore given by

$$\varphi_{\bar{k}}^{(\sigma)}(\mathbf{r}) = (-1)^{\frac{1}{2}+\sigma}\left(\varphi_k^{(-\sigma)}\right)^*. \tag{A4}$$

Because we are describing an even-even nucleus, we can choose the single-particle states to be even or odd under time-reversal symmetry and restrict to the former. Therefore, the expansion coefficients $C^{(k)}_{Nn_z\Lambda\sigma\tau}$ are real and the spin-σ component of the single-particle wave function $\varphi_k^{(\sigma)}(\mathbf{r})$ takes the form

$$\varphi_k^{(\sigma)}(\mathbf{r}) = f_k^{(\sigma)}(\rho, z)\frac{e^{i\Lambda_k^{(\sigma)}\theta}}{\sqrt{2\pi}}, \tag{A5}$$

where the function $f_k^{(\sigma)}(\rho, z)$ is real. From Eq. (A4) we obtain $f_{\bar{k}}^{(\sigma)}(\rho, z) = (-1)^{\frac{1}{2}+\sigma} f_k^{(-\sigma)}(\rho, z)$, that is,

$$f_{\bar{k}}^{+}(\rho, z) = -f_k^{-}(\rho, z), \tag{A6}$$

$$f_{\bar{k}}^{-}(\rho, z) = f_k^{+}(\rho, z). \tag{A7}$$

The matrix elements of the δ interaction in the $T = 0$ and $T = 1$ channels for any single-particle states $|i\rangle$, $|j\rangle$, $|k\rangle$, $|\ell\rangle$ can thus be written in cylindrical coordinates (ρ, z) as

$$\begin{aligned}\langle ij|\hat{V}_\delta^{(T=0)}|\widetilde{kl}\rangle = {} & \frac{V_0^{(T=0)}}{4\pi}\delta_{\Omega_i+\Omega_j,\Omega_k+\Omega_\ell}\left(\delta_{\tau_i\tau_k}\delta_{\tau_j\tau_\ell} - \delta_{\tau_i\tau_\ell}\delta_{\tau_j\tau_k}\right) \\ & \times \int_{-\infty}^{\infty} dz \int_0^{\infty} d\rho\, \rho\, [(f_i^+ f_j^- + f_i^- f_j^+)(f_k^+ f_\ell^- + f_k^- f_\ell^+) + 2(f_i^+ f_j^+ f_k^+ f_\ell^+ + f_i^- f_j^- f_k^- f_\ell^-)],\end{aligned} \tag{A8}$$

$$\langle ij|\hat{V}_\delta^{(T=1)}|\widetilde{kl}\rangle = \frac{V_0^{(T=1)}}{4\pi}\delta_{\Omega_i+\Omega_j,\Omega_k+\Omega_\ell}\left(\delta_{\tau_i\tau_k}\delta_{\tau_j\tau_\ell} + \delta_{\tau_i\tau_\ell}\delta_{\tau_j\tau_k}\right)\int_{-\infty}^{\infty} dz \int_0^{\infty} d\rho\, \rho\, (f_i^+ f_j^- - f_i^- f_j^+)(f_k^+ f_\ell^- - f_k^- f_\ell^+), \tag{A9}$$

where we have omitted the ρ and z dependence in the notation of the integrated functions. The two-body matrix elements of $\hat{V}_\delta$ are therefore real, and so are the many-body matrix elements of $\hat{V}_{\text{res}}$.

APPENDIX B: MATRIX ELEMENTS OF THE COULOMB INTERACTION IN THE CYLINDRICAL HARMONIC-OSCILLATOR BASIS

Apart from the spin degree of freedom, the quantum numbers characterizing the cylindrical harmonic-oscillator basis states considered in Appendix A are chosen here to be n_z, $\alpha = (n_\perp + \Lambda)/2$, and $\beta = (n_\perp - \Lambda)/2$, where $n_\perp = N - n_z$. Using the method described in detail in Ref. [31], we can write the matrix element of the Coulomb interaction in the cylindrical harmonic-oscillator basis in the form

$$\begin{aligned}&\left\langle n_{z_i}\alpha_i\beta_i, n_{z_j}\alpha_j\beta_j\left|\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}\right|n_{z_k}\alpha_k\beta_k, n_{z_l}\alpha_l\beta_l\right\rangle \\ &= \sqrt{\frac{2}{\pi}}\, e^2 c_0^3 \sum_{n=n_{\min}}^{n_{z_i}+n_{z_j}} f_n\left(n_{z_i}, n_{z_j}, n_{z_k}, n_{z_l}\right) \sum_{p=|n-n'|}^{n+n'} \mathcal{C}(n, n', p)\mathcal{A}(p) \sum_{a=a_{\min}}^{\alpha_i+\alpha_j} \sum_{b=b_{\min}}^{\beta_i+\beta_j} g_{a,b}(\alpha_i, \beta_i, \alpha_j, \beta_j, \alpha_k, \beta_k, \alpha_l, \beta_l)\, \delta_{a-b,a'-b'} \\ &\quad \times \frac{(a+b')!}{\sqrt{a!\,a'!\,b!\,b'!}} \sum_{k=0}^{k_{\max}} \frac{\binom{b}{k}\binom{b'}{k}}{\binom{a+b'}{k}} \mathfrak{I}^{c_z,c_\perp}_{p/2,|a-b|,k,a+b'+1-k},\end{aligned} \tag{B1}$$

with $e^2 = 1.439\,965$ MeV fm, and

$$n_{\min} = \max\left(0, n_{z_i} + n_{z_j} - n_{z_k} - n_{z_l}\right), \tag{B2}$$

$$a_{\min} = \max(0, \alpha_i + \alpha_j - \alpha_k - \alpha_l), \tag{B3}$$

$$b_{\min} = \max(0, \beta_i + \beta_j - \beta_k - \beta_l), \quad \text{and} \tag{B4}$$

$$k_{\max} = \min\left(\frac{a+b-|a-b|}{2}, \frac{a'+b'-|a'-b'|}{2}\right). \tag{B5}$$

The expression (B1) is obtained using a Moshinsky transformation [37] from the coordinate system of two particles $|n_{z_1}\alpha_1\beta_1, n_{z_2}\alpha_2\beta_2\rangle$ to the one of center-of-mass (c.m.) and relative coordinates $|nab, NAB\rangle$.

The Moshinsky coefficients $\langle n_1 n_2||nN\rangle$ can be written in terms of Wigner's reduced rotation matrix as

$$\langle n_1 n_2||nN\rangle = \delta_{n_1+n_2,n+N}\, d^{(n_1+n_2)/2}_{(n-N)/2,(n_1-n_2)/2}\left(\frac{\pi}{2}\right), \quad \text{(B6)}$$

which takes the explicit form

$$d^{(n_1+n_2)/2}_{(n-N)/2,(n_1-n_2)/2}\left(\frac{\pi}{2}\right) = \sqrt{\frac{n_1!\,n_2!\,n!\,N!}{2^{n_1+n_2}}} \sum_{\ell=\max(0,n_2-N)}^{\min(n_2,n)} \times \frac{(-1)^\ell}{(n_2-\ell)!\,(N-n_2+\ell)!\,\ell!\,(n-\ell)!}. \quad \text{(B7)}$$

The conservation of the phonon number imposed by the Moshinsky coefficients and the fact that the Coulomb interaction does not act in the c.m. coordinate system implies the following relation between the quantum numbers n', a', b' and n, a, b:

$$n' = n - n_{z_i} - n_{z_j} + n_{z_k} + n_{z_l}, \quad \text{(B8)}$$

$$a' = a - \alpha_{z_i} - \alpha_{z_j} + \alpha_{z_k} + \alpha_{z_l}, \quad \text{(B9)}$$

$$b' = b - \beta_{z_i} - \beta_{z_j} + \beta_{z_k} + \beta_{z_l}. \quad \text{(B10)}$$

The functions f_n and $g_{a,b}$ are products of Moshinsky coefficients given by

$$f_n = \langle n_{z_i} n_{z_j}||nN\rangle\langle n_{z_k} n_{z_l}||n'N\rangle, \quad \text{(B11)}$$

$$g_{a,b} = \langle\alpha_i\alpha_j||aA\rangle\langle\beta_i\beta_j||bB\rangle\langle\alpha_k\alpha_l||a'A\rangle\langle\beta_k\beta_l||b'B\rangle. \quad \text{(B12)}$$

In addition, the positive constant c_0 is such that $c_0^3 = c_z c_\perp^2$, where $c_z = \sqrt{m\omega_z/\hbar}$ and $c_\perp = \sqrt{m\omega_\perp/\hbar}$ are the oscillator constants associated, respectively, with the oscillator frequencies ω_z along the symmetry axis z and $\omega_\perp$ along the perpendicular direction. In the definitions of c_z and $c_\perp$, m is the average nucleon mass. The coefficients $\binom{i}{j}$ are the usual binomial coefficients, and $\mathcal{C}(n,n',k)$ and $\mathcal{A}(\ell)$ are defined by

$$\mathcal{C}(n,n',k) = \frac{\sqrt{n!\,n'!\,k!}}{\left(\frac{n+n'-k}{2}\right)!\left(\frac{n'+k-n}{2}\right)!\left(\frac{k+n-n'}{2}\right)!}, \quad \text{(B13)}$$

$$\mathcal{A}(\ell) = \begin{cases} \frac{(-)^{\ell/2}\sqrt{\ell!}}{2^{\ell/2}(\ell/2)!} & \text{if } \ell \text{ is even,} \\ 0 & \text{otherwise.} \end{cases} \quad \text{(B14)}$$

Finally, the $\mathfrak{I}^{c_z,c_\perp}_{k,\ell,m,n}$ integrals are defined by

$$\mathfrak{I}^{c_z,c_\perp}_{k,\ell,m,n} = \int_0^{+\infty} \frac{(c_\perp^2\sigma^2)^\ell (c_\perp^2\sigma^2-1)^m \sigma\, d\sigma}{(1+c_\perp^2\sigma^2)^n \sqrt{\left(1+c_z^2\sigma^2\right)^{2k+1}}} \quad \text{(B15)}$$

and have to be used with the following restrictions: (i) k, ℓ, and m are non-negative integers and $n \geqslant 0$; (ii) $\ell + m < n$.

Reference [31] provides a complete analytical method based on recursive expressions to evaluate the $\mathfrak{I}^{c_z,c_\perp}_{k,\ell,m,n}$ integrals, but this method is extremely sensitive to the computational accuracy for the quantum numbers n_z, α, and β involved in this work (we include 11 major oscillator shells in our basis). In practice, to evaluate these integrals with a sufficient precision and in a tractable way, we express $c_\perp^2\, \mathfrak{I}^{c_z,c_\perp}_{k,\ell,m,n}$ on the [0; 1] range as

$$c_\perp^2\, \mathfrak{I}^{c_z,c_\perp}_{k,\ell,m,n} = \frac{1}{2}\int_0^1 \left(\frac{x}{x+1}\right)^\ell \left(\frac{x-1}{x+1}\right)^m \frac{dx}{(x+1)^n(1+qx)^{k+\frac{1}{2}}} + \int_0^1 \left(\frac{1}{1+x^2}\right)^\ell \left(\frac{1-x^2}{1+x^2}\right)^m \frac{x^{2(k+n-1)}\,dx}{(1+x^2)^n(x^2+q)^{k+\frac{1}{2}}}, \quad \text{(B16)}$$

where $q = (c_z/c_\perp)^2$. We then interpolate the functions to be integrated using a cubic spline and integrate the resulting functions.

APPENDIX C: MATRIX ELEMENTS OF THE $\hat{\mathbf{T}}^4$ OPERATOR IN THE MANY-BODY BASIS

Let us start from the following form of the $\hat{\mathbf{T}}^2$ operator:

$$\hat{\mathbf{T}}^2 = \hat{T}_z(\hat{T}_z+1) + \hat{T}_-\hat{T}_+, \quad \text{(C1)}$$

where $\hat{T}_-$ and $\hat{T}_+$ are the usual isospin ladder operators defined by $\hat{T}_\pm = \hat{T}_x \pm i\hat{T}_y$. Because the product $\hat{T}_-\hat{T}_+$ commutes with any function of the $\hat{T}_z$ operator, and using the commutation relations

$$[\hat{T}_+, \hat{T}_-] = 2\hat{T}_z, \quad \text{(C2)}$$

$$[\hat{T}_z, \hat{T}_\pm] = \pm\hat{T}_\pm, \quad \text{(C3)}$$

we can express the $\hat{\mathbf{T}}^4$ operator as a function of powers of $\hat{T}_-$ and $\hat{T}_+$,

$$\hat{\mathbf{T}}^4 = (\hat{T}_z+1)^2\left(\hat{T}_z^2 + 2\hat{T}_-\hat{T}_+\right) + \hat{T}_-^2\hat{T}_+^2. \quad \text{(C4)}$$

The product $\hat{T}_-^2\hat{T}_+^2$ is the sum of two-body, three-body, and four-body operators:

$$\hat{T}_-^2\hat{T}_+^2 = 2\sum_{i\neq j}(\hat{t}_-\hat{t}_+)(i)\otimes(\hat{t}_-\hat{t}_+)(j) + \sum_{i\neq j\neq k}(\hat{t}_-\hat{t}_+)(i)\otimes\hat{t}_-(j)\otimes\hat{t}_+(k) + \sum_{i\neq j\neq k\neq\ell}\hat{t}_-(i)\otimes\hat{t}_-(j)\otimes\hat{t}_+(k)\otimes\hat{t}_+(\ell). \quad \text{(C5)}$$

Its nonvanishing matrix elements between Slater determinants $|\Phi\rangle$ and $|\Phi'\rangle$ built from the same single-particle basis involve five different cases.

(i) $|\Phi'\rangle = |\Phi\rangle$ (diagonal matrix element):

$$\langle\Phi|\hat{T}_-^2\hat{T}_+^2|\Phi\rangle = 2(Z-1)\left(Z - \langle\Phi|\hat{F}|\Phi\rangle\right) + \tfrac{1}{2}\langle\Phi|\hat{F}|\Phi\rangle^2 - \langle\Phi|\hat{F}\hat{\rho}_\Phi\hat{F}|\Phi\rangle, \quad \text{(C6)}$$

where the one-body operator $\hat{F}$ is defined in terms of the reduced one-body density $\hat{\rho}_\Phi$ associated with the Slater determinant $|\Phi\rangle$ and the single-particle isospin ladder operators $\hat{t}_\pm$ by

$$\hat{F} = \hat{t}_-\hat{\rho}_\Phi\hat{t}_+ + \hat{t}_+\hat{\rho}_\Phi\hat{t}_-. \quad \text{(C7)}$$

(ii) $|\Phi'\rangle = \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_b \hat{a}_a |\Phi\rangle$ (2p2h relative excitation):

$$\langle\Phi|\hat{T}_-^2\hat{T}_+^2|\Phi'\rangle = 4[(Z-1-\tfrac{1}{2}\langle\Phi|\hat{F}|\Phi\rangle)\langle ab|\hat{G}|\widetilde{\alpha\beta}\rangle + \langle ab|\hat{F}\otimes\hat{F}|\widetilde{\alpha\beta}\rangle + \langle ab|\hat{F}\hat{\rho}_\Phi\hat{G}|\widetilde{\alpha\beta}\rangle], \tag{C8}$$

with the two-body operator $\hat{G} = \hat{t}_-\otimes\hat{t}_+ + \hat{t}_+\otimes\hat{t}_-$ and $|\widetilde{\alpha\beta}\rangle = |\alpha\beta\rangle - |\beta\alpha\rangle$.

(iii) $|\Phi'\rangle = \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}^\dagger_\gamma \hat{a}^\dagger_\delta \hat{a}_d \hat{a}_c \hat{a}_b \hat{a}_a |\Phi\rangle$ (4p4h relative excitation):

$$\langle\Phi|\hat{T}_-^2\hat{T}_+^2|\Phi'\rangle = 4\,\langle abcd|(\hat{G}\otimes\hat{G}) + (\hat{t}_-\otimes\hat{t}_-)\otimes(\hat{t}_+\otimes\hat{t}_+) + (\hat{t}_+\otimes\hat{t}_+)\otimes(\hat{t}_-\otimes\hat{t}_-)|\widetilde{\alpha\beta\gamma\delta}\rangle, \tag{C9}$$

with

$$|\widetilde{\alpha\beta\gamma\delta}\rangle = |\widetilde{\alpha\beta}\rangle\otimes|\widetilde{\gamma\delta}\rangle - |\widetilde{\alpha\gamma}\rangle\otimes|\widetilde{\beta\delta}\rangle + |\widetilde{\alpha\delta}\rangle\otimes|\widetilde{\beta\gamma}\rangle + |\widetilde{\beta\gamma}\rangle\otimes|\widetilde{\alpha\delta}\rangle - |\widetilde{\beta\delta}\rangle\otimes|\widetilde{\alpha\gamma}\rangle + |\widetilde{\gamma\delta}\rangle\otimes|\widetilde{\alpha\beta}\rangle. \tag{C10}$$

APPENDIX D: ISOSPIN PROBABILITIES IN THE DCA FRAMEWORK

Let us start with the normalized state $|\Psi\rangle$

$$|\Psi\rangle = a_0\,|\Phi_0\rangle + \sum_{MP,k,T,i} a^{(k)}_{\mathrm{MP},T,i}\,\big|\Psi^{(k)}_{\mathrm{MP},T,i}\big\rangle, \tag{D1}$$

satisfying thus the condition

$$a_0^2 + \sum_{MP,k,T,i} \big|a^{(k)}_{\mathrm{MP},T,i}\big|^2 = 1. \tag{D2}$$

In the DCA framework one has

$$\langle\Psi|\hat{\mathbf{T}}^{2j}|\Psi\rangle = a_0^2\,\langle\Phi_0|\hat{\mathbf{T}}^{2j}|\Phi_0\rangle + \sum_{MP,k,T,i} \big|a^{(k)}_{\mathrm{MP},T,i}\big|^2 \big\langle\Psi^{(k)}_{\mathrm{MP},T,i}\big|\hat{\mathbf{T}}^{2j}\big|\Psi^{(k)}_{\mathrm{MP},T,i}\big\rangle. \tag{D3}$$

Starting from Eq. (23), one can write the general probability $P^{(n)}_\Psi(T)$ in the form

$$P^{(n)}_\Psi(T) = \delta_{TT_0} + \sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\big[\langle\Psi|\hat{\mathbf{T}}^{2j}|\Psi\rangle - T_0^j(T_0+1)^j\big] \tag{D4}$$

$$= \delta_{TT_0} + \sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\left[a_0^2\,\langle\Phi_0|\hat{\mathbf{T}}^{2j}|\Phi_0\rangle + \sum_{MP,k,T',i}\big|a^{(k)}_{\mathrm{MP},T',i}\big|^2\big\langle\Psi^{(k)}_{\mathrm{MP},T',i}\big|\hat{\mathbf{T}}^{2j}\big|\Psi^{(k)}_{\mathrm{MP},T',i}\big\rangle - T_0^j(T_0+1)^j\right] \tag{D5}$$

$$= \delta_{TT_0} + \sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\big[\langle\Phi_0|\hat{\mathbf{T}}^{2j}|\Phi_0\rangle - T_0^j(T_0+1)^j\big] + \sum_{\mathrm{MP},k,T',i}\big|a^{(k)}_{\mathrm{MP},T',i}\big|^2\sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\big[\big\langle\Psi^{(k)}_{\mathrm{MP},T',i}\big|\hat{\mathbf{T}}^{2j}\big|\Psi^{(k)}_{\mathrm{MP},T',i}\big\rangle - \langle\Phi_0|\hat{\mathbf{T}}^{2j}|\Phi_0\rangle\big]. \tag{D6}$$

The result (D6) is obtained thanks to the normalization relation (D2).

Noting that

$$\sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\big\langle\Psi^{(k)}_{\mathrm{MP},T',i}\big|\hat{\mathbf{T}}^{2j}\big|\Psi^{(k)}_{\mathrm{MP},T',i}\big\rangle = P^{(n)}_{\Psi^{(k)}_{\mathrm{MP},T',i}}(T) - \delta_{TT_0} - \sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\,T_0^j(T_0+1)^j$$

and

$$\sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\,\langle\Phi_0|\hat{\mathbf{T}}^{2j}|\Phi_0\rangle = P^{(n)}_{\Phi_0}(T) - \delta_{TT_0} - \sum_{j=1}^{n}\Gamma^{(n)}_{T-T_0,j}\,T_0^j(T_0+1)^j, \tag{D7}$$

one can finally write the contribution $P^{(n)}_{\mathrm{corr}}(T)$ coming from the correlations to the probability $P^{(n)}_\Psi(T)$ as

$$P^{(n)}_{\mathrm{corr}}(T) = \sum_{\mathrm{MP},k,T',i}\big|a^{(k)}_{\mathrm{MP},T',i}\big|^2\left(P^{(n)}_{\Psi^{(k)}_{\mathrm{MP},T',i}}(T) - P^{(n)}_{\Phi_0}(T)\right). \tag{D8}$$

The isospin-mixing parameter $\alpha = 1 - P_\Psi(T_d)$ finally becomes

$$\alpha = \alpha_0 + C_{\mathrm{corr}}, \tag{D9}$$

with

$$\alpha_0 = 1 - P^{(n)}_{\Phi_0}(T_d) \tag{D10}$$

and

$$C_{\mathrm{corr}} = \sum_{\mathrm{MP},k,T',i}\big|a^{(k)}_{\mathrm{MP},T',i}\big|^2\left(P^{(n)}_{\Phi_0}(T_d) - P^{(n)}_{\Psi^{(k)}_{\mathrm{MP},T',i}}(T_d)\right). \tag{D11}$$

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