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Neutron-proton pairing and double-beta decay in the interacting boson model

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Background: The interacting boson model has been used extensively to calculate the matrix elements governing neutrinoless double-beta decay. Studies within other models—the shell model, the quasiparticle random-phase approximation, and nuclear energy-density functional theory—indicate that a good description of neutron-proton pairing is essential for accurate calculations of those matrix elements, even though the isotopes used in experiment have significantly more neutrons than protons. The usual interacting boson model is based only on like-particle pairs, however, and the extent to which it captures neutron-proton pairing is not clear.

Purpose: To determine whether neutron-proton pairing should be explicitly included as neutronproton bosons in interacting-boson-model calculations of neutrinoless double-beta decay matrix elements. In this initial work we restrict ourselves to nuclei in the lower half of the pf shell, where exact shell model calculations are possible.

Method: An isospin-invariant version of the nucleon-pair shell model is applied to carry out shellmodel calculations in a large space and in a collective subspace, and to define effective operators in the latter. A democratic mapping is then used to define corresponding boson operators for the interacting boson model, with and without an isoscalar neutron-proton pair boson.

Results: Interacting-boson-model calculations with and without the isoscalar boson are carried out for nuclei near the beginning of the pf shell, with a realistic shell-model Hamiltonian and neutrinoless double-beta-decay operator as the starting point. Energy spectra and double-beta matrix elements are compared to those obtained in the underlying shell model.

Conclusions: The isoscalar boson is not important for energy spectra but improves the results for the double-beta matrix elements. To be useful at the level of precision we need, the mapping procedure must be further developed to better determine the dependence of the boson Hamiltonian and decay operator on particle number and isospin, and extended to heavier nuclei. But the benefits provided by the isoscalar boson in the nuclei examined here suggest that through an appropriate combination of mappings and fitting, it would make interacting-boson-model matrix elements more accurate in the heavier nuclei used in experiments.

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I. INTRODUCTION

Experiments to measure the rate of neutrinoless double-beta $(0\nu\beta\beta)$ decay, in which two neutrons decay to two protons and two electrons, are growing in number and expense [1–4]. A nonzero rate would imply that neutrinos are Majorana particles [5] and provide information about neutrino masses [6, 7], and possibly about exotic new particles [8]. To efficiently plan and interpret the experiments, however, one must know with reasonable accuracy the nuclear matrix elements that govern the decay. The matrix elements cannot be measured, and so calculating them with controlled precision has become an important theoretical goal.

A variety of many-body methods have been loosed on the matrix element problem [9]. Of these, most are embedded in phenomenological models that describe energy levels and other decay processes well in heavy nuclei. The interacting boson model (IBM) [10], in which the fundamental constituents are spin-zero and spin-two bosons that stand both for like-nucleon pairs and the collective quadrupole degree of freedom, is a good example [11– 13]. The version called IBM-2 [14], in which neutron and proton bosons are distinguishable, successfully describes spectra and electromagnetic transitions [10] plus single- β decay [15] in a wide variety of nuclei.

Because the IBM is equivalent to the Bohr-Mottelson collective model in certain limits, one might expect the important physics in the IBM to mirror that in approaches such as nuclear energy-density functional (EDF) theory, in which quadrupole degrees of freedom are emphasized. Similarly, because the IBM's bosons are related to collective shell-model excitations, the important physics in the IBM and the shell model should have something in common. In both EDF-based methods—in particular, the generator coordinate method (GCM) and in the shell model, $0\nu\beta\beta$ matrix elements tend to be too large unless care is taken with the J = 1, T = 0(isoscalar) pairing interaction. That component of the nuclear Hamiltonian has been known to be important from QRPA calculations [16, 17] for nearly 30 years. More recently, Ref. [18] showed that the inclusion of the isoscalar-pairing amplitude as a generator coordinate reduces matrix elements significantly, and Ref. [19] showed

that the isoscalar pairing in the Hamiltonian does the same in the shell model. Here we investigate whether it plays a similar role in the IBM. More explicitly, we ask whether we need to add a spin-1 isoscalar boson to the model to avoid over-estimating $0\nu\beta\beta$ matrix elements, and try to provide an answer.

To address the question, one would like to modify the IBM $0\nu\beta\beta$ calculations of Refs. [11–13] by adding the isoscalar spin-1 boson, which we will label p. But because the IBM Hamiltonian is phenomenological, we do not know *a priori* how to add to and alter its Hamiltonian so as to correctly include the physics of the new boson. One might examine single- β decay and other processes in which the boson could play a significant role in order to pin down new terms in the Hamiltonian, but that task is beyond what we are able to do here. Instead, we try to derive the boson Hamiltonian and the corresponding decay operator, not in nuclei that actually undergo $0\nu\beta\beta$ decay, but rather in light pf-shell nuclei for which exact shell model results are available, both for spectra and for $0\nu\beta\beta$ matrix elements [19]. Since the IBM is supposed to represent collective dynamics in a major shell, we construct a mapping of operators from the pf shell to a set of bosons, including not only the usual bosons of the IBM-2 but "neutron-proton" bosons as well. Ref. [11] developed a mapping to obtain a boson $0\nu\beta\beta$ operator; here, starting from square one, we map the Hamiltonian as well. Though this procedure will not tell us how much a p boson would change the realistic IBM $0\nu\beta\beta$ predictions, it will give us a good idea of the extent to which a p boson is required to faithfully reflect shell-model results.

It is not obvious that the extra boson will improve the description of $0\nu\beta\beta$ decay. Certainly it will capture some of the isoscalar-pair correlations that elude the IBM-2. But because the product of two isoscalar J = 1pair creation operators can be rewritten as a superposition of products of proton pair creation operators and neutron pair creation operators, some of the physics of isoscalar pairing is probably already in the IBM-2. Furthermore, the use of too many boson types can cause a model to degrade for a related reason: an over-counting, roughly speaking, of the independent collective degrees of freedom. Thus, though an independent isoscalar-pairing coordinate is clearly important in GCM calculations of $0\nu\beta\beta$ matrix elements, an isoscalar boson may or may not improve the corresponding IBM calculations.

We carry out the mapping from shell model to IBM in two steps, the first of which relies on the nucleonpair shell model (NPSM) [20–22] to define a collective subspace. We briefly review the NPSM in Secs. II and III, with the main purpose of introducing notation for an isospin-invariant formulation of the model [23]; with a collective subspace specified by the NPSM, we show in Sec. IV that we can use the method of Suzuki and Lee [24] to construct effective operators for the subspace. The second step, which we describe in Sec. V, involves the mapping of the (effective) Hamiltonian and the $0\nu\beta\beta$ decay operator from the fermion to boson spaces. In Sec. VI we apply the formalism to the energy spectra of and $0\nu\beta\beta$ -transition strengths between nuclei in the lower part of the pf shell, taking into account correlations in the entire shell. Finally, in Sec. VII, we present our conclusions.

II. THE NUCLEON-PAIR SHELL MODEL

We introduce the following notation for pairs of fermions:

$$P^{\dagger}_{\alpha\Gamma M_{\Gamma}} \equiv (a^{\dagger}_{\gamma_{1}} \times a^{\dagger}_{\gamma_{2}})^{(\Gamma)}_{M_{\Gamma}}, \qquad (1)$$

where γ_i denotes the angular momentum j_i and isospin t_i (which is always $\frac{1}{2}$) of a single nucleon, Γ stands for the coupled angular momentum J and isospin T (which can be 0 or 1) of the nucleons with γ_1 and γ_2 (with α standing for γ_1, γ_2), and M_{Γ} represents the corresponding projections (i.e., $M_{\Gamma} = M_J M_T$). We write an arbitrary n-pair state of the NPSM as

$$|\alpha_{1}\Gamma_{1}\dots\alpha_{n}\Gamma_{n}\Lambda_{2}\dots\Lambda_{n}\rangle \equiv \left(\cdots \left(\left(P_{\alpha_{1}\Gamma_{1}}^{\dagger} \times P_{\alpha_{2}\Gamma_{2}}^{\dagger}\right)^{(\Lambda_{2})} \times P_{\alpha_{3}\Gamma_{3}}^{\dagger}\right)^{(\Lambda_{3})} \times \cdots \times P_{\alpha_{n}\Gamma_{n}}^{\dagger}\right)^{(\Lambda_{n})} |O\rangle, \qquad (2)$$

or,

$$|P_r\rangle \equiv |\alpha_1\Gamma_1\dots\alpha_n\Gamma_n\Lambda_2\dots\Lambda_n\rangle, \ r=1,\dots,\Theta, \quad (3)$$

for short. The state $|O\rangle$ in Eq. (2) is the bare fermion vacuum, and the index r in Eq. (3) stands for the set of quantum numbers $\{\alpha_1\Gamma_1 \dots \alpha_n\Gamma_n\Lambda_2 \dots \Lambda_n\}$, which specifies the character of the n pairs $\alpha_q\Gamma_q$, the set Λ_q of intermediate angular momenta and isospins, and Λ_n , the state's total angular momentum and isospin.

In general the basis in Eq. (2) is non-orthonormal and

overcomplete. A calculation in this basis therefore requires the diagonalization of the overlap matrix $\langle P_r | P_s \rangle$, the elements of which can be computed with a recurrence relation presented in Ref. [21] and generalized to include isospin in Ref. [23]. Here we need matrix elements between one- and two-pair states; these are trivial for n = 1 and summarized in Appendix A for n = 2. Vanishing eigenvalues of the matrix $\langle P_r | P_s \rangle$ indicate the overcompleteness of the pair basis. In a subspace of Ω pair states in which all eigenvalues of the overlap matrix are non-zero, one can construct an orthonormal set given by:

$$|\bar{P}_r\rangle = \sqrt{\frac{1}{O_r}} \sum_{s=1}^{\Omega} C_{rs} |P_s\rangle \equiv \sum_{s=1}^{\Omega} \bar{C}_{rs} |P_s\rangle, \ r = 1, \dots, \Omega,$$
(4)

where O_r is the r^{th} eigenvalue of the $\Omega \times \Omega$ overlap matrix:

$$O_{rs} \equiv \langle P_r | P_s \rangle, \ r, s = 1, \dots, \Omega, \tag{5}$$

and the coefficients $\{C_{rs}, s = 1, \ldots, \Omega\}$ specify the corresponding eigenvector. If Ω is the dimension of the original shell-model space \mathbb{H} , which we call the "complete" shell-model space, then the vectors $\{|\bar{P}_r\rangle, r = 1, \ldots, \Omega\}$ form a basis of \mathbb{H} .

It is important to distinguish between the total number Θ of possible *n*-pair states in Eq. (3) and the number $\Omega \leq \Theta$ of linearly independent states among them. To apply the NPSM in a collective subspace, one needs to expand an arbitrary *n*-pair state in terms of the orthogonal basis states,

$$|P_r\rangle = \sum_{s=1}^{\Omega} A_{rs} |\bar{P}_s\rangle, \ r = 1, \dots, \Theta, \qquad (6)$$

where the coefficients A_{rs} are given by

$$A_{rs} \equiv \langle P_r | \bar{P}_s \rangle = \sum_{t=1}^{\Omega} \bar{C}_{st} \langle P_r | P_t \rangle, \qquad (7)$$

with $r = 1, \ldots, \Theta$ and $s = 1, \ldots, \Omega$. We assume here and henceforth that the matrix elements are real, that is, that $\langle P_r | P_s \rangle = \langle P_s | P_r \rangle$ and $\langle \bar{P}_r | P_s \rangle = \langle P_s | \bar{P}_r \rangle$.

An arbitrary shell-model operator \hat{T}^{f} (where f stands for "fermion") between two sets of orthogonal basis states,

$$|\bar{P}'_{r'}\rangle = \sum_{s'=1}^{\Omega'} \bar{C}'_{r's'} |P'_{s'}\rangle, \ r' = 1, \dots, \Omega',$$

$$|P''_{r''}\rangle = \sum_{s''=1}^{\Omega''} \bar{C}''_{r''s''} |P''_{s''}\rangle, \ r'' = 1, \dots, \Omega'',$$

$$(8)$$

has the matrix elements

$$\langle \bar{P}'_{r'} | \hat{T}^{\rm f} | \bar{P}''_{r''} \rangle = \sum_{s'=1}^{\Omega'} \sum_{s''=1}^{\Omega''} \bar{C}'_{r's'} \bar{C}''_{r''s''} \langle P'_{s'} | \hat{T}^{\rm f} | P''_{s''} \rangle$$

$$= (\bar{C}' \times T^{\rm f} \times \bar{C}''^{T})_{r'r''} .$$
(9)

Here M^T is the transposed matrix of M and \bar{C}', T^f , and \bar{C}'' are the following matrices:

$$\bar{\boldsymbol{C}}' : \{ \bar{C}'_{r's'}, r' = 1, \dots, \Omega', s' = 1, \dots, \Omega' \},
\boldsymbol{T}^{\mathrm{f}} : \{ \langle P'_{s'} | \hat{T}^{\mathrm{f}} | P''_{s''} \rangle, s' = 1, \dots, \Omega', s'' = 1, \dots, \Omega'' \},
\bar{\boldsymbol{C}}'' : \{ \bar{C}''_{r''s''}, r'' = 1, \dots, \Omega'', s'' = 1, \dots, \Omega'' \}.$$
(10)

For the Hamiltonian operator, $\hat{T}^{\rm f} = \hat{H}^{\rm f}$, the dimensions in bra and ket of Eq. (9) are the same, $\Omega' = \Omega'' \equiv \Omega$, and the diagonalization of the $\Omega \times \Omega$ Hamiltonian matrix leads to the eigenstates

$$\left|\bar{E}_{t}\right\rangle = \sum_{r=1}^{\Omega} E_{tr} \left|\bar{P}_{r}\right\rangle, \ t = 1, \dots, \Omega, \qquad (11)$$

where the coefficients $\{E_{tr}, r = 1, \ldots, \Omega\}$ are the components of the eigenvector associated with the eigenvalue E_t . If \hat{T}^{f} is another operator, e.g. a transition operator, its action on eigenstates of \hat{H}^{f} in the complete Hilbert space \mathbb{H} is given by

$$\langle \bar{E}_{t'}^{\prime} | \hat{T}^{\mathrm{f}} | \bar{E}_{t''}^{\prime\prime} \rangle = \sum_{r'=1}^{\Omega'} \sum_{r''=1}^{\Omega''} E_{t'r'}^{\prime} E_{t''r''}^{\prime\prime} \langle \bar{P}_{r'}^{\prime} | \hat{T}^{\mathrm{f}} | \bar{P}_{r''}^{\prime\prime} \rangle$$

$$= (\boldsymbol{E}^{\prime} \times \bar{\boldsymbol{C}}^{\prime} \times \boldsymbol{T}^{\mathrm{f}} \times \bar{\boldsymbol{C}}^{\prime\prime T} \times \boldsymbol{E}^{\prime\prime T})_{t't''},$$

$$(12)$$

with $t' = 1, ..., \Omega'$ and $t'' = 1, ..., \Omega''$.

All this shows us that it is possible to carry out standard shell-model calculations in the NPSM, albeit in a complicated way. The advantage of the NPSM is that it allows a truncation to a shell-model subspace constructed in terms of collective pairs.

III. COLLECTIVE SUBSPACE

A collective fermion pair is a superposition of pairs built from orbits with different γ_1 and γ_2 , all coupled to the same Γ . It can be specified by its coefficients $\alpha_{\gamma_1\gamma_2}^{\Gamma}$:

$$B^{\dagger}_{\alpha\Gamma M_{\Gamma}} \equiv \sum_{\gamma_{1}\gamma_{2}} \alpha^{\Gamma}_{\gamma_{1}\gamma_{2}} (a^{\dagger}_{\gamma_{1}} \times a^{\dagger}_{\gamma_{2}})^{(\Gamma)}_{M_{\Gamma}} , \qquad (13)$$

where the subscript α is to emphasize the dependence of the pair on its coefficients. After selecting a particular set of collective pairs $\{B_{\Gamma}\}$, we can construct NPSM states from them, *viz*.

$$|\alpha_{1}\Gamma_{1}\dots\alpha_{n}\Gamma_{n}\Lambda_{2}\dots\Lambda_{n}\rangle \equiv \left(\dots\left(\left(B_{\alpha_{1}\Gamma_{1}}^{\dagger}\times B_{\alpha_{2}\Gamma_{2}}^{\dagger}\right)^{(\Lambda_{2})}\times B_{\alpha_{3}\Gamma_{3}}^{\dagger}\right)^{(\Lambda_{3})}\times\dots\times B_{\alpha_{n}\Gamma_{n}}^{\dagger}\right)^{(\Lambda_{n})}|0\rangle.$$
(14)

Although the formalism does not require it, we shall henceforth consider only one collective pair for a given Γ (i.e., J and T). This step enables us to dispense

with the indices α_q , reducing the necessary labels to $\{\Gamma_1 \dots \Gamma_n \Lambda_2 \dots \Lambda_n\}$ and leading to the abbreviation

$$|B_i\rangle \equiv |\Gamma_1 \dots \Gamma_n \Lambda_2 \dots \Lambda_n\rangle, \ i = 1, \dots, \omega, \qquad (15)$$

where ω is the number of couplings $\{\Gamma_1 \dots \Gamma_n \Lambda_2 \dots \Lambda_n\}$.

The collective NPSM states in Eq. (14) can be expressed as linear combinations of the non-collective ones in Eq. (2):

$$|B_i\rangle = \sum_{r=1}^{\Theta} a_{ir} |P_r\rangle = \sum_{r=1}^{\Theta} \sum_{s=1}^{\Omega} a_{ir} A_{rs} |\bar{P}_s\rangle$$

$$= \sum_{s=1}^{\Omega} (\boldsymbol{a} \times \boldsymbol{A})_{is} |\bar{P}_s\rangle, \ i = 1, \dots, \omega,$$
 (16)

with coefficients a_{ir} that are functions of $\alpha_{\gamma_1\gamma_2}^{\Gamma}$. Results analogous to those in Sec. II can now be obtained by diagonalizing the collective overlap matrix

$$o_{ij} \equiv \langle B_i | B_j \rangle = \sum_{r=1}^{\Omega} (\boldsymbol{a} \times \boldsymbol{A})_{ir} (\boldsymbol{a} \times \boldsymbol{A})_{jr}$$

= $(\boldsymbol{a} \times \boldsymbol{A} \times \boldsymbol{A}^T \times \boldsymbol{a}^T)_{ij}, \ i, j = 1, \dots, \omega.$ (17)

The number of linearly independent vectors $|B_i\rangle$ is given by the number of non-zero eigenvalues of the matrix o_{ij} . We assume here that all eigenvalues of the matrix (17) are non-zero, which will be the case for any reasonable choice of the collective subspace. As we have noted, the NPSM is interesting because when one restricts oneself to a set of collective pairs, the resulting space has a much lower dimension than does \mathbb{H} itself, *i.e.*, $\omega \ll \Omega$.

To carry out a shell-model calculation in the collective subspace, we employ notation that is analogous to what we used for the full space \mathbb{H} . Thus, we work with orthonormal states

$$\begin{split} |\bar{B}_{i}\rangle &= \sqrt{\frac{1}{o_{i}}} \sum_{j=1}^{\omega} c_{ij} |B_{j}\rangle \equiv \sum_{j=1}^{\omega} \bar{c}_{ij} |B_{j}\rangle \\ &= \sum_{r=1}^{\Omega} (\bar{\boldsymbol{c}} \times \boldsymbol{a} \times \boldsymbol{A})_{ir} |\bar{P}_{r}\rangle \equiv \sum_{r=1}^{\Omega} b_{ir} |\bar{P}_{r}\rangle \,, \end{split}$$
(18)

where o_i is the *i*th eigenvalue of the overlap matrix $(i = 1, \ldots, \omega)$ and the coefficients $\{c_{ij}, j = 1, \ldots, \omega\}$ make up the corresponding eigenvector. A shell-model operator \hat{T}^{f} has the matrix elements

$$\langle \bar{B}_{i'}' | \hat{T}^{\mathrm{f}} | \bar{B}_{i''}'' \rangle = \sum_{r'=1}^{\Omega'} \sum_{r''=1}^{\Omega''} b_{i'r'} b_{i''r''} \langle \bar{P}_{r'}' | \hat{T}^{\mathrm{f}} | \bar{P}_{r''}'' \rangle$$

$$= (\boldsymbol{b}' \times \bar{\boldsymbol{C}}' \times \boldsymbol{T}^{\mathrm{f}} \times \bar{\boldsymbol{C}}''^T \times \boldsymbol{b}''^T)_{i'i''},$$

$$(19)$$

with $i' = 1, \ldots, \omega'$ and $i'' = 1, \ldots, \omega''$. For the Hamiltonian operator, $\hat{T}^{f} = \hat{H}^{f}$, the matrix (19) has dimension $\omega \times \omega$ and its diagonalization leads to the eigenstates

$$|\bar{e}_k\rangle = \sum_{i=1}^{\omega} e_{ki} |\bar{B}_i\rangle = \sum_{r=1}^{\Omega} (\boldsymbol{e} \times \boldsymbol{b})_{kr} |\bar{P}_r\rangle, \qquad (20)$$

with $k = 1, ..., \omega$ and with the coefficients $\{e_{ki}, i = 1, ..., \omega\}$ given by the components of the eigenvector associated with the eigenvalue e_k . If \hat{T}^{f} is some other operator, its matrix elements in the basis of eigenstates of \hat{H}^{f} are given by

$$\langle \bar{e}'_{k'} | \hat{T}^{\mathrm{f}} | \bar{e}''_{k''} \rangle = (\boldsymbol{e}' \times \boldsymbol{b}' \times \bar{\boldsymbol{C}}' \times \boldsymbol{T}^{\mathrm{f}} \times \bar{\boldsymbol{C}}''^T \times \boldsymbol{b}''^T \times \boldsymbol{e}''^T)_{k'k''},$$
(21)
with $k' = 1, \dots, \omega'$ and $k'' = 1, \dots, \omega''.$

IV. EFFECTIVE SHELL-MODEL OPERATORS IN A COLLECTIVE SUBSPACE

The eigenspectrum of \hat{H}^{f} and the matrix elements of transition operators \hat{T}^{f} in the restricted Hilbert space differ from the corresponding eigenspectrum and matrix elements of the operators in the complete Hilbert space \mathbb{H} . We need an effective Hamiltonian \hat{H}_{eff}^{f} and, more generally, effective operators \hat{T}_{eff}^{f} in the restricted Hilbert space that preserve the original eigenvalues and matrix elements. We begin their construction by letting \mathbb{H}_{P} be the restricted Hilbert space and \mathbb{H}_{Q} the excluded Hilbert space, with $\mathbb{H} = \mathbb{H}_{P} \cup \mathbb{H}_{Q}$. The operators \hat{P} and \hat{Q} project onto the corresponding spaces, so that $\hat{P}\mathbb{H} =$ \mathbb{H}_{P} and $\hat{Q}\mathbb{H} = \mathbb{H}_{Q}$. The eigenstates of \hat{H}^{f} in \mathbb{H} are given by $\{|\bar{E}_{t}\rangle, t = 1, \ldots, \Omega\}$ and those of \hat{H}^{f} in \mathbb{H}_{P} by $\{|\bar{e}_{k}\rangle, k = 1, \ldots, \omega\}$. For each eigenstate $|\bar{e}_{k}\rangle$ we identify a corresponding eigenstate $|\bar{E}_{k}\rangle$, usually by requiring a maximum overlap

$$\langle \bar{E}_k | \bar{e}_k \rangle = \sum_{r=1}^{\Omega} E_{tr} (\boldsymbol{e} \times \boldsymbol{b})_{kr} = (\boldsymbol{E} \times \boldsymbol{b}^T \times \boldsymbol{e}^T)_{tk}.$$
 (22)

This procedure defines a set of ω eigenstates $\{|\bar{E}_{t_k}\rangle, k = 1, \ldots, \omega\}$ and an associated $\omega \times \Omega$ matrix \tilde{E} with the elements

$$\tilde{\boldsymbol{E}}: \{\tilde{E}_{kr} \equiv E_{t_kr}, \ k = 1, \dots, \omega, \ r = 1, \dots, \Omega\}.$$
(23)

For each of the eigenstates $|\bar{E}_{t_k}\rangle$ we define its component in \mathbb{H}_P ,

$$|e_k\rangle \equiv \hat{P} |\bar{E}_{t_k}\rangle, \ k = 1, \dots, \omega,$$
 (24)

and assume that the states $\{|e_k\rangle, k = 1, \ldots, \omega\}$ are linearly independent and therefore span the entire restricted Hilbert space \mathbb{H}_P .

We use the method of Suzuki and Lee [24] to determine effective operators in \mathbb{H}_P . The method employs an operator $\hat{\eta}$ that maps states in \mathbb{H}_P to states in \mathbb{H}_Q such that

$$\hat{\eta} |e_k\rangle = \hat{Q} |\bar{E}_{t_k}\rangle, \ k = 1, \dots, \omega.$$
 (25)

Since $\hat{\eta} = \hat{Q}\hat{\eta}\hat{P}$, the operator $\hat{\eta}$ satisfies the relations

$$\hat{P}\hat{\eta} = \hat{\eta}\hat{Q} = 0, \quad \hat{\eta}\hat{P} = \hat{Q}\hat{\eta} = \hat{\eta}, \quad \hat{\eta}^2 = 0.$$
 (26)

It follows that

$$|\bar{E}_{t_k}\rangle = (\hat{P} + \hat{Q}) |\bar{E}_{t_k}\rangle = |e_k\rangle + \hat{\eta} |e_k\rangle = (\hat{I} + \hat{\eta}) |e_k\rangle, \quad (27)$$

and, inversely, that

$$|e_k\rangle = (\hat{I} - \hat{\eta})(\hat{I} + \hat{\eta}) |e_k\rangle = (\hat{I} - \hat{\eta}) |\bar{E}_{t_k}\rangle.$$
(28)

The transformed (non-hermitian) Hamiltonian $\hat{\mathcal{H}}^{f} \equiv (\hat{I} - \hat{\eta})\hat{H}^{f}(\hat{I} + \hat{\eta})$ satisfies the relation

$$\hat{\mathcal{H}}^{\mathrm{f}} |e_k\rangle = (\hat{I} - \hat{\eta})\hat{H}^{\mathrm{f}} |\bar{E}_{t_k}\rangle = E_{t_k}(\hat{I} - \hat{\eta}) |\bar{E}_{t_k}\rangle = E_{t_k} |e_k\rangle,$$
(29)

which shows that the states $\{|e_k\rangle, k = 1, \dots, \omega\}$ are eigenstates of $\hat{\mathcal{H}}^{\mathrm{f}}$, with eigenvalues $\{E_{t_k}, k = 1, \dots, \omega\}$.

A matrix element of $\hat{\eta}$ is nonzero only if the bra is in \mathbb{H}_Q and the ket in \mathbb{H}_P . The operator is therefore determined by the matrix elements

$$\langle \bar{P}_r | \hat{\eta} | \bar{B}_i \rangle, \ r = 1, \dots, \Omega, \ i = 1, \dots, \omega,$$
 (30)

where $|\bar{P}_r\rangle \in \mathbb{H}$ and $|\bar{B}_i\rangle \in \mathbb{H}_P$. To calculate the matrix elements in Eq. (30), we first note that although the states $\{|e_k\rangle, k = 1, \ldots, \omega\}$ span the entire Hilbert space \mathbb{H}_P , they do not form an orthonormal basis. A biorthogonal basis $\{\langle \tilde{e}_k | , k = 1, \ldots, \omega\}$ can be defined such that

$$\langle \tilde{e}_k | e_{k'} \rangle = \delta_{kk'} \,, \tag{31}$$

which implies that the operator \hat{P} , which is nothing but the identity operator on \mathbb{H}_P , can be written as

$$\hat{P} = \sum_{k=1}^{\omega} |e_k\rangle \langle \tilde{e}_k|.$$
(32)

Thus we have

$$\langle \bar{P}_r | \hat{\eta} | \bar{B}_i \rangle = \sum_{k=1}^{\omega} \langle \bar{P}_r | \hat{\eta} | e_k \rangle \langle \tilde{e}_k | \bar{B}_i \rangle.$$
(33)

The first matrix element in this sum can be written as

$$\langle \bar{P}_r | \hat{\eta} | e_k \rangle = \langle \bar{P}_r | \bar{E}_{t_k} \rangle - \sum_{i=1}^{\omega} \langle \bar{P}_r | \bar{B}_i \rangle \langle \bar{B}_i | \bar{E}_{t_k} \rangle , \quad (34)$$

where we have used the relation $\hat{P} = \sum |\bar{B}_i\rangle \langle \bar{B}_i|$. With the help of Eqs. (11) and (18) we deduce the relations

$$\langle \bar{P}_r | \bar{E}_{t_k} \rangle = \tilde{E}_{kr} , \; \langle \bar{P}_r | \bar{B}_i \rangle = b_{ir} , \; \langle \bar{B}_i | \bar{E}_{t_k} \rangle = (\boldsymbol{b} \times \boldsymbol{\tilde{E}}^T)_{ik} ,$$
(35)

which lead to the following expression for the first matrix element in the sum in Eq. (33):

$$\langle \bar{P}_r | \hat{\eta} | e_k \rangle = \tilde{E}_{kr} - (\tilde{\boldsymbol{E}} \times \boldsymbol{b}^T \times \boldsymbol{b})_{kr} .$$
 (36)

To determine the second matrix element in the sum in Eq. (33), we note that

$$\langle \bar{B}_i | \bar{B}_j \rangle = \sum_{k=1}^{\omega} \langle \bar{B}_i | e_k \rangle \, \langle \tilde{e}_k | \bar{B}_j \rangle = \delta_{ij} \,, \qquad (37)$$

which implies that the matrix $\langle \tilde{e}_k | \bar{B}_i \rangle$ is the inverse of the matrix with the elements

$$d_{ik} \equiv \langle \bar{B}_i | e_k \rangle = \langle \bar{B}_i | \hat{P} | \bar{E}_{t_k} \rangle = (\boldsymbol{b} \times \tilde{\boldsymbol{E}}^T)_{ik} .$$
(38)

We conclude that the matrix elements of the operator $\hat{\eta}$ are

$$\eta_{ri} \equiv \langle \bar{P}_r | \hat{\eta} | \bar{B}_i \rangle = \left((\boldsymbol{I}_{\Omega} - \boldsymbol{b}^T \times \boldsymbol{b}) \times \tilde{\boldsymbol{E}}^T \times \boldsymbol{d}^{-1} \right)_{ri}, \quad (39)$$

with $r = 1, \ldots, \Omega$ and $i = 1, \ldots, \omega$, and I_{Ω} given by the $\Omega \times \Omega$ identity matrix. The matrix elements η_{ri} can be defined entirely in terms of the Ω^2 NPSM overlap matrix elements in Eq. (5).

With an expression for the matrix elements of $\hat{\eta}$, we are now finally in a position to define effective operators for the collective subspace. To any operator \hat{T}^{f} , which acts on states in a Hilbert space \mathbb{H}'' to give states in a Hilbert space \mathbb{H}' , there corresponds an effective, hermitian operator [25]

$$\hat{T}_{\text{eff}}^{\text{f}} = \hat{P}' \hat{T}_{\eta}'^{-1/2} (\hat{I}' + \hat{\eta}'^{\dagger}) \hat{T}^{\text{f}} (\hat{I}'' + \hat{\eta}'') \hat{T}_{\eta}''^{-1/2} \hat{P}'' , \quad (40)$$

where

$$\hat{T}'_{\eta} \equiv (\hat{I}' + \hat{\eta}'^{\dagger} \hat{\eta}'), \quad \hat{T}''_{\eta} \equiv (\hat{I}'' + \hat{\eta}''^{\dagger} \hat{\eta}'').$$
 (41)

The operator $\hat{T}_{\text{eff}}^{\text{f}}$ acts on states in the restricted Hilbert space $\mathbb{H}_{P}^{\prime\prime}$ to give states in the restricted Hilbert space $\mathbb{H}_{P}^{\prime\prime}$. Its matrix elements involve sums over the inverse square root of the matrix

$$\langle \bar{B}_i | \hat{T}_\eta | \bar{B}_j \rangle = (\boldsymbol{I}_\omega + \boldsymbol{\eta}^T \times \boldsymbol{\eta})_{ij}, \ i, j = 1, \dots, \omega.$$
 (42)

Since $\hat{\eta}$ defines a positive-definite metric, the square root of the matrix in Eq. (42) can be taken through diagonalization. And the matrix elements of the other part of the operator in Eq. (40) are given by

$$\langle \bar{B}'_{j'} | (\hat{I}' + \hat{\eta}'^{\dagger}) \hat{T}^{\rm f} (\hat{I}'' + \hat{\eta}'') | \bar{B}''_{j''} \rangle$$

$$= ((\boldsymbol{b}' + \boldsymbol{\eta}'^T) \times \bar{\boldsymbol{C}}' \times \boldsymbol{T}^{\rm f} \times \bar{\boldsymbol{C}}''^T \times (\boldsymbol{b}''^T + \boldsymbol{\eta}''))_{j'j''},$$

$$(43)$$

with $j' = 1, ..., \omega'$ and $j'' = 1, ..., \omega''$.

Equation (40) gives the effective version of any operator. For the Hamiltonian operator an alternative expressions exists [25]:

$$\hat{H}_{\text{eff}}^{\text{f}} \equiv \hat{P}' \hat{T}_{\eta}'^{+1/2} \hat{H}^{\text{f}} (\hat{I}'' + \hat{\eta}'') \hat{T}_{\eta}''^{+1/2} \hat{P}'' , \qquad (44)$$

which involves the matrix elements

$$\langle \bar{B}'_{j'} | \hat{H}^{\mathrm{f}}(\hat{I}'' + \hat{\eta}'') | \bar{B}''_{j''} \rangle$$

$$= (\boldsymbol{b}' \times \bar{\boldsymbol{C}}' \times \boldsymbol{H}^{\mathrm{f}} \times \bar{\boldsymbol{C}}''^T \times (\boldsymbol{b}''^T + \boldsymbol{\eta}''))_{j'j''},$$

$$(45)$$

with $j' = 1, ..., \omega'$ and $j'' = 1, ..., \omega''$.

V. MAPPING TO BOSON OPERATORS

To study the IBM, we need to map the collective fermion pairs onto bosons. Given a choice of collective pairs $\{B_{\Gamma}\}$ we can introduce a corresponding set of bosons $\{b_{\Gamma}\}$. The boson analog of the state in Eq. (14) is

6

$$b_i \rangle \equiv \left(\cdots \left(\left(b_{\Gamma_1}^{\dagger} \times b_{\Gamma_2}^{\dagger} \right)^{(\Lambda_2)} \times b_{\Gamma_3}^{\dagger} \right)^{(\Lambda_3)} \times \cdots \times b_{\Gamma_n}^{\dagger} \right)^{(\Lambda_n)} |\mathbf{o}\rangle, \ i = 1, \dots, \omega,$$

$$(46)$$

where the $|o\rangle$ is the boson vacuum and the index *i* is again short-hand for the labels { $\Gamma_1 \dots \Gamma_n \Lambda_2 \dots \Lambda_n$ }. In general, the boson states in Eq. (46) do not form an orthonormal basis, leading to complications described in Ref. [26]. For a mapping that is limited to operators with at most two-body terms between the bosons, however, only boson states with n = 1 and n = 2 are needed, in which case the overlap matrix $\langle b_i | b_j \rangle$ is diagonal and no such complications arise. The boson states that correspond to the orthogonalized fermion-pair states are obtained from the unitary transformation

$$\bar{b}_i \rangle = \sum_{j=1}^{\omega} c_{ij} |b_j\rangle, \ i = 1, \dots, \omega,$$
(47)

with the coefficients c_{ij} taken from the orthogonalization process in the collective fermion subspace [see Eq. (18)].

In the standard method for carrying out the boson mapping, introduced in the IBM by Otsuka, Arima, and Iachello (OAI) [27], one uses the Gram-Schmidt procedure to orthogonalize the fermion basis (not the boson basis). The procedure proposed in Eq. (47), known as democratic mapping [28], is different from OAI because it relies on the diagonalization of the overlap matrix for the non-orthogonal fermion basis. It is thus similar to Löwdin's symmetric orthogonalization procedure [29], introduced in quantum chemistry, which yields the orthogonal basis that is "closest" to the original non-orthogonal one [30, 31]. The democratic mapping has the additional advantage that it imposes no Graham-Schmidt-like hierarchy on the basis states, and as a result is more useful for models with several kinds of bosons, such as those to be considered here, for which an ordering would be arbitrary.

In the democratic mapping the boson image \hat{T}^{b} of a fermion operator, which can be \hat{T}^{f} or its effective version \hat{T}_{eff}^{f} , is determined by the relation

$$\langle \bar{b}'_{i'} | \hat{T}^{\mathbf{b}} | \bar{b}''_{i''} \rangle \doteq \langle \bar{B}'_{i'} | \hat{T}^{\mathbf{f}} | \bar{B}''_{i''} \rangle, \ i'' = 1, \dots, \omega'', \quad (48)$$

where the symbol \doteq indicates that the equality holds by virtue of the mapping. In terms of the original basis states $|b_i\rangle$, this relation leads to the boson matrix elements

$$\langle b_{i'}' | \hat{T}^{\mathbf{b}} | b_{i''}'' \rangle \doteq \sum_{j'=1}^{\omega'} \sum_{j''=1}^{\omega''} c_{j'i'}' c_{j''i''}'' \langle \bar{B}_{j'}' | \hat{T}^{\mathbf{f}} | \bar{B}_{j''}'' \rangle$$

$$= (\boldsymbol{c}'^{T} \times \boldsymbol{b}' \times \bar{\boldsymbol{C}}' \times \boldsymbol{T}^{\mathbf{f}} \times \bar{\boldsymbol{C}}''^{T} \times \boldsymbol{b}''^{T} \times \boldsymbol{c}'')_{i'i''},$$

$$(49)$$

with $i' = 1, ..., \omega'$ and $i'' = 1, ..., \omega''$.

In the most general mapping several technical issues arise, including the elimination of spurious boson states and ambiguities for n > 2, which are described in Ref. [26]. No such difficulties exist for a mapping to a collective subspace with no more than two-body operators, $n \leq 2$. Even so, one must carefully define boson operators order by order. For example, for the Hamiltonian operator, $\hat{T} = \hat{H}$, one determines the single-boson energy from

$$\epsilon_{\Gamma} \equiv \langle b_{\Gamma} | \hat{H}^{\rm b} | b_{\Gamma} \rangle = \langle \bar{b}_{\Gamma} | \hat{H}^{\rm b} | \bar{b}_{\Gamma} \rangle \doteq \langle \bar{B}_{\Gamma} | \hat{H}^{\rm f} | \bar{B}_{\Gamma} \rangle , \quad (50)$$

and subsequently the two-body part of the boson Hamiltonian from

$$\begin{aligned} v^{\Lambda}_{\Gamma'_1\Gamma'_2\Gamma''_1\Gamma''_2} &\equiv \langle b_{\Gamma'_1}b_{\Gamma'_2}; \Lambda | \hat{H}_2^{\rm b} | b_{\Gamma''_1}b_{\Gamma''_2}; \Lambda \rangle \\ &= \langle b_{\Gamma'_1}b_{\Gamma'_2}; \Lambda | \hat{H}^{\rm b} | b_{\Gamma''_1}b_{\Gamma''_2}; \Lambda \rangle - (\epsilon_{\Gamma'_1} + \epsilon_{\Gamma'_2}) \delta_{\Gamma'_1\Gamma''_1}\delta_{\Gamma'_2\Gamma''_2}, \end{aligned}$$
(51)

where we have assumed that the two-boson states are normalized and that the labels Γ'_i and Γ''_i appear in some standard order (i.e., $\Gamma'_1 \leq \Gamma'_2$ and $\Gamma''_1 \leq \Gamma''_2$). Similar reasoning leads to somewhat more complicated expressions for the $0\nu\beta\beta$ -decay operator because it is non-scalar in isospin. The order-by-order mapping of non-scalar operators is explained in Appendix B.

VI. APPLICATION TO $0\nu\beta\beta$ DECAY IN THE pfSHELL

To test the role of an isoscalar-pair boson in the IBM, we now apply the formalism presented above to nuclei in the lower part of the pf shell. We will map both the Hamiltonian and the $0\nu\beta\beta$ operator from the pf shell to a system of bosons.

Like Ref. [19], we use two fermion Hamiltonians: the modified Kuo-Brown Hamiltonian KB3G [32], which is used throughout the pf shell [33], and a multi-separable collective approximation to it [34]. The collective Hamiltonian contains a monopole term, isovector pairing, isoscalar paring, a quadrupole-quadrupole interaction, and a particle-hole spin-isospin interaction. Its virtue is that it allows us to selectively remove particular pieces of the Hamiltonian, for example isoscalar pairing, which has been shown to be important [19] and which we are interested in investigating within the IBM. The detailed results we report now, however, are produced by KB3G. We will turn to the collective interaction towards the end of this section.

We now construct two boson models designed to test the ability of the IBM, with and without an explicit isoscalar-pair degree of freedom, to capture the physics important to $0\nu\beta\beta$ decay. The first consists of isovector bosons with angular momentum $\ell = 0$ (s) and $\ell = 2$

TABLE I. Two-boson interaction matrix elements $\langle JT | \hat{H}_2^b | JT \rangle$ (in MeV), mapped from the KB3G interaction (IBMb, top), from the effective fermion interaction (IBMe, middle), and from the $1f_{7/2}$ interaction of Ref. [37] (bottom).

		J = 0		J = 1		J = 2		J = 3	J = 4
T	$\langle s^2 \hat{V} s^2 \rangle$	$\langle d^2 \hat{V} d^2 \rangle$	$\langle s^2 \hat{V} d^2 \rangle$	$\langle d^2 \hat{V} d^2 angle$	$\langle sd \hat{V} sd angle$	$\langle d^2 \hat{V} d^2 \rangle$	$\langle sd \hat{V} d^2\rangle$	$\langle d^2 \hat{V} d^2 angle$	$\langle d^2 \hat{V} d^2 \rangle$
	-4.440	-4.258	-3.402		-6.350	-4.916	0.661		-5.116
0	-6.379	-5.013	-3.489		-8.263	-7.873	-0.563		-8.642
	-7.200	-6.650	-2.090		-8.290	-6.600	0.960		-8.500
				-3.029	-2.284			-3.106	
1	—		—	-4.861	-4.224			-4.831	
				-5.620	-4.460			-5.280	
	2.985	3.229	3.490		0.896	0.899	-0.822		0.719
2	1.438	1.699	2.072		0.473	0.297	-0.520		-0.282
	0.210	∞	0		0.210	0.710	0		-0.380

(d), and with isospin t = 1. This set corresponds to the isospin-invariant version of the IBM known as IBM-3 [35]. In the second model the set is enlarged by adding an isoscalar (p) boson with $\ell = 1$ and t = 0 (and positive parity). The result is not the full SU(4)-invariant version of the interacting boson model known as IBM-4 [36], but it incorporates that model's most important isoscalar correlations and therefore is situated somewhere between IBM-3 and IBM-4. We refer generically to the boson models here simply as the IBM. To refer specifically to the versions without or with the isoscalar boson, we use the terms IBM and p-IBM.

A. Mapping of the Hamiltonian

We use the order-by-order mapping described earlier to obtain the boson Hamiltonian from two- and fournucleon systems, that is, from the A = 42 and A = 44nuclei. The first yields the boson energies, which turn out to be $\epsilon_s = -2.692$, $\epsilon_d = -1.322$, and $\epsilon_p = -2.350$, in MeV. It also determines the structure coefficients $\alpha^{\Gamma}_{\gamma_1\gamma_2}$ of the collective S, D, and P pairs. In principle these may vary with mass number A to reflect the changing structure of the collective pairs. Here, however, we derive (boson) operators completely from the two- and fournucleon systems. A strategy to account for the variation of the boson Hamiltonian with A is discussed below. Actually, in the two-nucleon calculation there is no need to introduce effective two-body operators since the eigenvalues and eigenvectors in the restricted Hilbert space \mathbb{H}_P do not differ from those in the complete Hilbert space \mathbb{H} .

We thus derive the two-body interaction matrix elements between the bosons from an analysis of the fournucleon system. The first step here is to diagonalize the shell-model Hamiltonian in a complete two-pair basis H, following the procedure outlined in Sec. II to overcome the non-orthogonality of this basis. The resulting eigenspectrum should coincide with the one obtained with any standard shell-model code, allowing a rigorous check of the formalism and its implementation. Next, we diagonalize the Hamiltonian in the restricted Hilbert space

 \mathbb{H}_P , which is the collective subspace defined in terms of the pairs derived from the two-nucleon system. We will report two different types of result: (i) one with the original "bare" shell-model Hamiltonian, and (ii) one with an effective Hamiltonian, defined by the procedure outlined in Sec. IV. The third and final step is to use the mapping procedure of Sec. V to determine the two-body part of the boson Hamiltonian. If S and D pairs are mapped onto s and d bosons, without considering an isoscalar P pair, then we call the resulting boson model IBMb or IBMe, depending on whether the bare or the effective shellmodel Hamiltonian is used. Likewise, if S, D, and P pairs are mapped onto s, d, and p bosons, the resulting models are referred to as *p*-IBMb or *p*-IBMe. We emphasize that, unlike in the two-nucleon system, for four nucleons a realistic shell-model Hamiltonian in general couples the collective subspace to the rest of the space with potentially important renormalization effects. Therefore, the mapped two-body matrix elements in IBMb and IBMe may differ significantly.

The two-body matrix elements between the s and dbosons appear in Table I, both for the "bare" KB3G interaction (IBMb) and for its effective version renormalized to the collective subspace (IBMe). Because the largest components of the S and D pairs are in the $1f_{7/2}$ shell, we can compare the IBMe Hamiltonian with that obtained by Thompson *et al.* [37] from a $1f_{7/2}$ shellmodel interaction. The middle row of Table I indeed shows that the IBMe Hamiltonian resembles the one of Ref. [37], which is given in the bottom row. There are some differences, notably in the J = 0, T = 2 matrix elements, which suffer from a spurious d^2 state in the $1f_{7/2}$ mapping (a problem that is absent from the pf mapping), and smaller differences appear because the shellmodel interactions and mapping procedures (OAI versus democratic) are not exactly the same. But overall, the correspondence is good.

The two-body matrix elements between the s and d bosons appear in Table I, both for the "bare" KB3G interaction (IBMb) and for its effective version renormalized to the collective subspace (IBMe). Because the largest components of the S and D pairs are in the $1f_{7/2}$

TABLE II. Two-boson interaction matrix elements $\langle JT = 0 | \hat{H}_2^b | JT = 0 \rangle$ (in MeV), mapped from the KB3G interaction (*p*-IBMb, top) and from the effective fermion interaction (*p*-IBMe, bottom).

J = 0				J = 2				J = 4		
	$ s^2\rangle$	$ d^2 angle$	$ p^2\rangle$		$ sd\rangle$	$ d^2 angle$	$ p^2\rangle$			$ d^2\rangle$
$\langle s^2 $	$-3.718 \\ -3.909$	$-2.476 \\ -2.093$	$3.792 \\ 4.418$	$\langle sd $	$-6.078 \\ -7.978$	$0.477 \\ -0.601$	$-1.721 \\ -1.195$		$\langle d^2 $	$-5.116 \\ -8.642$
$\langle d^2 $		$-3.436 \\ -4.147$	$2.187 \\ 1.984$	$\langle d^2 $		$-4.802 \\ -7.898$	$0.826 \\ -0.065$			
$\langle p^2 $			$-0.620 \\ -1.975$	$\langle p^2 $			$-0.327 \\ -2.088$			

TABLE III. Two-boson interaction matrix elements $\langle JT = 1 | \hat{H}_2^b | JT = 1 \rangle$ (in MeV), mapped from the KB3G interaction (*p*-IBMb, top) and from the effective fermion interaction (*p*-IBMe, bottom).

J = 1				J = 2				J = 3		
	sp angle	$ d^2\rangle$	dp angle		sd angle	dp angle		$ d^2 angle$	dp angle	
$\langle sp $	$0.468 \\ 0.117$	$0.422 \\ 0.710$	$-1.032 \\ -0.949$	$\langle sd $	$-2.075 \\ -2.518$	$-1.327 \\ -1.990$	$\langle d^2 $	$-3.019 \\ -4.649$	$0.861 \\ 0.559$	
$\langle d^2 $		$-2.328 \\ -3.020$	$1.754 \\ 1.678$	$\langle dp $		-1.441 -2.256	$\langle dp $		$-0.435 \\ -2.123$	
$\langle dp $			$-0.664 \\ -1.267$							

shell, we can compare the IBMe Hamiltonian with that obtained by Thompson *et al.* [37] from a $1f_{7/2}$ shellmodel interaction. The bottom row of Table I indeed shows that the IBMe Hamiltonian resembles the one of Ref. [37]. There are some differences, notably in the J = 0, T = 2 matrix elements, which suffer from a spurious d^2 state in the $1f_{7/2}$ mapping (a problem that is absent from the pf mapping), and smaller differences appear because the shell-model interactions and mapping procedures (OAI *versus* democratic) are not exactly the same. But overall, the agreement is good.

The two-body matrix elements between the s, d, and p bosons, both for the p-IBMb and p-IBMe, are shown in Table II for T = 0 and in Table III for T = 1. The P pair does not influence the T = 2 matrix elements, which therefore can be taken from Table I. A general feature of the results, either with s and d, or with s, d, and p bosons, is that the diagonal matrix elements of the effective Hamiltonians are more attractive (or less repulsive) than corresponding matrix elements of the bare Hamiltonians. This is to be expected because the renormalization takes account of correlations from outside the collective subspace.

Figure 1 shows four-nucleon spectra for T = 2, T = 1, and T = 0, corresponding to low-lying levels in the nuclei ⁴⁴Ca, ⁴⁴Sc, and ⁴⁴Ti. In each case the figure shows the levels calculated in the shell model (SM) with the KB3G interaction. Some of these levels are exactly reproduced with an effective Hamiltonian constructed for a particular subspace: SM levels in dashed blue pertain to the *SDP* subspace and those in dotted red to the *SDP* subspace, while SM levels in dash-dotted purple are calculated in both subspaces. For comparison, the figure also shows the results produced by the bare KB3G Hamiltonian in the two collective subspaces.

All levels in Fig. 1 result from *fermionic* calculations, in which the Pauli principle is fully taken into account, though possibly in a truncated Hilbert space. The various fermionic systems are mapped onto corresponding bosonic systems, consisting of either s and d bosons, or s, d, and p bosons. For a four-nucleon system and a boson Hamiltonian containing up to two-body interactions between the bosons, the mapping is exact. Therefore, the levels in the left (middle) columns of Fig. 1 are also obtained in the *boson* calculation with the bare Hamiltonian of the IBMb (p-IBMb) while the colored levels in the right column are obtained in IBMe (p-IBMe).

In summary, the two-boson calculations (with the IBMe or p-IBMe Hamiltonians) exactly reproduce the energy of some eigenstates of the four-nucleon shell-model calculation. As explained in Sec. IV, the normal procedure is to select those that have maximal overlap with the eigenstates in the two-pair basis. This set usually includes the yrast state but not necessarily the yrare state. For example, the shell model gives a J = 0, T = 0 ground state at -13.668 MeV, which we also include in the (p)-IBMe; the next J = 0, T = 0 state in the two-boson calculation is at -5.601 MeV and corresponds to the *third* shell-model state with those quantum numbers. For the J = 4 states, both with T = 0 and T = 2, we find that the D^2 pair state is fragmented over the yrast and yrare shell-model states.



FIG. 1. Four-nucleon spectra for T = 2 (a), T = 1 (b), and T = 0 (c), corresponding to low-lying levels in the nuclei ⁴⁴Ca, ⁴⁴Sc, and ⁴⁴Ti. The left column (dashed blue) shows all levels obtained with the bare Hamiltonian in the collective subspace constructed from S and D pairs. The middle column (dotted red) shows the same for S, D, and P pairs. The right column shows the low-energy levels obtained in the shell model with the KB3G interaction; the ones that are exactly reproduced with an effective Hamiltonian in the SD and SDP subspaces are drawn in dash-dotted purple and those that are reproduced only in the SDP subspace in dotted red.

state to the lowest one, irrespective of the overlap; this choice conforms to the one of Thompson *et al.* [37].

From Fig. 1 it is apparent that the dash-dotted purple SM levels are concentrated in the low-energy region, indicating that the s and d bosons capture the essential collective degrees of freedom. The same statement cannot be made about the dotted red levels, which also occur at higher energies. This is a first indication that the isoscalar p boson is not crucial for describing lowlying spectra, a fact that is not surprising in light of past work [38].

B. Mapping of the $0\nu\beta\beta$ -decay operator

The boson $0\nu\beta\beta$ -decay operator $(0\nu\beta\beta$ operator for short) is also determined by the A = 42 and A = 44nuclei. Although the $0\nu\beta\beta$ operator has no fermion onebody term, its boson one-body terms are non-zero and determined by the analog of Eq. (50). The shell-model $0\nu\beta\beta$ operator, together with the KB3G interaction applied to A = 42, leads to $\langle s \| \hat{T}^{\rm b}_{1,\beta\beta} \| s \rangle = -11.395$ and $\langle d \| \hat{T}^{\rm b}_{1,\beta\beta} \| d \rangle = -15.179$. No $0\nu\beta\beta$ transition occurs between P pairs with T = 0, and hence $\langle p \| \hat{T}^{\rm b}_{1,\beta\beta} \| p \rangle = 0$. The two-body part of the $0\nu\beta\beta$ operator is specified by the reduced matrix elements $\langle b_1 b_2; JT_{\rm f} \| \hat{T}^{\rm b}_{2,\beta\beta} \| b'_1 b'_2; JT_{\rm i} \rangle$. For the $T_{\rm i} = 2 \rightarrow T_{\rm f} = 0$, $T_{\rm i} = 2 \rightarrow T_{\rm f} = 1$, and $T_{\rm i} = 1 \rightarrow T_{\rm f} = 1$ transitions the p boson can contribute while the $T_{\rm i} = 2 \rightarrow T_{\rm f} = 2$ transitions are independent of the p boson.

The total $0\nu\beta\beta$ operator, both in the IBMb and

p-IBMb, and their effective versions, the IBMe and *p*-IBMe, is completely specified by the reduced matrix elements $\langle b_1 b_2; JT_{\rm f} || \hat{T}^{\rm b}_{2,\beta\beta} || b_1' b_2'; JT_{\rm i} \rangle$. Of course, similar mappings can be executed for separate pieces of the $0\nu\beta\beta$ operator, such as its Gamow-Teller part. The effectiveoperator theory of Suzuki and Lee [24] ensures that the transition matrix elements between eigenstates in the restricted Hilbert space \mathbb{H}_P coincide *exactly* with those between some of the eigenstates in the complete Hilbert space \mathbb{H} .

We conclude this and the previous subsection by reemphasizing that the formalism developed in this paper allows us to derive a boson Hamiltonian and, in general, boson operators that exactly reproduce the properties of a subset of the shell-model eigenstates of all two- and four-nucleon systems.

C. Results for the energies

We now turn to systems with more nucleons and consider nuclei for which a shell-model calculation is feasible in the complete Hilbert space, in order to compare its results with those of the IBM. Our procedure incorporates no A dependence into the IBM operators, so that we have neither the mass-dependent structure coefficients $\alpha_{\gamma_1\gamma_2}^{\Gamma}$ mentioned earlier nor a dependence of the IBM Hamiltonian on the boson number n and isospin T, which is discussed in Refs. [39, 40]. Not only is it difficult to combine the two effects but in addition the (n, T)-dependence as derived in Refs. [39, 40] applies only to a seniority-based mapping, the generalization of which to an arbitrary system of bosons is not obvious. For the purpose of this paper, therefore, we propose the following heuristic method to obtain an A-dependent IBM Hamiltonian and, in general, A-dependent IBM operators.

As explained in Subsec. VIA, for a given bosonic system (e.g., sd or sdp) the mapping defines a bare boson Hamiltonian $\hat{H}_{\rm b}^{\rm b}$ —obtained from the bare fermion Hamiltonian—as well as an effective one $\hat{H}_{\rm e}^{\rm b}$. The former underbinds the two-boson system, when compared with the shell-model result for four nucleons, while the latter exactly reproduces the shell-model binding energy. In the use of these Hamiltonians for systems with more bosons, we have consistently found that, for a given boson number n, angular momentum J, and isospin T, $\hat{H}_{\rm b}^{\rm b}$ underestimates the corresponding (positive) shell-model binding energy and $\hat{H}_{\rm e}^{\rm b}$ overestimates it. Therefore, although we have no formal proof of it, we conjecture the following inequalities:

$$\langle \hat{H}_{e}^{b} \rangle_{n,J,T} \leq \langle \hat{H}^{f} \rangle_{2n,J,T} \leq \langle \hat{H}_{b}^{b} \rangle_{n,J,T} , \qquad (52)$$

where $\langle \hat{H}^{\mathrm{f}} \rangle_{2n,J,T}$ is the lowest eigenvalue, for a given nucleon number 2n, angular momentum J, and isospin T, of the shell-model Hamiltonian in the complete Hilbert space \mathbb{H} . These inequalities suggest the use of an (n,T)-dependent boson Hamiltonian of the form

$$\hat{H}^{\rm b} = x\hat{H}^{\rm b}_{\rm b} + (1-x)\hat{H}^{\rm b}_{\rm e},$$
 (53)

with x an (n, T)-dependent parameter between 0 and 1 that we consider adjustable, to be determined by a comparison with the spectrum of the shell-model Hamiltonian in the complete Hilbert space \mathbb{H} . By construction x = 0 for n = 2 bosons and we expect x to increase with increasing n and T.

Figure 2 shows spectra of nuclei with mass number A = 46; the results of the interpolation procedure can be called satisfactory. The panels in the figure are labeled with the nuclei and spectra refer to their low-energy levels with isospin $T = |T_z|$. Since isospin symmetry is conserved in both the shell model and the IBM, the calculated spectra in 46 Ca and 46 Ti are identical to those of the mirror nuclei 46 Fe and 46 Cr. (Because both the shell model and the IBM produce absolute energies, one would need different Coulomb corrections in the mirror nuclei.) The levels in 46 Ca have isospin T = 3 and are not affected by the p bosons; the ⁴⁶Ca spectra in IBM and *p*-IBM are consequently identical. For the T = 1levels of 46 Ti, on the other hand, the IBM and *p*-IBM yield different results. In the IBM a value of x can be chosen such that the binding energies and the excitation spectra are reasonably well reproduced. That is not the case in the p-IBM: If x is adjusted to reproduce the shellmodel binding energy of ⁴⁶Ti, then an unrealistic excitation spectrum results, with a 0^+-2^+ energy splitting that is far too low. This difficulty confirms our suspicion that the isoscalar p boson does not play a vital role in the spectroscopy of light pf-shell nuclei. Not only does it

render the mapping to the bosonic system more complex but it also worsens the results of the simpler IBM. We have, however, yet to examine its role in $0\nu\beta\beta$ decay.

Figure 3 shows spectra for nuclei with mass number A = 48. The boson approximation clearly breaks down in ⁴⁸Ca, a fact that is unsurprising because the sub-shell closure at neutron number N-28 should cause the structure of the collective pairs to change dramatically from we constructed in A = 42 nuclei. The binding energy of the ⁴⁸Ca ground state is not badly wrong, however, and that particular state, which consists mostly of eight neutrons in the $f_{7/2}$ shell but also includes correlations from the $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$, may still be described well enough to use in calculating the $0\nu\beta\beta$ matrix element. The spectra for A = 48, however, again confirm our statement p bosons do not improve spectra.

Finally, Fig. 4 shows spectra for nuclei with mass number A = 50. The neutron sub-shell closure at N = 28causes problems again in ⁵⁰Ti. Unlike ⁴⁸Ca, for which only T = 2 matrix elements enter the boson calculation, ⁵⁰Ti has ground-state structure that depends on *all* boson matrix elements, including those with T = 1 and T = 0. The many significant matrix elements might lead the IBM and *p*-IBM to overestimate the degree of correlation in the ⁵⁰Ti ground state. The same seems to be true in the IBM without *p* bosons for ⁵⁰Cr. We could improve the excitation energies in these nuclei, if we wanted, by relaxing the requirement of matching the binding energies.

D. Results for $0\nu\beta\beta$ -decay transitions

We turn finally to $0\nu\beta\beta$ matrix elements. Our main interest at this point is a comparison of the results of the shell model, as reported by Menéndez *et al.* [19], with those of the IBM and *p*-IBM. The matrix elements depend on the values of the Hamiltonian-interpolation parameter x in the initial and final nuclei. We can also assign a similar parameter $x_{\beta\beta}$ to the $0\nu\beta\beta$ operator, that is we can use a linear combination of the bare and effective $0\nu\beta\beta$ operators the same way we do for the Hamiltonian in Eq. (53). Here we make the simplest choice for $x_{\beta\beta}$, setting it equal to the average of the Hamiltonian xparameters in the initial and final nuclei.

The results for the total $0\nu\beta\beta$ matrix elements are shown in Fig. 5. Because isospin is conserved both in the shell model and in the IBM, transition matrix elements for mirror sets of nuclei (e.g., ⁴⁴Ca \rightarrow ⁴⁴Ti and ⁴⁴Ti \rightarrow ⁴⁴Cr) are equal and we show them for only one set here and in what follows. The shaded area in the figure indicates the values of the $0\nu\beta\beta$ matrix elements obtained by varying the Hamiltonian and $0\nu\beta\beta$ operators together between their bare and effective limits. Such limits probably overestimate the errors on the calculated matrix elements, but at least give some idea of the uncertainties. It would be helpful to have similar error estimates on the shell-model matrix elements but these are



FIG. 2. Spectra of the A = 46 nuclei 46 Ca (T = 3) (a) and 46 Ti (T = 1) (b). The shell-model spectra (SM) are produced by the KB3G interaction with six nucleons in the pf shell. The IBM spectra, with three bosons (sd or sdp), are produced by a Hamiltonian interpolated between the bare \hat{H}_{b}^{b} and the effective \hat{H}_{e}^{b} (see text).



FIG. 3. Spectra of the A = 48 nuclei ⁴⁸Ca (T = 4) (a), ⁴⁸Ti (T = 2) (b), and ⁴⁸Cr (T = 0) (c). The shell-model spectra (SM) are produced by the KB3G interaction with eight nucleons in the pf shell. The IBM spectra, with four bosons (sd or sdp), are produced by a Hamiltonian interpolated between the bare \hat{H}_{b}^{b} and the effective \hat{H}_{e}^{b} (see text).

not available to our knowledge. The shaded area is very large in the IBM and significantly reduced if effects of the *p* boson are included. Figure 6 shows the results for the Gamow-Teller part of the $0\nu\beta\beta$ matrix elements, $M_{0\nu}^{\rm GT}$. The *p*-IBM is clearly superior to IBM in matching the shell-model trends, although it systematically overestimates the $0\nu\beta\beta$ matrix elements. One conspicuous feature of the shell-model calculation is the enhancement of transitions between mirror nuclei (i.e., $^{42}\text{Ca} \rightarrow ^{42}\text{Ti}$, $^{46}\text{Ti} \rightarrow ^{46}\text{Cr}$, and $^{50}\text{Cr} \rightarrow ^{50}\text{Fe}$). This *p*-IBM reproduces the resulting "kink" in the calculated set of matrix Gamow-Teller matrix elements, but the IBM does not.

Despite the better performance of the p-IBM, the range of possibilities it predicts—reflected by the shaded areas that represent the plausible amount of phenomenological modification to the mapped effective operators—is large enough that one could question whether a p boson is really essential in IBM calculations of matrix elements for the more complicated nuclei that are used in experiments. To provide a better measure of the p-boson's importance, we examine the degree to which the IBM captures the effects of isoscalar pairing (shown repeatedly to be im-



FIG. 4. Spectra of the A = 50 nuclei ⁵⁰Ti (T = 3) (a) and ⁵⁰Cr (T = 1) (b). The shell-model spectra (SM) are produced by the KB3G interaction with ten nucleons in the pf shell. The IBM spectra, with five bosons (sd or sdp), are produced by a Hamiltonian interpolated between the bare $\hat{H}_{\rm b}^{\rm b}$ and the effective $\hat{H}_{\rm e}^{\rm b}$ (see text).

portant for $\beta\beta$ decay [16, 19]) with and without the new degree of freedom. There is not a unique prescription for isolating the isoscalar-pairing part of the KB3G interaction, so we substitute the multi-separable collective interaction employed in Ref. [19]. This "collective" Hamiltonian supplements the KB3G monopole part with separable like-particle pairing, isoscalar-pairing, quadrupolequadrupole , and spin-isospin interactions, with coefficients determined through the methods presented in Ref. [34]. With this Hamiltonian, it is a simple matter to turn the isoscalar pairing on or off for tests.

To carry out such tests, we repeat the entire mapping procedure with the new Hamiltonian, with and without isoscalar pairing. Figure 7 shows the results for the matrix elements of $M_{0\nu}^{\rm GT}$. The left column contrasts these matrix elements for our *sd* IBM, with (c) and without (a) isoscalar pairing. Without isoscalar pairing the IBM reproduces the shell-model matrix elements fairly well, and the range of predictions associated with the shaded band, though not small, is not unreasonable. When isoscalar pairing is turned on, shell-model matrix elements shrink considerably, except for the mirror transitions. Though the IBM matrix elements also shrink on average, the range of predictions is much larger.

The results of the *p*-IBM in the right column are different, not so much in the top figure (b), where, as expected, the *p* boson makes little difference in the absence of isoscalar pairing, but in the bottom figure (d). When the T = 0 pairing interaction is on, the *p*-IBM with the best value of *x* reproduces the shell model results nearly perfectly, and the range of predictions is much smaller than when the pairing is off or when the *p* boson is absent. Clearly, the *p* boson is required to fully capture the effects of isoscalar pairing. Even with it, however, the range of predictions grows noticeably after the boson number reaches about four.

We can look in a little more detail at how the two models attempt to capture the physics of the Gamow-Teller matrix element. Figure 8 shows its decomposition into pieces produced by different terms in the corresponding boson operator for the decay of 44 Ca. The contribution of all terms involving particular creation and destruction operators are grouped together, with all possible values for the angular momentum and isospin of pairs of creation (and annihilation) operators summed over. As in the realistic IBM-2 calculations of Ref. [11], the largest contribution is from the $s^{\dagger}s$ term, which converts a neutron s boson into a proton s boson. And as in those calculations, the contribution of $d^{\dagger}d$, representing transitions between d bosons, is negative and relatively small. Here, however, other terms that are absent or suppressed in Ref. [11] contribute significantly. When the p boson is included, the largest contribution, outside of that from $s^{\dagger}s$, is from $p^{\dagger}p^{\dagger}ss$. This operator, roughly speaking, replaces one neutron with a proton in each of two J = 0neutron pairs, while recoupling the resulting pairs to angular momentum J = 1 and isospin T = 0. The isoscalarpairing interaction ensures that both the initial and final configurations are well represented in the corresponding ground states. In the absence of a p boson, the IBM attempts to mock up the isoscalar pairs in the final nucleus by isovector proton-neutron s bosons, through the term $s^{\dagger}s^{\dagger}ss$. Not surprisingly, the physics of isoscalar pairing is not as well captured. In the IBM-2, which does not contain neutron-proton bosons of any kind, $d^{\dagger}d$ is the only term compensating $s^{\dagger}s$. One suspects that the effects of isoscalar pairing are overlooked.



SM 5 IBM 4 3 $|M_{0\nu}^{
m GT}|$ 2 1 (a) 0 Ti_{24 20} Ca_{26 22} 22 SM 5 p·IBM 3 $|M_{0V}^{
m GT}$ 2 1 (b) 0 26 22

FIG. 5. Eight $0\nu\beta\beta \ 0_1^+ \rightarrow 0_1^+$ matrix elements between $f_{7/2}$ -shell nuclei, calculated in the shell model [19] and in the IBM (a) and the *p*-IBM (b). The full black lines connect the shell-model results and the dashed blue (dotted red) lines the IBM (*p*-IBM) results with an *x* parameter fit to energy spectra (see text). The shaded areas indicate upper and lower limits defined by x = 1 (bare operators) and x = 0 (effective operators).

VII. CONCLUSIONS

Our results clearly suggest that although the isoscalarpair bosons have a deleterious effect on spectra—the inevitable result of diluting collectivity—they are important for $\beta\beta$ decay. In our calculations with the realistic KB3G interaction, the improvement they offer is only modest, but the reason, undoubtedly, is that our mapping is exact only for two and four nucleons and we do not know how best to extrapolate it to larger numbers. This problem plagues almost all applications of the Lee Suzuki mapping procedure.

What are the implications for the realistic IBM-2 calculations of Refs. [11–13, 41]? Would they be improved by the addition of a p boson? Isoscalar paring is probably more effective in light pf-shell nuclei discussed here than, e.g., in ⁷⁶Ge, so we have to be a little careful in extrapolating blindly. But many studies have shown isoscalar pairing to affect $\beta\beta$ matrix elements in most of the nuclei

FIG. 6. Same as Fig. 5 for the Gamow-Teller part of eight $0\nu\beta\beta \ 0^+_1 \rightarrow 0^+_1$ matrix elements between $f_{7/2}$ -shell nuclei.

used in experiments, and the p boson thus has the potential to improve the fidelity with which they are treated. One could take the first steps in these nuclei by mapping the $0\nu\beta\beta$ operator, either with the democratic procedure developed here or by extending the mapping used in Ref. [11].

A useful extension of the IBM-2, however, would require some careful phenomenology. Unlike the $0\nu\beta\beta$ operator, the IBM-2 Hamiltonian is entirely phenomenological and without a guiding principle and careful fitting, it is not obvious how best to modify it. One might try to map the Hamiltonian as we do here, select from the result the most important terms that contain *p*-boson operators, and then modify the coefficients by fitting, e.g., to single- β decay rates (which require their own mapped operator) or other observables. Until an attempt is made, we cannot know how successful such a program would be. Our results, however, imply that an attempt would be worthwhile.



FIG. 7. Same as Fig. 5 for the collective Hamiltonian without isoscalar pairing in the IBM (a), without isoscalar pairing in the p-IBM (b) with isoscalar pairing in the IBM (c), and with isoscalar pairing in the p-IBM (d).



FIG. 8. Contributions to the Gamow-Teller matrix element $M_{0\nu}^{GT}$ from different terms in the boson Hamiltonian (see text) for the IBM (cross-hatched) and *p*-IBM (solid).

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Appendix A: Matrix elements in a two-pair basis

We summarize in this appendix the expressions for the matrix element of a generic one- or two-body operator between two-pair states. For n = 2 we rewrite the pair state (2) in a more explicitly as

$$\begin{aligned} &|\gamma_a \gamma_b \gamma_c \gamma_d [\Gamma_1 \Gamma_2] \Lambda M_\Lambda \rangle \equiv |abcd[\Gamma_1 \Gamma_2] \Lambda M_\Lambda \rangle \end{aligned} \tag{A1} \\ &\propto \mathcal{A} \sum_{M_1 M_2} (\Gamma_1 M_1 \Gamma_2 M_2 | \Lambda M_\Lambda) |ab; \Gamma_1 M_1 \rangle |cd; \Gamma_2 M_2 \rangle \,, \end{aligned}$$

where the pair states on the last line are normalized and anti-symmetric, and \mathcal{A} is a four-nucleon anti-symmetrization operator. Coupling to definite angular momentum and isospin together with antisymmetrization leads to an expansion in terms of coefficients of fractional parentage (CFPs),

$$|abcd[\Gamma_{1}\Gamma_{2}]\Lambda M_{\Lambda}\rangle = \sum_{qrst} \sum_{\bar{\Gamma}_{1}'\bar{\Gamma}_{2}'} [qr(\bar{\Gamma}_{1}')st(\bar{\Gamma}_{2}')\Lambda|]abcd[\Gamma_{1}\Gamma_{2}]\Lambda] \times |qr(\bar{\Gamma}_{1}')st(\bar{\Gamma}_{2}');\Lambda M_{\Lambda}\rangle, \qquad (A2)$$

where the sum $\{qrst\}$ is over all permutations of $\{abcd\}$.

Consider now an operator $\hat{T}_{m_{\lambda}}^{(\lambda)}$, where λ refers to the operator's tensor character in angular momentum and isospin, and m_{λ} to the respective projections. By virtue of the Wigner-Eckart theorem [42], the matrix elements of $\hat{T}_{m_{\lambda}}^{(\lambda)}$ can be written as

$$\begin{aligned} \langle a'b'c'd'[\Gamma_1'\Gamma_2']\Lambda'M_\Lambda'|\hat{T}_{m_\lambda}^{(\lambda)}|a''b''c''d''[\Gamma_1''\Gamma_2'']\Lambda''M_\Lambda''\rangle \\ &= (-)^{\Lambda'-M_\Lambda'} \begin{pmatrix} \Lambda' & \lambda & \Lambda'' \\ -M_\Lambda' & m_\lambda & M_\Lambda'' \end{pmatrix} \\ &\times \langle a'b'c'd'[\Gamma_1'\Gamma_2']\Lambda''|\hat{T}^{(\lambda)}||a''b''c''d''[\Gamma_1''\Gamma_2'']\Lambda''\rangle . \end{aligned}$$
(A3)

The matrix element on the right side of this equation is reduced in angular momentum J and isospin T and the symbol in round brackets, consequently, refers to a product of Wigner coefficients, one pertaining to J and the other to T. The reduced matrix element in turn can be expressed as

$$\begin{split} \langle a'b'c'd'[\Gamma_{1}'\Gamma_{2}']\Lambda' \|\hat{T}^{(\lambda)}\|a''b''c''d''[\Gamma_{1}''\Gamma_{2}'']\Lambda'' \rangle \\ &= p \sum_{q'r's't'} \sum_{\bar{\Gamma}_{1}'\bar{\Gamma}_{2}'} [q'r'(\bar{\Gamma}_{1}')s't'(\bar{\Gamma}_{2}')\Lambda'] \}a'b'c'd'[\Gamma_{1}'\Gamma_{2}']\Lambda'] \\ &\times \sum_{q''r''s''t''} \sum_{\bar{\Gamma}_{2}''} [q''r''(\bar{\Gamma}_{1}')s''t''(\bar{\Gamma}_{2}')\Lambda''] \}a''b''c''d''[\Gamma_{1}''\Gamma_{2}'']\Lambda''] \\ &\times \langle q'r'; \bar{\Gamma}_{1}'|q''r''; \bar{\Gamma}_{1}'\rangle \langle s't'; \bar{\Gamma}_{2}'\|\hat{T}^{(\lambda)}\|s''t''; \bar{\Gamma}_{2}''\rangle \\ &\times (-)^{\bar{\Gamma}_{1}'+\bar{\Gamma}_{2}''+\Lambda'+\lambda} [\Lambda'][\Lambda''] \Big\{ \frac{\bar{\Gamma}_{2}'}{\Lambda''} \frac{\Lambda'}{\bar{\Gamma}_{2}''} \frac{\bar{\Gamma}_{1}'}{\lambda} \Big\}, \tag{A4}$$

with $[x] \equiv \sqrt{2x+1}$, p = 2 for a one-body and p = 6 for a two-body operator, and

$$\langle q'r'; \bar{\Gamma}'_1 | q''r''; \bar{\Gamma}'_1 \rangle$$

$$= \frac{1}{1 + \delta_{q'r'}} \left(\delta_{q'q''} \delta_{r'r''} - (-)^{\gamma_{q'} + \gamma_{r'} - \bar{\Gamma}'_1} \delta_{q'r''} \delta_{q'r''} \right).$$
(A5)

The symbol in curly brackets in Eq. (A4) refers to a product of Racah coefficients [42] in angular momentum and isospin space,

$$\begin{cases} \Gamma_2' & \Lambda' & \Gamma_1' \\ \Lambda'' & \Gamma_2'' & \lambda \end{cases} \equiv \begin{cases} J_2' & J' & J_1' \\ J'' & J_2'' & \lambda_j \end{cases} \begin{cases} T_2' & T' & T_1' \\ T'' & T_2'' & \lambda_t \end{cases} .$$
 (A6)

An important case occurs if $(\lambda) = (0,0)$, that is, the tensor operator is scalar in angular momentum as well as isospin. Then $\Lambda' = \Lambda'' \equiv \Lambda$ and the expression (A4) for the matrix element reduces to

$$\begin{split} \langle a'b'c'd'[\Gamma_{1}'\Gamma_{2}']\Lambda | \hat{T}_{0}^{(0)} | a''b''c''d''[\Gamma_{1}''\Gamma_{2}'']\Lambda \rangle \\ &= p \sum_{q'r's't'} \sum_{\bar{\Gamma}_{1}'\bar{\Gamma}_{2}'} [q'r'(\bar{\Gamma}_{1}')s't'(\bar{\Gamma}_{2}')\Lambda | \}a'b'c'd'[\Gamma_{1}'\Gamma_{2}']\Lambda] \\ &\times \sum_{q''r''s''t''} [q''r''(\bar{\Gamma}_{1}')s''t''(\bar{\Gamma}_{2}')\Lambda | \}a''b''c''d''[\Gamma_{1}''\Gamma_{2}'']\Lambda] \\ &\times \langle q'r'; \bar{\Gamma}_{1}' | q''r''; \bar{\Gamma}_{1}' \rangle \langle s't'; \bar{\Gamma}_{2}' | \hat{T}_{0}^{(0)} | s''t''; \bar{\Gamma}_{2}' \rangle . \end{split}$$
(A7)

This formula (with p = 6) applies to the matrix elements of a scalar two-body interaction, in which case the last factor in Eq. (A7) is the two-body matrix element,

$$\langle s't'; \Gamma | \hat{T}_0^{(0)} | s''t''; \Gamma \rangle = \upsilon_{s't's''t''}^{\Gamma}.$$
(A8)

The $0\nu\beta\beta$ operator can be assumed scalar in angular momentum but not in isospin, and therefore requires the application of the more general expression in Eq. (A4).

Appendix B: Order-by-order mapping of non-scalar operators

For a non-scalar operator, it is better to define the boson image by requiring the equality of *reduced* matrix elements in angular momentum and isospin, defined through the Wigner-Eckart theorem [42]. The one-boson term follows from

$$\langle b_{\Gamma'} \| \hat{T}^{\mathbf{b}(\lambda)} \| b_{\Gamma''} \rangle = \langle \bar{b}_{\Gamma'} \| \hat{T}^{\mathbf{b}(\lambda)} \| \bar{b}_{\Gamma''} \rangle \doteq \langle \bar{B}_{\Gamma'} \| \hat{T}^{\mathbf{f}(\lambda)} \| \bar{B}_{\Gamma''} \rangle.$$
(B1)

The fermion matrix element on the right-hand side of Eq. (B1) is given by

$$\begin{split} \langle \bar{B}_{\Gamma'} \| \hat{T}^{\mathrm{f}(\lambda)} \| \bar{B}_{\Gamma''} \rangle \\ &= \sum_{\gamma'_1 \gamma'_2} \sum_{\gamma''_1 \gamma''_2} \bar{\alpha}_{\gamma'_1 \gamma'_2}^{\Gamma''} \bar{\alpha}_{\gamma''_1 \gamma''_2}^{\Gamma''} (-)^{\Gamma' - M'_{\Gamma}} \begin{pmatrix} \Gamma' & \lambda & \Gamma'' \\ -M'_{\Gamma} & m_{\lambda} & M''_{\Gamma} \end{pmatrix}^{-1} \\ &\times \langle \gamma'_1 \gamma'_2; \Gamma' M'_{\Gamma} | \hat{T}^{\mathrm{f}(\lambda)}_{m_{\lambda}} | \gamma''_1 \gamma''_2; \Gamma'' M''_{\Gamma} \rangle \,, \end{split}$$
(B2)

where $\langle \gamma'_1 \gamma'_2; \Gamma' M'_{\Gamma} | \hat{T}^{\mathrm{f}(\lambda)}_{m_{\lambda}} | \gamma''_1 \gamma''_2; \Gamma'' M''_{\Gamma} \rangle$ are matrix elements in the complete shell-model space and $\bar{\alpha}^{\Gamma}_{\gamma_1 \gamma_2}$ are structure coefficients of normalized collective pairs,

$$\bar{B}^{\dagger}_{\Gamma M_{\Gamma}} | \mathbf{O} \rangle = \sum_{\gamma_{1} \gamma_{2}} \bar{\alpha}^{\Gamma}_{\gamma_{1} \gamma_{2}} | \gamma_{1} \gamma_{2}; \Gamma M_{\Gamma} \rangle .$$
(B3)

Equations (B1) and (B2) define entirely the one-body part $\hat{T}_{1,m_{\lambda}}^{\mathrm{b}(\lambda)}$ of the mapped boson operator. This object can be written in second quantization as

$$\hat{T}_{1,m_{\lambda}}^{\mathrm{b}(\lambda)} = \sum_{\Gamma'\Gamma''} t_{\Gamma'\Gamma''} (b_{\Gamma'}^{\dagger} \times \tilde{b}_{\Gamma''})_{m_{\lambda}}^{(\lambda)}, \qquad (\mathrm{B4})$$

with

$$t_{\Gamma'\Gamma''} \equiv \frac{\langle \bar{B}_{\Gamma'} \| \hat{T}^{f(\lambda)} \| \bar{B}_{\Gamma''} \rangle}{\sqrt{2\lambda + 1}},\tag{B5}$$

an expression showing that in general $\hat{T}_{1,m_{\lambda}}^{\mathrm{b}(\lambda)}$ is nondiagonal in the boson basis.

The two-body part of the mapped boson operator follows from the obvious identity

$$\langle b_{\Gamma_1'} b_{\Gamma_2'}; \Lambda' \| \hat{T}^{\mathrm{b}(\lambda)} \| b_{\Gamma_1''} b_{\Gamma_2''}; \Lambda'' \rangle$$

= $\langle b_{\Gamma_1'} b_{\Gamma_2'}; \Lambda' \| \hat{T}_1^{\mathrm{b}(\lambda)} + \hat{T}_2^{\mathrm{b}(\lambda)} \| b_{\Gamma_1''} b_{\Gamma_2''}; \Lambda'' \rangle .$ (B6)

The matrix element on the left side is the boson image of the fermion operator and can be computed from Eq. (48). By using the operator representation in Eq. (B4), one can work out the first (one-body) term on the right side, obtaining

$$\langle b_{\Gamma_1'} b_{\Gamma_2'}; \Lambda' \| \hat{T}_1^{\mathrm{b}(\lambda)} \| b_{\Gamma_1''} b_{\Gamma_2''}; \Lambda'' \rangle$$

$$= [\Lambda'][\lambda][\Lambda''] \hat{P}(-)^{\Gamma_1' + \Gamma_2' + \Lambda'' + \lambda} t_{\Gamma_1' \Gamma_1''} \left\{ \begin{array}{cc} \Gamma_1' & \Lambda' & \Gamma_2' \\ \Lambda'' & \Gamma_1'' & \lambda \end{array} \right\} \delta_{\Gamma_2' \Gamma_2''} ,$$

$$(B7)$$

where the operator \hat{P} takes care of the different permu-

tations: $\hat{P} \equiv \hat{P}_{\Gamma'_1 \Gamma'_2 \Lambda'} \hat{P}_{\Gamma''_1 \Gamma''_2 \Lambda''}$ with

$$\hat{P}_{\Gamma_1\Gamma_2\Lambda} \equiv \frac{f(\Gamma_1, \Gamma_2, \Lambda) + (-)^{\Gamma_1 + \Gamma_2 - \Lambda} f(\Gamma_2, \Gamma_1, \Lambda)}{\sqrt{1 + \delta_{\Gamma_1\Gamma_2}}}.$$
 (B8)

Equation (B6) therefore entirely defines the two-body part $\hat{T}_{2,m_{\lambda}}^{\mathrm{b}(\lambda)}$ of the mapped boson operator.

As an example, we apply the above formulas to the $0\nu\beta\beta$ operator, which is a non-scalar tensor $\hat{T}_{m_{\lambda}}^{(\lambda)}$ with $\lambda = (0, 2)$ and $m_{\lambda} = (0, -2)$. It is of two-body character in the fermions and we calculate its image up to twobody terms in the bosons. We assume, as is the case in the applications discussed in this paper, that off-diagonal matrix elements between pair states vanish, that is, that $\langle \bar{B}_{\Gamma'} || \hat{T}^{f\beta\beta} || \bar{B}_{\Gamma''} \rangle = 0$ if $\Gamma' \neq \Gamma''$. This relation obtains because the pairs have different angular momenta (S, D and P) and the $0\nu\beta\beta$ operator is assumed scalar in angular momentum. For two-particle states, $0\nu\beta\beta$ decay takes place from an initial state with $T = 1, M'_T = +1$ to a final state with $T = 1, M'_T = -1$, and the matrix element (B2) reduces to

$$\langle \bar{B}_{JT} \| \hat{T}^{f\beta\beta} \| \bar{B}_{JT} \rangle$$

$$= \sqrt{5(2J+1)} \langle JT, M'_T = -1 | \hat{T}^{f\beta\beta} | JT, M''_T = +1 \rangle .$$

$$(B9)$$

The contribution (B7) of the one-body part of the boson operator between two-boson states also simplifies because $\Gamma'_1 = \Gamma''_1 \equiv \Gamma_1$ and $\Gamma'_2 = \Gamma''_2 \equiv \Gamma_2$, and can be written explicitly as

$$\langle b_{\Gamma_1} b_{\Gamma_2}; \Lambda' \| \hat{T}_1^{\mathrm{b}(\lambda)} \| b_{\Gamma_1} b_{\Gamma_2}; \Lambda'' \rangle = [\Lambda'] [\lambda] [\Lambda''] (-)^{\Gamma_1 + \Gamma_2 + \lambda} \Big[(-)^{\Lambda''} t_{\Gamma_1 \Gamma_1} \Big\{ \begin{array}{cc} \Gamma_1 & \Lambda' & \Gamma_2 \\ \Lambda'' & \Gamma_1 & \lambda \end{array} \Big\} + (-)^{\Lambda'} t_{\Gamma_2 \Gamma_2} \Big\{ \begin{array}{cc} \Gamma_2 & \Lambda' & \Gamma_1 \\ \Lambda'' & \Gamma_2 & \lambda \end{array} \Big\} \Big].$$

$$(B10)$$

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