

Weak entanglement approximation for nuclear structure

Oliver C. Gorton ^{*}

*Lawrence Livermore National Laboratory, Livermore, California 94550, USA
and Department of Computational Science, San Diego State University, San Diego, California 92182, USA*

Calvin W. Johnson [†]

Department of Physics, San Diego State University, San Diego, California 92182, USA



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The interacting shell model, a configuration-interaction method, is a venerable approach for low-lying nuclear structure calculations, but it is hampered by the exponential growth of its basis dimension as one increases the single-particle space and/or the number of active particles. Recent, quantum-information-inspired work has demonstrated that the proton and neutron sectors of a nuclear wave function are weakly entangled. Furthermore, the entanglement is smaller for nuclides away from $N = Z$, such as heavy, neutron-rich nuclides. Here we implement a weak entanglement approximation to bipartite configuration-interaction wave functions, approximating low-lying levels by coupling a relatively small number of many-proton and many-neutron states. This truncation scheme, which we present in the context of past approaches, reduces the basis dimension by many orders of magnitude while preserving essential features of nuclear spectra.

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I. INTRODUCTION

In 1949, Haxel, Jensen, and Suess [1] and Goeppert-Meyer [2] introduced the noninteracting shell model for nuclear levels. A decade later, Kurath [3], followed by Halbert and French [4], among others, introduced configuration mixing, also known as the configuration-interaction method or shell-model diagonalization. In configuration-interaction, one expands the nuclear wave function in a basis of many-body states,

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle, \quad (1)$$

computes the matrix elements of the nuclear Hamiltonian \hat{H} in that basis, $H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle$, and then solves the matrix eigenvalue problem,

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}. \quad (2)$$

In the 1970s, Whitehead *et al.* introduced the Lanczos algorithm to the interacting shell model [5], allowing one to efficiently find extremal eigenstates in basis dimensions for which full diagonalization would be prohibitive. On today's supercomputers one can tackle basis dimensions in the few tens of billions [6,7].

Even modern supercomputers are not enough, however. The many-body basis dimension goes like N_s choose $N_p = N_s! / N_p! (N_s - N_p)!$, where N_s is the number of available

single-particle states and N_p is the number of active particles. (Selection rules reduce these dimensions but the scaling remains the same.) As the factorial leads to an unfavorable exponential scaling, this motivates alternate methods, such as coupled clusters [8], which scale polynomially rather than exponentially.

Nonetheless, configuration-interaction methods see continued development due to their numerous advantages including: relative ease of generating excited states, ability to handle even and odd numbers of particles equally well, relevance to open-shell nuclides, flexibility with choice of interactions, and so on. Examples of alternate truncations include the so-called Monte Carlo shell model [9], truncations based on algebraic structures [10,11], energy-based importance truncations [12], and beyond-mean-field-based truncations [13].

A surge in the interest in and applications of quantum information theory has given new lenses for truncation schemes. The nucleus can be naturally described as a bipartite systems with proton and neutron components, and nearly all shell-model codes utilize such a partitioning [14–16]. Recent work has indicated that the proton and neutron components are only weakly entangled [17], and in fact among different partitioning schemes, proton-neutron partitioning leads to the smallest entanglement [18].

We use these observations to motivate our *weak entanglement approximation*, where our lowest-order calculation, generating the proton and neutron bases independently, implicitly assumes zero entanglement. This approach can be related to density-matrix renormalization group calculations [19–21] as well as the singular-value-decomposition variational wave-function [22,23] approaches. Our proton and neutron approximate shell-model (PANASh) is, however, more straightforward than either of those approaches, as we do not

^{*}Contact author: gorton3@llnl.gov

[†]Contact author: cjohnson@sdsu.edu

iterate to optimize the basis. Nonetheless, as we demonstrate here, our simplified protocol provides a very good description of nuclear spectra for a variety of different cases.

In Sec. II we briefly review entanglement of bipartite systems. In Sec. III we outline the PANASH scheme. We then present results: In Sec. IV we compare against full configuration interaction cases, while in Sec. IV A we demonstrate the utility of PANASH by presenting an application too large to tackle in the standard shell model. After comparing in Sec. V to related methods which rely on singular-value-decomposition, we briefly outline work yet to be done. In Appendix we give details of coupling together the proton and neutron components.

II. PROTON-NEUTRON ENTANGLEMENT

In this section we briefly review the theory of entanglement and what we mean by “weak” entanglement. Entanglement starts by considering two independent Hilbert spaces, which here we write as \mathcal{P} , \mathcal{N} to reflect the proton and neutron spaces relevant to the shell model. One then constructs a product Hilbert space $\mathcal{H} = \mathcal{P} \otimes \mathcal{N}$. This can be done explicitly by writing basis states $\{|\alpha\rangle\}$ of \mathcal{H} as simple tensor products of basis states from the component spaces, $\{|p\rangle\} \in \mathcal{P}$ and $\{|n\rangle\} \in \mathcal{N}$, so that each $|\alpha\rangle = |p\rangle \otimes |n\rangle$. The dimension of the bipartite Hilbert space \mathcal{H} is multiplicative:

$$\dim \mathcal{H} = \dim \mathcal{P} \times \dim \mathcal{N}. \quad (3)$$

(In practice quantum number selection rules, such as on total J_z , can make the Hamiltonian block-diagonal and thus reduce the working dimension.) For configuration-interaction calculations, one then simply expands in the basis as in Eq. (1), or, explicitly representing the bipartite nature of the space,

$$|\Psi\rangle = \sum_{p,n} \psi_{p,n} |p\rangle \otimes |n\rangle. \quad (4)$$

Any interaction which couples two systems will generate an entangled state. An entangled state can no longer be written as a simple product $|\Psi\rangle = |\tilde{p}\rangle \otimes |\tilde{n}\rangle$, but will necessarily involve a superposition (sum) of product states, as in Eq. (4). This relationship can be formalized using density operators. A system with a density operator $\hat{\rho}$ is said to be entangled if its von Neumann entropy,

$$S(\hat{\rho}) = -\text{tr}(\hat{\rho} \ln \hat{\rho}), \quad (5)$$

is nonzero. The density operator for any wave function is $\hat{\rho} = |\Psi\rangle\langle\Psi|$ and the elements of the density matrix are

$$\rho_{pn,p'n'} = \psi_{pn}^* \psi_{p'n'}. \quad (6)$$

We often compute Eq. (5) using the eigenvalues of $\hat{\rho}$. For an isolated system, the density matrix has unit trace if the wave function is normalized, and as the density matrix is idempotent ($\hat{\rho}^2 = \hat{\rho}$) the eigenvalues of the density matrix are either 0 or 1. Therefore, its entanglement entropy $S(\rho)$ is identically 0. However, we can consider the entanglement between partitions within our isolated system which are interacting. This is done using *reduced density matrix* which is found by tracing over one of the subspaces: $\rho^{(x)} = \text{tr}_y \rho^{(xy)}$. For example, tracing over the neutron partition yields a reduced density

matrix with proton indices:

$$\rho_{p,p'}^{(p)} = \sum_n \rho_{pn,p'n} = \sum_n \psi_{pn}^* \psi_{p'n}. \quad (7)$$

The reduced density matrix still has unit trace, but its eigenvalues can be between 0 and 1, inclusive. This happens whenever there is an interaction coupling the two partitions. If any eigenvalues are not zero or 1, then the two partitions are *entangled*, and the entropy $S(\hat{\rho}^x) > 0$.

By the singular-value decomposition theorem, the eigenvalues of the reduced density matrix do not depend on which partition index is summed over. Indeed, one can simply view entanglement through the lens of singular-value decomposition (SVD), also called Schmidt decomposition. The proton-neutron coefficients of Eq. (4) form a matrix on which we can perform a SVD: $\Psi = USV^T$, which can be seen as a transformation of the proton and neutron basis factors using the orthogonal matrices U and S to one in which the Ψ matrix is diagonal (S). This is equivalent to using the eigenvectors of the proton density matrix $\rho^{(p)} = US^2U^T$ as the proton basis factors and the eigenvectors of $\rho^{(n)} = VS^2V^T$ as the neutron basis factors; simultaneously we see that the eigenvalues of the reduced density matrix are nothing but squares of the singular values.

Now we can summarize the relation between entanglement, SVD, and wave-function factorization: a state with zero entanglement has singular values of only 1s and 0s, and thus can be written as a single term, a simple product of one proton factor and one neutron factor. Not coincidentally, both density matrix renormalization group calculations [19–21] and variational wave-function truncations [22,23] rely on SVD.

In recent work [17] we found empirical evidence that low-lying shell-model states have weak proton-neutron entanglement, that is, entanglement much smaller than the maximum; furthermore nuclei with $N > Z$ have systematically lower entanglement than their $N = Z$ counterparts. These results suggest that a truncation scheme based on proton-neutron factorization may be even more effective for neutron-rich nuclei, where the need for reduced dimensions is greatest. It has also been shown that among orbital equipartitions, the proton-neutron bipartition has the weakest entanglement [18]. In the limit of zero entanglement, an eigenstate can be written as a simple tensor product of one proton wave function times one neutron wave function. In such a case, the effective dimension of the joint model space would be greatly reduced to an additive one:

$$\lim_{\text{entanglement} \rightarrow 0} \dim \mathcal{H} = \dim \mathcal{P} + \dim \mathcal{N}. \quad (8)$$

It is this effective reduction of dimensionality that drives our method. We surmise that our method should therefore outperform other orbital-partitioning truncation schemes such as [24].

In this paper we present the proton and neutron approximate shell model which builds on the weak entanglement limit. In simple terms, we first solve the Hamiltonian in the zero-entanglement limit [setting $\hat{H}^{(pm)}$ to zero]. This leaves us with the uncoupled proton and neutron wave functions which we call the proton and neutron factors. Second, we couple

these factors together, now in all combinations suitable to form basis states with good total angular momentum. The number of factors from each subspace is truncated to suit a chosen reduction in overall basis dimension (generally limited by computer resources). Third, the full interaction including $\hat{H}^{(pn)}$ is diagonalized in this truncated basis.

III. PROTON AND NEUTRON APPROXIMATE SHELL MODEL

We now explain how the weak entanglement limit is used with a proton-neutron factorization to approximate exact shell-model states. The shell-model Hamiltonian represents a system of interacting single-particle harmonic oscillator states with a mean-field (one-body) and effective two-body interaction:

$$\hat{H} = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \quad (9)$$

The creation/destruction operators $\hat{a}_i^\dagger/\hat{a}_i$ create/destroy particles in the valence space orbital i , which has harmonic oscillator labels n_i, l_i, j_i (and magnetic quantum number m_i for single-particle states).

With two species of particles, protons and neutrons, we have the following Hamiltonian:

$$\hat{H} = \hat{H}^{(p)} + \hat{H}^{(pp)} + \hat{H}^{(n)} + \hat{H}^{(nn)} + \hat{H}^{(pn)}, \quad (10)$$

where the superscript in parenthesis indicates the type of operator: (p) is a one-body proton operator, (pp) is a two-body proton operator, and equivalently for neutrons (n), (nn); and finally there is the remaining proton-neutron two-body interaction (pn). The proton-only and neutron-only operators,

$$\hat{P} \equiv \hat{H}^{(p)} + \hat{H}^{(pp)} \quad (11)$$

$$\hat{N} \equiv \hat{H}^{(n)} + \hat{H}^{(nn)}, \quad (12)$$

each have the form of Eq. (9). Furthermore, each is an operator constrained to its own subspace: $\hat{P} : \mathcal{P} \rightarrow \mathcal{P}$ and $\hat{N} : \mathcal{N} \rightarrow \mathcal{N}$. The direct product of these two subspaces is the bipartite proton-neutron space $\mathcal{H} = \mathcal{P} \otimes \mathcal{N}$, which is where the total Hamiltonian acts:

$$\hat{H} = \hat{P} + \hat{N} + \hat{H}^{(pn)}. \quad (13)$$

Each subspace operator has its own eigenstates and eigenenergies:

$$\hat{P}|p\rangle = E_p|p\rangle \quad (14)$$

$$\hat{N}|n\rangle = E_n|n\rangle. \quad (15)$$

The dimensions of these subspaces are orders of magnitude smaller than the full space, and often can be solved without any truncation. In the weak entanglement limit, these subspace eigenstates approximate the optimal basis factors $|\tilde{p}_j\rangle, |\tilde{n}_j\rangle$, i.e., eigenstates of the exact reduced density matrix. This motivates us to use these proton and neutron eigenstates directly as factors for a basis:

$$[|p\rangle \otimes |n\rangle]_{J^\pi} = |pn; J^\pi\rangle. \quad (16)$$

We work in the J scheme so that any truncation of this basis will produce wave functions with well-defined J . [This is similar to the methodology of the J -scheme (fixed total J) configuration-interaction code NuShellX [25], except, crucially, we carry out an energy truncation on the proton and neutron components.]

We can write the matrix elements of the Hamiltonian in this basis as

$$\begin{aligned} \langle p_f n_f; J^\pi | \hat{H} | p_i n_i; J^\pi \rangle &= \delta_{n_f n_i} E_p + \delta_{p_f p_i} E_n \\ &+ \langle p_f n_f; J^\pi | \hat{H}^{(pn)} | p_i n_i; J^\pi \rangle, \end{aligned} \quad (17)$$

where the matrix elements of $\hat{H}^{(pn)}$ are expressed in terms of one-body density matrices computed from the $|p\rangle$ and $|n\rangle$ eigenstates. The details for computing the proton-neutron matrix elements are given in Appendix. By diagonalizing in a truncated basis set, we obtain approximate solutions of the form:

$$|\tilde{\Psi}\rangle = \sum_{pn}^{m_n, m_p} \psi_{pn} |pn; J^\pi\rangle \approx |\Psi\rangle, \quad (18)$$

where $|\Psi\rangle$ is an exact eigenstate of \hat{H} . Setting $m_p = d_p \equiv \dim(\hat{P})$ and $m_n = d_n \equiv \dim(\hat{N})$ leads to the full configuration interaction solution. In the next section we show we can obtain good results with $m_p \ll d_p, m_n \ll d_n$; the energies follow the usual variational principle.

IV. RESULTS

Here we compare the low-lying spectra obtained from the weak entanglement factorization against untruncated, full configuration-interaction (FCI) calculations. Given specifications from the phenomenological interactions used, we also compute the total binding energies using the formulas given in Refs. [26–28]. We compare the most-bound levels for four benchmark nuclei, ^{78}Ge , ^{70}As , ^{60}Ni , and ^{79}Rb . In each case, multiple calculations are performed with increasing fidelity: Each uses an increasing fraction of the proton and neutron subspace factors and therefore an increasing computational cost which scales like the cube of the model space dimension.

We perform calculations in two model spaces. The first is the $0f_{7/2}, 1p_{3/2}, 0f_{5/2}, 1p_{1/2}$ space with the GX1A interaction [28], and the second is the $0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2}$ space with the JUN45 interaction [27]. The nuclei modeling in each space and their dimensions are shown in Table I. These nuclei were selected to span a large range of M -scheme model space dimensions (from 10^6 to 10^9), as well as several properties which affect the difficulty of capturing the many-body physics. Even-even nuclei have more regular, collective excitation spectra than odd-A (^{79}Rb) or odd-odd (^{70}As) nuclei. We consider two even-even cases: one more spherical (^{60}Ni) expected to exhibit seniority-like spectra, and one more deformed (^{78}Ge) expected to exhibit rotational spectra.

Since PANASH uses a J -scheme basis, each J^π block of the Hamiltonian can be solved independently with a much smaller basis, typically an order of magnitude than the equivalent M -scheme basis. The J -scheme matrix elements have a much higher cost per element, however, and the BIGSTICK code

TABLE I. PANASH benchmark calculations and their interaction used (Int.), M -scheme FCI dimension in millions (Mdim), number of protons (Z), number of valence protons (Z_{val}), proton subspace M -scheme dimension (Z_{dim}), (the equivalent for neutrons), and properties for which the nucleus was selected as a benchmark.

Nucleus	Interaction	M scheme		Z (Z_{val})	Z dim.	N (N_{val})	N dim.	Properties
		FCI dim. ($\times 10^6$)						
^{78}Ge	JUN45	3.7		32 (4)	701	46 (18)	701	Even-even, deformed
^{70}As	JUN45	760		33 (5)	2 293	37 (9)	36 998	Odd-odd, deformed
^{60}Ni	GX1A	1090		28 (8)	12 022	32 (12)	12 022	Even-even, spherical
^{79}Rb	JUN45	8600		37 (9)	36 998	42 (14)	24 426	Odd-A, spherical

is more efficient for a fixed-size basis. For this reason we use BIGSTICK to compute the FCI results for the untruncated basis where the advantages of the weak-entanglement approximation are lost.

The results for ^{78}Ge , an even-even deformed nucleus, are shown in Fig. 1. In each panel the PANASH basis is constructed with m proton and neutron factors as an increasing fraction of the available subspace factors $d_n = d_p = 701$ (see also Table I). Also given is the maximum J -scheme dimension d solved. In the first panel, with 1% of the basis factors resulting in four orders of magnitude reduction in the dimension of the model space, we reproduce the spectral structure characteristic of a deformed, rotational nucleus: nondegenerate low-lying 0^+ , 2^+ , 4^+ states. We also obtain the ground-state binding energy well within the 1-percent level (1.6 MeV/676 MeV). Notice that in addition to the yrast band we also reproduce the yrare $K = 2$ band. The last panel, $m = 1.0d_n$, is equivalent to the FCI calculation. Unlike the next three benchmark cases, it is practical to compute the FCI results with PANASH, since the dimensions are relatively modest (10^5).

The results for ^{60}Ni , an even-even spherical nucleus, are shown in Fig. 2. The format of the figure is the same as in Fig. 1, except for the last panel showing the FCI calculation. Here it was not practical to get the FCI results using PANASH due to the large dimensions, and instead the FCI code BIGSTICK was used. Therefore, the dimension indicated is in the M scheme rather than the J scheme (which would have been about an order of magnitude smaller). The spectral structure here is not so different from ^{78}Ge , but we do see seniority-like spectra as one might expect for a spherical, semimagic nucleus [29]. The ground-state binding energies obtained using only 1% of the basis factors (four orders of magnitude reduction in dimension) is within 1 MeV, and the excitation energy of the first 2^+ state is about 350 keV too high, about twice the typical shell-model uncertainty. Using 5% of the basis factors (still three orders of magnitude reduction), the ground-state binding energy is within 160 keV of FCI, and the first 2^+ is within 81 keV.

The results for ^{70}As , an odd-odd, deformed nucleus, are shown in Fig. 3. Compared to even-even nuclei with a 0^+ ground state and orderly low-lying excitations, the spectra for

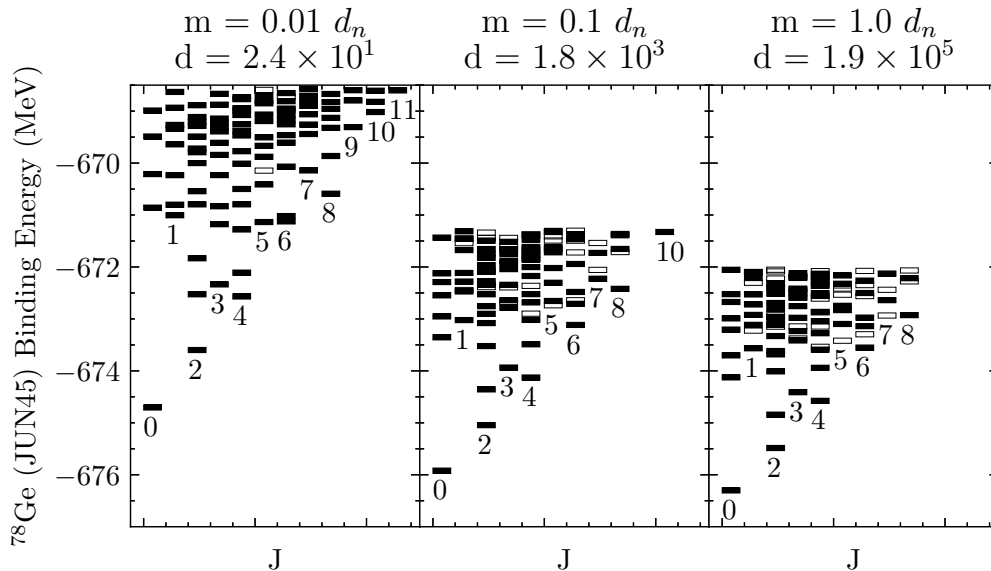


FIG. 1. Binding energies of 100 levels of ^{78}Ge computed with the weak entanglement approximation. Each panel has two labels: the number of components used as a fraction of the neutron subspace dimension and the largest J -scheme basis dimension required (across all values of J). Each stack of bars is a set of levels with a given total angular momentum J ; full bars are positive parity and empty bars are negative parity.

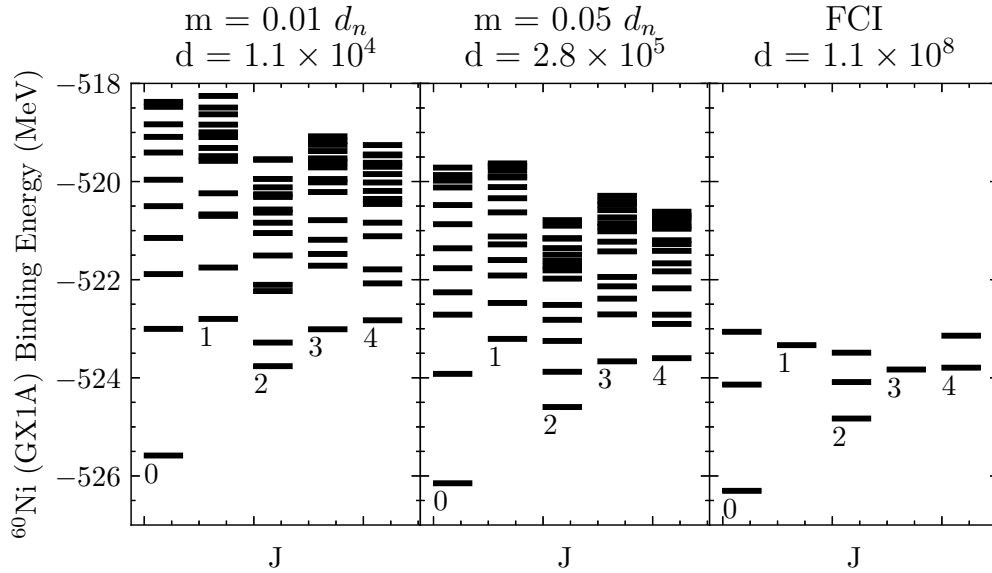


FIG. 2. Same as Fig. 1 but for ^{60}Ni . The final panel, labeled FCI, was performed with the M -scheme code BIGSTICK at a dimension of 1.1×10^9 but lists the equivalent J -scheme dimension. See text for a full discussion.

the odd-odd ^{70}As is much denser with a 4^+ ground state. While the 1% calculation which in the previous two cases came very close to the final ground-state binding energy, here the discrepancy is almost 3 MeV. This comports with our expectation that the odd proton and neutron are forced to couple, increasing the proton neutron entanglement entropy and reducing the effectiveness of the PANASH method. Despite this, we are still able to obtain the approximate ordering of the low-lying states and obtain hundreds of states where FCI can only manage a few with significant resources. For the 9% calculation, the 2^- ground state is off by 0.75 MeV

and resolves above the first 4^+ MeV state which is nearly degenerate.

The results for ^{79}Rb , an odd- A , spherical nucleus, are shown in Fig. 4. As an odd- A nucleus, there will be one unpaired nucleon leading to half-integer spins (represented in the figure in decimal values). The M -scheme dimension for this nucleus is 8.6×10^9 , which is approaching the limits of our computing capabilities. Using BIGSTICK, we could only obtain the lowest four states of each parity in a reasonable amount of time. In the J scheme it would have been 7.1×10^8 . Using 1% of the basis factors, four orders of magnitude basis

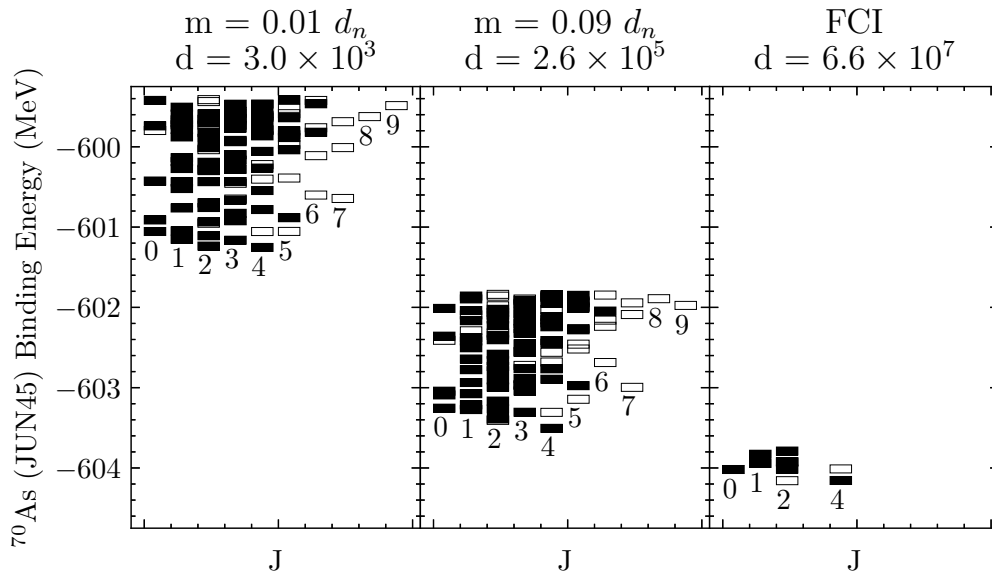


FIG. 3. Same as Fig. 1 but for ^{70}As . The final panel, labeled FCI, was performed with the M -scheme code BIGSTICK at a dimension of 7.1×10^8 but lists the equivalent J -scheme dimension.

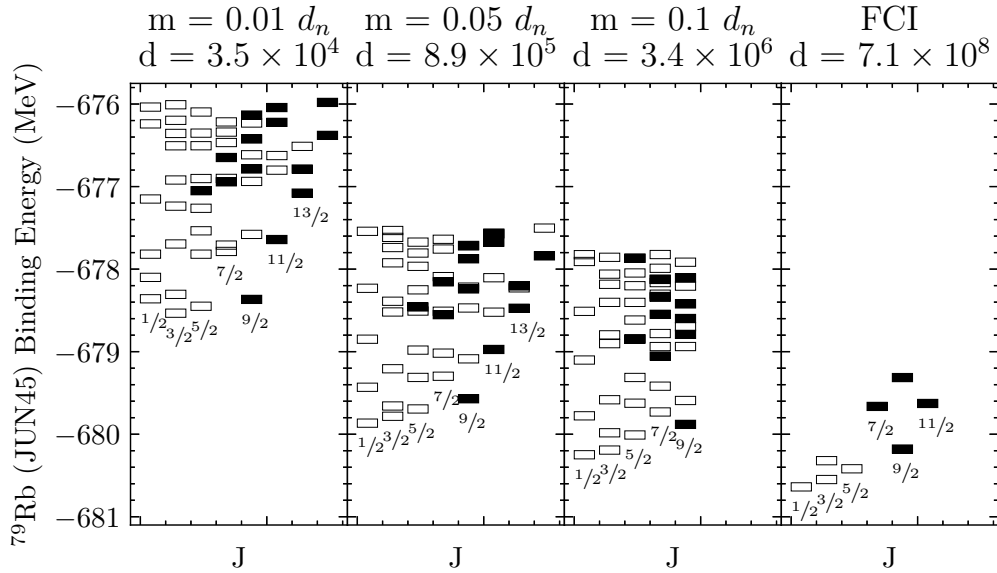


FIG. 4. Same as Fig. 1 but for ^{79}Rb . The right-most panel was computed with the FCI code BIGSTICK at a dimension of 8.6×10^9 , but lists the equivalent J -scheme dimension.

reduction, the ground-state binding energy is too high by 2.1 MeV, and the ordering of the first few states does not match the converged results. This is not too surprising given the high level density. Furthermore, this truncation error is comparable to the error of FCI compared to the experimental binding energy: $\text{BE}_{\text{exp}} = -679.5$ MeV, $\text{BE}_{\text{FCI}} = -680.7$ MeV (error = 1.2 MeV). Increasing to 5% of the basis factors and an order of magnitude increase in dimension, we get the right ordering of at least the first five states compared to FCI. The error in the ground-state binding energy is 770 keV. Doubling the basis factors to 10% does not significantly improve convergence despite quadrupling the basis dimension. This is evidence that we can extract most of the physics from the lowest-energy basis factors.

The significant basis reduction achieved by the weak entanglement approximation is useful in two extremes. The first, is that it makes possible calculations which cannot be attempted in FCI—we will be able to study the structure of a few low-lying states in model spaces that were previously computationally impossible. The second extreme can already be seen by the small number of levels in the FCI panel of last three figures: Using this basis reduction method we can obtain a far greater number of states for a comparable computational cost. We can choose to sacrifice some quality for a larger quantity of states. This might not sound desirable, but for statistical quantities such as average electromagnetic properties of highly excited states, it is exactly the right trade-off.

Finally, we explored how the weak entanglement approximation is reflected in the convergence properties of our four benchmark cases. Using the formalism described in Sec. II, we computed the proton-neutron entanglement entropy of the first five levels of each benchmark case. In Fig. 5 we show there is a correlation between the error in the binding energy as computed with our PANASH code and the relative strength of the proton-neutron entanglement (which we normalized to 1). This matches our expectations and the assumptions of

the weak entanglement approximation. It should be noted that the proton-neutron entanglement entropies were computed using the approximate PANASH wave functions indicated in the caption of Fig. 5, and are thus approximations themselves.

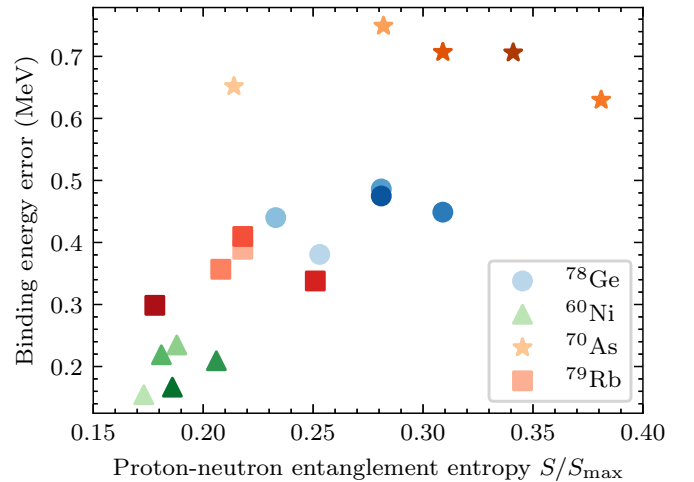


FIG. 5. Error in the binding energy using a similar truncation for the five lowest states of the benchmark cases, as a function of the relative proton-neutron entanglement entropy. Nuclei with weaker entanglement tend to have a smaller error in the PANASH basis, as predicted in Ref. [17]. Markers are shaded darker with increasing excitation energy; lower excited states tend to have lower entanglement. The binding energy and entanglements are computed from the largest truncation performed in Figs. 1–5 (^{78}Ge : $m = 0.10d_n$, ^{60}Ni : $m = 0.05d_n$, ^{70}As : $m = 0.09d_n$, ^{79}Rb : $m = 0.10d_n$). The error is relative to the FCI (untruncated) values. The proton-neutron entanglement entropies are computed using the method described in Sec. II and as in Ref. [17] and are divided by their maximum value in each model space to give a value between 0 and 1.

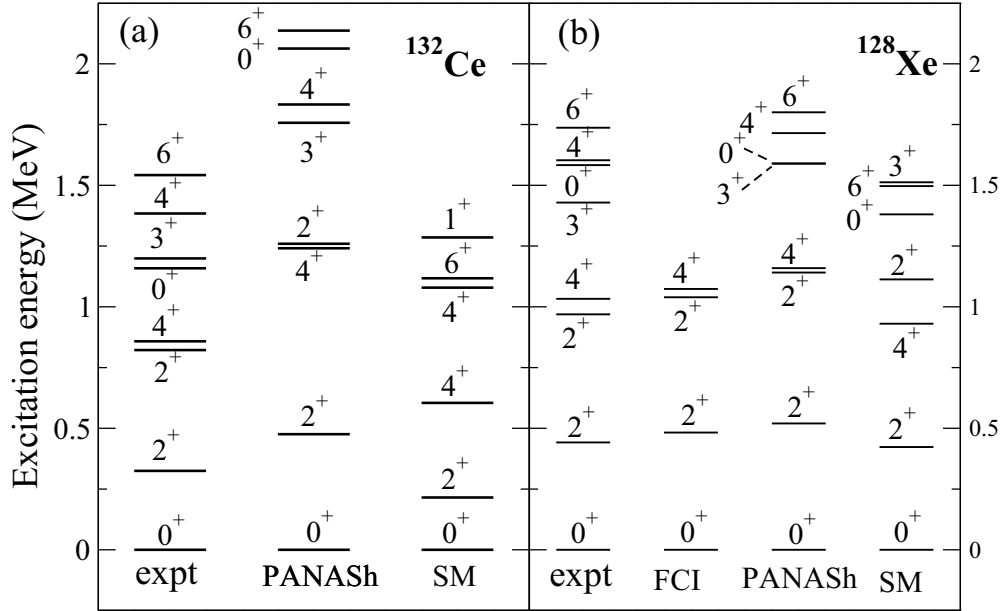


FIG. 6. Excitation spectra for (a) ^{132}Ce and (b) ^{128}Xe , including from experiment (Refs. [31,34], respectively). We assume a ^{100}Sn core and a valence space of the orbitals between magic numbers 50 and 82, and use the interaction in Ref. [32], including the recommended 0.9 reduction of neutron-neutron two-body matrix elements. Only for ^{128}Xe is a full configuration-interaction (FCI) calculation possible, with an M -scheme dimension of 9.3 billion; the FCI M -scheme dimension for ^{132}Ce would be 2.4 trillion. The PANASH calculations have neutron fractions $m = 0.015 d_n$; the $J = 6$ PANASH dimensions are 377 000 for ^{128}Xe and 432 000 for ^{132}Ce . Also shown are truncated (see text for details) configuration-interaction shell-model (SM) levels, with M -scheme dimensions of 507 million for ^{128}Xe and 1.29 billion for ^{132}Ce .

A. Aspirational calculation

In the benchmark results presented above, at least a few of the low-lying states can be extracted from the full shell model using state-of-the-art codes like [30]. In order to demonstrate the potential reach of PANASH, we chose a case— ^{132}Ce in the valence space bounded by magic numbers 50 and 82, with a ^{100}Sn core (that is, valence orbitals $0g_{7/2}$, $2s_{1/2}$, $1d_{3/2}$, $1d_{5/2}$, $0h_{11/2}$)—whose FCI M -scheme dimension, 2.4 trillion, is far beyond current capabilities. Because no FCI result is possible, we compare to the experimental excitation spectrum [31]. The interaction we use is tuned to tellurium isotopes [32] and provides a reasonable description of xenon isotopes [33]. (Following Ref. [32], we reduce the strength of the neutron-neutron two-body matrix elements by 0.9.) As a partial benchmark, we also compute in this space with this interaction ^{128}Xe , which has in this space an FCI M -scheme dimension of 9.3 billion, still tractable with suitable supercomputing power; we take its experimental excitation energies from Ref. [34].

Figure 6 presents the excitation spectra for ^{132}Ce and ^{128}Xe . In both cases we used 1000 proton and 1000 neutron levels to construct the PANASH basis; this corresponds to a neutron basis fraction of $m = 0.015 d_n$, and proton basis fractions also $0.15 d_p$ for ^{132}Ce and $m = 0.34 d_p$ for ^{128}Xe . For ^{132}Ce the largest PANASH J -scheme dimension used was 432 000 for $J = 6$, compared to the FCI $J = 6$ dimension of 133 billion. For ^{128}Xe , the corresponding PANASH $J = 6$ dimension was 377 000, compared to the FCI $J = 6$ of 614 million.

In addition to a calculation with PANASH, we carried out truncated calculation with the BIGSTICK code. We assign to

each orbital a an integer weight w_a . Each many-body configuration is then assigned a total weight W which is the sum of the weights of the occupied orbitals. The M -scheme Hilbert space is truncated by keeping all configurations with weights up to a defined maximum W_{\max} , defined relative to the minimum in the space W_{\min} : $W_{\text{ex}} = W_{\max} - W_{\min}$. With suitable choice of weights, this truncation scheme [30] is flexible enough to include the standard N_{\max} truncation scheme for the no-core shell model, as well as particle-hole truncations. We assigned the following weights w to each of the orbitals: $w(0g_{7/2}) = 0$; $w(1d_{5/2}) = 1$; $w(1d_{3/2}) = w(2s_{1/2}) = w(9h_{11/2}) = 2$. This choice of weights approximates a truncation based on the centroids (average energies) of orbital configurations [35,36]. Under this truncation scheme with $W_{\text{ex}} = 6$, ^{128}Xe has an M -scheme dimension of 507 million, while ^{132}Ce has an M -scheme dimension of 1.29 billion.

For ^{128}Xe we get relatively good agreement for all three calculations as well as with experiment. The truncated shell-model (SM) calculation has a slightly compressed yrast 0-2-4 band, while the PANASH band is slightly expanded. This behavior is exaggerated for ^{132}Ce . One can speculate that the PANASH calculation, because it only partially couples the proton and neutron sectors, underestimates the proton-neutron quadrupole collectivity, while the SM calculation, which has reduced proton and neutron spaces, underestimates the pairing collectivity in the ground state. We leave investigating this speculation to future work.

Nonetheless, by comparing ground-state energies we can demonstrate that PANASH builds in substantial correlations. Table II shows the ground-state energies obtained from our calculations. The absolute values of these energies are not

TABLE II. Ground-state (GS) energies from three shell-model calculations of ^{132}Ce and ^{128}Xe shown in Fig. 6. The value does not have a direct interpretation on its own since the interaction was not fit to the total binding energy. However, the variational principle guarantees that all truncations are less bound than FCI, and so the GS energy serves as a proxy for convergence. These values show that the PANASH calculation is more converged than the SM truncation while using a smaller basis.

Calculation	^{132}Ce			^{128}Xe		
	FCI	PANASH	SM trunc.	FCI	PANASH	SM trunc.
J -scheme ($J = 6$) dimension	1.33×10^{11}	4.32×10^5	—	6.14×10^8	3.77×10^5	—
M -scheme dimension	2.4×10^{12}	—	1.29×10^9	9.3×10^9	—	5.07×10^8
GS energy (MeV)	—	-291.17	-287.79	-264.41	-263.98	-262.88
First 2^+ (MeV)	—	-290.69	-287.58	-263.93	-263.46	-262.46

meaningful on their own, as the interaction was not fitted to absolute binding energies, but they serve as a proxy for overall convergence due to the variational principle of basis truncation methods. For ^{128}Xe , the truncated SM ground state is 1.53 MeV above the FCI ground state, but the PANASH ground state is only 0.43 MeV above. While the FCI ground-state energy for ^{132}Ce is not available, the PANASH ground-state energy is 3.37 MeV lower than the truncated SM ground state.

The FCI dimension for ^{132}Ce is two orders of magnitude larger than any published shell-model calculation [6,7]. Although the PANASH excitation spectrum is not perfect, it captures the main features of the experimental spectrum, and clearly builds in correlations beyond what can be captured by a traditional truncated shell-model calculation. As discussed briefly in Sec. VI, this will provide motivation to push PANASH further and to carefully investigate extrapolation to the full space with appropriate uncertainty quantification.

V. COMPARISON TO OTHER SVD TRUNCATIONS

Our weak entanglement factorization has precursors in the density matrix renormalization group (DMRG) [19–21,37] and variational wave-function factorization (VWF) or simply wave-function factorization (as called by its creators [22,23]). Both of these methods are based on a bipartite decomposition of the Hilbert space, followed by some sort of truncation. Both also directly or indirectly consider a singular-value decomposition of the bipartite representation of the wave functions.

In a DMRG approach to the nuclear shell model, one splits the single-particle space into two subgroups which are iteratively improved. At each step of the DMRG method, (1) the effective interaction in each subspace is diagonalized exactly, (2) the approximate ground state's SVD is used to inform which states to keep in a truncation to m factors from that subspace, and (3) the solution to the full space is taken as a product state of the two subspace solutions. Various flavors of DMRG deal with how to define the subgroups, and how to change the subgroups at each iteration.

Variational wave-function factorization is also an iterative method which works with a bipartite representation. A complete description can be found in the literature by Papenbrock *et al.* [22,23]; a short summary will be given here. VWF seeks the optimal set of proton and neutron factors $|\bar{p}\rangle$ and $|\bar{n}\rangle$ which

for $m \ll \min(d_p, d_n)$ yield a good approximation,

$$|\Psi\rangle \approx \sum_j^m s_j |\bar{p}_j\rangle |\bar{n}_j\rangle. \quad (19)$$

It is known that the optimal factors are given by the SVD, but VWF deals with the scenario where it is too computationally expensive to solve even the ground state of the system. One starts with an ansatz state composed of random proton and neutron many-body wave functions and writes down a variational condition. Then, one solves the coupled set of nonlinear equations that follow. This is computed as a generalized eigenvalue problem. After each iteration, the number of basis factors m is increased until satisfactory convergence is reached.

Like DMRG, VWF relies on the fact that the singular values of realistic shell model ground states fall off rapidly so that an accurate approximation can be achieved with only a small number of factors [21]. Empirically, the spectra tends to converge exponentially with the number of states m retained [22].

A major cost of both DMRG and VWF is the iterative approach to finding the optimal basis factors. The weak entanglement approximation avoids this cost by assuming that the eigenstates of the proton and neutron subgroups are sufficient approximations of the optimal proton and neutron factors. Interestingly, our choice of metric for selecting the proton and neutron basis factors is reminiscent of Wilson's numerical renormalization group (NRG) [38,39], the precursor to DMRG. The downfall of NRG (which DMRG overcame) is that its truncation is based only on the energy of the subspace solutions and ignores the coupling of the subgroup to the rest of the system. It fails when long-range correlations exist. Our method does not have this problem, since within each bipartition we include all orbitals, and it is known that the entanglement between the proton and neutron subgroups is weak [17].

We can compare how close the weak entanglement approximation comes to the optimal basis given by SVD. The SVD basis is the one where $\Psi = USV^T$ yields a diagonal matrix S whose elements are the singular values s_i . The values s_i^2 are plotted and labeled "SVD" in Fig. 7(a). The PANASH basis is one where $\Psi = P\tilde{S}Q^T$ yields a matrix \tilde{S} (the proton-neutron wave function in the PANASH basis) which is approximately diagonal, and with strongly decaying diagonal elements ψ_{jj} . (The matrices P and Q would be formed by the proton and

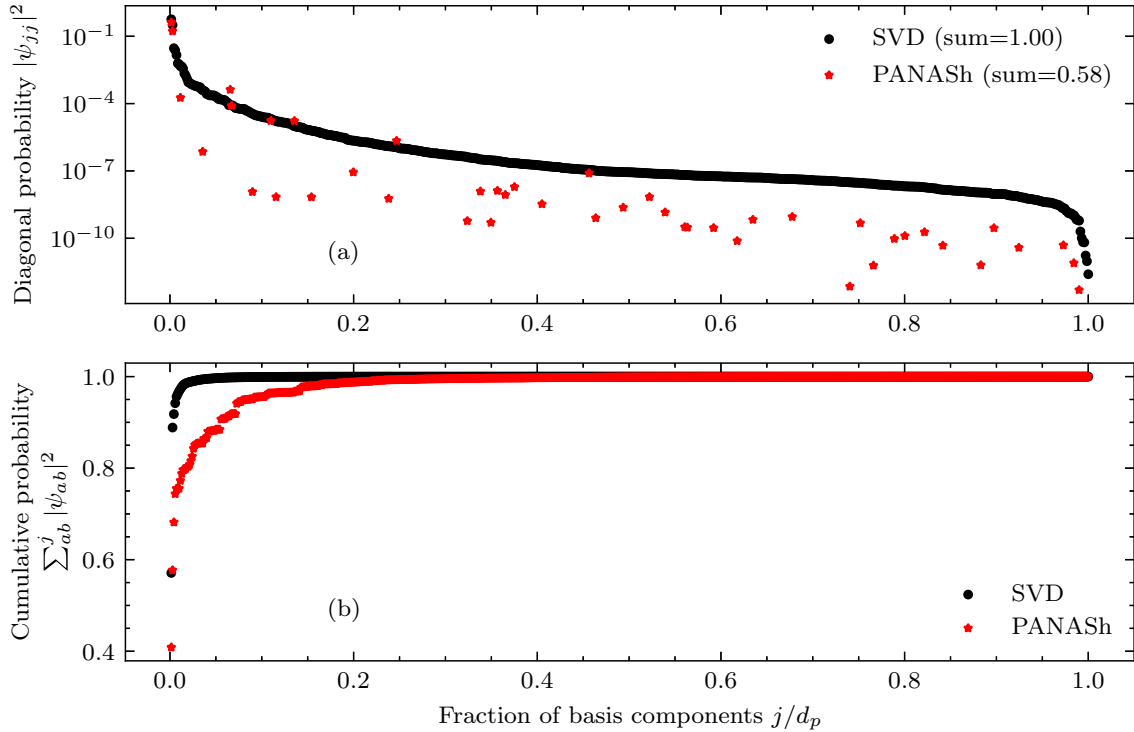


FIG. 7. Representation of the (JUN45) ^{78}Ge ground-state wave-function elements ψ_{ij} in two different proton-neutron bases: the SVD basis in which the wave function is exactly diagonal, and the PANASh basis which for this nucleus is 58% diagonal. (a) Diagonal elements (squared) of the wave function showing the PANASh basis follows the same exponentially decaying trend as the SVD basis. (b) Cumulative probability of the wave function captured as a function of the fraction of basis components. The PANASh basis is suboptimal but the cumulative probability still converges to 1 exponentially in the number of basis components. This demonstrates that a significant truncation can be performed while maintaining a high-fidelity wave function.

neutron basis factors.) The values $|\psi_{ij}|^2$ are plotted for an untruncated PANASh calculation and labeled “PANASh” in Fig. 7(a). The SVD matrix S is completely diagonal and its diagonal elements sum to 1. The PANASh matrix \tilde{S} has off diagonal elements and only sums to 0.58 in this case. The off-diagonal (0.42) strength is due to the fact that the PANASh basis is not optimal for nonzero proton-neutron entanglement; for this nucleus the proton-neutron entanglement is roughly 20% of its maximum value. In Fig. 7(b), we plot the cumulative fraction of the wave function as one includes more components, both of the ideal SVD basis and of the more practical PANASh basis. While the SVD basis more quickly captures the full wave function, as it must, the PANASh basis nonetheless provides a reasonable approximation with significantly less numerical burden.

VI. SUMMARY AND OUTLOOK

We have presented a “weak entanglement” approximation to the nuclear shell model, which relies on the observation [17,18] that the proton and neutron components, especially for neutron-rich nuclei, have relatively low entanglement. Thus, rather than requiring computationally expensive optimization of the basis, as is done in precursor methods DMRG and VWF, we simply construct the many-proton and many-neutron components independently as eigenpairs of their respective Hamiltonians, an approach

that arises from an assumption of zero entanglement. If the entanglement were truly zero, then the full solutions would be simple tensor products; instead, we couple the proton and neutron components through the proton-neutron interaction. We find this construction provides a “good enough” representation of the excitation spectra of complex nuclei, including cases beyond current shell-model capabilities, while retaining many of the advantages of configuration interaction, such as generating many excited states, addressing open-shell and odd-particle systems, and so on.

There are a number of issues to be tackled in the immediate future, among them: electromagnetic and weak transitions; improved basis construction; and extrapolation and uncertainty quantification. Basis construction might be improved by relaxing the “zero entanglement” assumption: We could add to (for example) the proton Hamiltonian a deformed field representing the average influence of the neutron component and vice versa. Such work is under way and will be reported on in a future paper.

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APPENDIX: RESIDUAL INTERACTION MATRIX ELEMENTS

To diagonalize the nuclear Hamiltonian $\hat{H} = \hat{P} + \hat{N} + \hat{H}^{(pn)}$ in the basis Eq. (16), we seek an explicit form in terms of proton and neutron one-body density matrices since these are a byproduct of the diagonalization of the subspace Hamiltonians as defined in Eq. (14). The \hat{P} and \hat{N} operators will naturally be diagonal in our basis. (This may be relaxed in the future.) The diagonal terms are $E^{(p)}$ and $E^{(n)}$. All that remains is to find the matrix elements of $\hat{H}^{(pn)}$ in terms of the original FCI single particle basis and matrix elements.

Starting from an explicit proton-neutron formalism, the (pn) part of the interaction can be written in the form:

$$\hat{H}^{(pn)} = \sum_{abcd} \sum_K V_{ab,cd;K}^{(pn)} \sum_M \hat{A}_{ab;KM}^{\dagger(pn)} \hat{A}_{cd;KM}^{(pn)}, \quad (\text{A1})$$

$$\langle f | \hat{\rho}_{ac;K}^{(p)} \cdot \hat{\rho}_{bd;K}^{(n)} | i \rangle = (-1)^{j_{pi} + j_{nf} + J} \begin{Bmatrix} J & j_{nf} & j_{pf} \\ K & j_{pi} & j_{ni} \end{Bmatrix} \langle p_f | | \hat{\rho}_{ac;K}^{(p)} | | p_i \rangle \langle n_f | | \hat{\rho}_{bd;K}^{(n)} | | n_i \rangle. \quad (\text{A7})$$

Here $|i\rangle = |p_i n_i; J\pi\rangle$ and $(J\pi)_i = (J\pi)_f = J\pi$. The matrix elements of the proton-neutron interaction is thus expressed in terms of the one-body transition density matrix elements of the proton and neutron factor wave functions.

The matrix elements of the pn -part of the Hamiltonian can be written in the simplified form:

$$\langle f | \hat{H}_J^{(pn)} | i \rangle = (-1)^{j_{pi} + j_{nf} + J} \sum_K \begin{Bmatrix} J & j_{nf} & j_{pf} \\ K & j_{pi} & j_{ni} \end{Bmatrix} \sum_{bd} P_{bd;K}^{p_f p_i} \rho_{bd;K}^{n_f n_i} \quad (\text{A8})$$

where the reduced one-body density matrix elements of the factor wave functions $|x\rangle$ are defined as

$$\rho_{ab;K}^{x_f x_i} \equiv \langle x_f | | \hat{\rho}_{ab;K}^{(x)} | | x_i \rangle / \sqrt{2K + 1}, \quad (\text{A9})$$

and where the partial sum $P_{bd;K}^{p_f p_i}$ is defined as

$$P_{bd;K}^{p_f p_i} = (2K + 1) \sum_{ac} \rho_{ac;K}^{p_f p_i} W_{ac,bd;K}^{(pn)} \quad (\text{A10})$$

where subscripts a and c will refer to proton single-particle orbits, and b and d to neutron single-particle orbits. The two-body operators are defined as:

$$\hat{A}_{ab;JM}^{\dagger(xy)} \equiv [x_a^\dagger \otimes y_b^\dagger]_{JM} = \sum_{m_a m_b} (j_a m_a, j_b m_b | JM) \hat{x}_{j_a m_a}^\dagger \hat{y}_{j_b m_b}^\dagger. \quad (\text{A2})$$

Using various commutation relations and vector-coupling identities [40], the following equivalent expression can be derived:

$$H^{(pn)} = \sum_{abcd} \sum_K W_{ac,bd;K}^{(pn)} \hat{\rho}_{ac;K}^{(p)} \cdot \hat{\rho}_{bd;K}^{(n)}, \quad (\text{A3})$$

where the one-body proton (neutron) density operators are defined as

$$\hat{\rho}_{ac;K\mu}^{(p)} \equiv \sum_{m_a m_c} (j_a m_a, j_c - m_c | K\mu) \pi_{j_a m_a}^\dagger \tilde{\pi}_{j_c - m_c}, \quad (\text{A4})$$

which carry total angular momentum K and z component μ , and the transformed proton-neutron interaction $W^{(pn)}$ is

$$W_{ac,bd;K}^{(pn)} \equiv \sum_{K'} (-1)^{K' + j_b + j_c} [K']^2 \begin{Bmatrix} j_a & j_b & K' \\ j_d & j_c & K \end{Bmatrix} V_{ab,cd;K'}^{(pn)}, \quad (\text{A5})$$

with $[x] = \sqrt{2x + 1}$. Finally, the scalar product of one-body density operators is defined as

$$\hat{\rho}_{ac;K}^{(p)} \cdot \hat{\rho}_{bd;K}^{(n)} = \sum_{\mu} (-1)^{-\mu} \hat{\rho}_{ac;K\mu}^{(p)} \hat{\rho}_{bd;K\mu}^{(n)}. \quad (\text{A6})$$

The $H^{(pn)}$ part of the interaction is a scalar product of two independent operators: $\hat{\rho}_{ac;K}^{(p)} \cdot \hat{\rho}_{bd;K}^{(n)}$. Standard vector-coupling relations allow us to write matrix elements of this operator in a j - j -coupled basis as products of matrix elements in the uncoupled basis [40]:

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