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Effective summation over intermediate states in double-beta decay

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We consider two separate schemes for eliminating the explicit summation over states in the intermediate nucleus in double-beta decay. The first, known as the operator expansion method, has recently been applied in several calculations; we show in a variety of simple models that the method fails and isolate its weaknesses. We then describe an efficient technique for generating Green's function matrix elements, based on the Lanczos algorithm, and apply it to a full *fp*-shell calculation in ^{48}Ca. The method efficiently generates an exact (to within machine accuracy) result while the operator expansion method is again inaccurate.

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Several recent papers [1–4] contend that the nuclear matrix elements governing two-neutrino double-beta decay can be easily and accurately evaluated without explicit consideration of the intermediate nucleus. The claim rests on a collection of approximations known as the operator expansion method (OEM). Briefly, the denominator in the second-order perturbation expression for the two-neutrino matrix element

$$M_{\rm GT}=\tfrac{1}{2}\sum_{i,j,N}\frac{\langle 0_F^+|\sigma(i)\tau_-(i)|1_N^+\rangle\cdot\langle 1_N^+|\sigma(j)\tau_-(j)|0_I^+\rangle}{\Delta+Z(E_N-E_I)}\ , \tag{1}$$

where in our convention τ_- changes a neutron to a proton, $\Delta=\frac{1}{2}(E_I-E_F)$, and Z is a parameter that must eventually be set to unity, is expanded in powers of Z, manipulated by replacing energies with Hamiltonian operators, and then partially resummed, with intractable terms discarded. Provided the two-body Hamiltonian can be written in the form [4]

$$V=\tfrac{1}{2}\sum_{i\neq j}[v_0(r_{ij})+v_\sigma(r_{ij})\boldsymbol{\sigma}(i)\cdot\boldsymbol{\sigma}(j)+v_\tau(r_{ij})\boldsymbol{\tau}(i)\cdot\boldsymbol{\tau}(j) +v_{\sigma\tau}(r_{ij})\boldsymbol{\sigma}(i)\cdot\boldsymbol{\sigma}(j)\boldsymbol{\tau}(i)\cdot\boldsymbol{\tau}(j)]\ , \tag{2}$$

the procedure, which amounts to an approximation for the nuclear Green's function $1/(E_0-H)$, can be followed, yielding the result

$$M_{\rm GT}^{\rm OEM}=\tfrac{1}{2}\sum_{i,j}\langle 0_F^+|\mathcal{M}_{ij}\tau_-(i)\tau_-(j)|0_I^+\rangle\ , \tag{3}$$

where

$$\mathcal{M}_{ij}=\frac{12[v_\sigma(r)-v_\tau(r)]\Omega_0(ij)}{\Delta^2-16[v_\sigma(r)-v_\tau(r)]^2} +\frac{4[v_{\sigma\tau}(r)-v_\sigma(r)-v_\tau(r)]\Omega_1(ij)}{\Delta^2-16[2v_{\sigma\tau}(r)-v_\sigma(r)-v_\tau(r)]^2}\ . \tag{4}$$

(Here Ω_0 and Ω_1 are projectors onto spin singlet and triplet states, and r is shorthand for r_{ij}.) Were this result correct, it would remarkably simplify two-neutrino double-beta decay calculations; the full nuclear Green's function has been replaced by a simple effective two-body operator. Accepting Eq. (4), however, requires several leaps of faith. The first is in the belief that the power-series expansion of the denominator in Eq. (1) can be carried out beyond its radius of convergence. The second is the assumption that the kinetic-energy operator T can be ignored in the resulting commutators, despite the usual argument that nuclei are weakly bound so that $\langle T\rangle\approx\langle V\rangle$. A third assumption is that only two-body terms need be retained in the commutators, contradicting the long-held view that the Green's function for strongly interacting systems contains many complex and highly linked contractions. While the authors argue that their approximations are reasonable, they neither test them nor posit any "small parameter" that would justify the exclusion of the omitted terms.

Properties of matrix elements calculated in the OEM immediately cast doubt on one or all of the assumptions involved. First of all, as is apparent from Eq. (4), a zero-range δ-force causes the matrix element to vanish, in clear contradiction to the results of other studies [5,6]. Equally puzzling is the lack of any significant dependence on the parameter g_{pp}, which multiplies the particle-particle force, when the method is used in conjunction with QRPA [3]. Reference [3] argues that the widely noted dependence is artificial, caused by QRPA-induced errors in the intermediate-nucleus states that the OEM avoids. Yet studies have shown that even the "closure" matrix elements (in which the intermediate-state sum is removed) are sensitive to g_{pp}, and a model calculation in the f shell clearly indicates that the same is true of the exact shell-model $M_{\rm GT}$ [6], for which no approximations in the intermediate nucleus are made.

This report has two purposes. First, to isolate the weaknesses of the OEM, we apply it to several simple models that can be solved exactly. The OEM fails these tests, generating matrix elements that are much too small. Second, we describe an efficient method for exactly evaluating the desired Green's function, and compare it to the OEM in an application to the decay of ^{48}Ca in a full fp shell-model space. Our method, based on a Lanczos algorithm for inverting linear operators, removes the need for Green's function approximations, particularly if they are as unreliable as those in the OEM.

We begin with a toy system in which two neutrons, bound in a charge-independent harmonic oscillator well, decay to two protons. Since there are only two particles in the model, we will be testing the omission of the kinetic energy in the OEM, independent of any additional errors caused by the neglect of higher-order ("multiparticle-scattering") terms in the OEM commutators. We assume that the oscillator $\hbar\omega$ is large enough compared to the residual interaction that the particles reside exclusively in the 0s orbital. The ground states in the initial and final nuclei are therefore both given by the product of two s-wave spatial wave functions and a singlet in spin space. The intermediate nucleus contains two states, a singlet and triplet, the splitting of which is determined by the residual two-body interaction, which we take to be a square well of radius a with independent strengths V_0 and V_1 in the singlet and triplet channels. To simplify matters even further, we neglect the Coulomb energy, so that $\Delta \rightarrow 0$; i.e., the initial and final ground states become degenerate (to prevent the intermediate ground state from lying lower we may choose V_0 to be more attractive than V_1; this of course is not the case in the real world). Double-beta decay proceeds only through the spin-triplet (isosinglet) state, and the complete matrix element can be easily calculated. The interaction may then be rewritten in the form Eq. (2) and the OEM matrix element just as easily evaluated. The result is

$$\frac{M_{\mathrm{GT}}^{\mathrm{OEM}}}{M_{\mathrm{GT}}} = F^2(a) \ , \tag{5}$$

where

$$F = \mathrm{erf}\left[\frac{a}{\sqrt{2}b}\right] - \frac{2a}{\sqrt{2\pi}b} e^{-a^2/2b^2} \ , \tag{6}$$

and b is the oscillator parameter. We show the function F^2 in Fig. 1. At small ranges a the ratio goes to zero like $(a/b)^6$; at very long ranges it approaches but never exceeds 1. These results are not mysterious. The OEM neglects derivatives of the potential, which arise in (repeated) commutators of the kinetic and potential energy operators. For a force with essentially no r dependence, the resulting error is small. For a short-range force, however, with a steep drop, the error is apparently very large; indeed, we have already remarked that a δ force yields no double-beta decay at all in the OEM. References [2–4] argue that the effects of the kinetic-energy operator should be small; these arguments, however, concern kinetic energies of the nuclear states rather than the commutators with the potential that appear in the OEM expansion, and are not convincing.

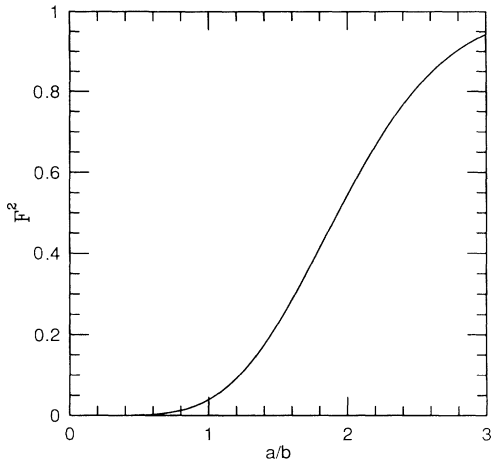

FIG. 1. The ratio F^2 of the OEM to exact two-neutrino matrix element for two nucleons in the $0s_{1/2}$ shell. The interaction is a square well of range a.

We now turn our attention to a somewhat more realistic model, the decay of ^{48}Ca in the approximation that only the $f_{7/2}$ orbital is active. In Ref. [2], the two-neutrino matrix element is calculated in the OEM with wave functions from Ref. [7] and compared to the results of closure calculations with energy denominators taken from Ref. [8]. One problem with this approach is that the interaction used in $\mathcal{M}_{ij}$ is not consistent with the $f_{7/2}$ two-body matrix elements that generate the wave functions. But consistency aside, working in closure with an estimated energy denominator is unnecessary because the full M_{GT} in the $f_{7/2}$ model space can be easily calculated. The transition proceeds through a single excited 1^+ state in ^{48}Sc, and so the closure approximation is exact, provided the energy denominator is taken from the energy of this excited state [9]. The wave functions of Ref. [7] yield a M_{GT} of 0.034, while the OEM method (with a Paris-potential-based force in $\mathcal{M}_{ij}$) gives 0.019. The comparison is complicated by the inconsistency between force and wave function, but once again, the OEM method underestimates M_{GT}, in part, at least, because it neglects kinetic energy.

A consistent calculation in the $f_{7/2}$ model space is easy to carry out. We begin by using an r-independent (schematic) force to eliminate possible errors in the OEM caused by neglect of the kinetic energy; our intention here is to test the truncation of the series expansion at the two-body level. In this limit, the OEM matrix element is simply proportional to the closure matrix element, where the constant of proportionality is the inverse of some "effective" energy denominator. (The same is true of the exact solution, as we have already noted.) To avoid issues associated with the Coulomb force, which is not consistently treated in the OEM, we take ground state energies directly from our calculation, without adjusting to obtain experimental Q values. We fit the four parameters in the most general r-independent force, Eq. (2), to the eight two-body matrix elements of Ref. [9] (the quality of

the fit, unfortunately, is not particularly good). With the prescription just described, the shell-model energy denominator is 4.04 MeV, while the OEM gives an effective denominator of 13.07 MeV. In this example, at least, the neglect of "multiparticle scattering" therefore has the same effect as ignoring the kinetic energy: it reduces M_{GT} from its true value. This conclusion is not changed substantially when we allow intermediate states with particles in the $f_{5/2}$ level, which can in principle be excited by our simple r-independent Green's function.

We may also use the $f_{7/2}$ model to test the accuracy of the OEM for more realistic finite range forces, where all the approximations come into play. To this end, we calculate the exact and OEM M_{GT} for a series of general Yukawa forces with different ranges. For each range, we fit the strengths of the four Yukawas in Eq. (2), again so as to best reproduce the two-body interaction matrix elements of Ref. [9]. We treat Coulomb effects in the usual way, by taking Δ and the ground-state energy of the intermediate nucleus ^{48}Sc from experiment. Figure 2 shows the exact and OEM results. The exact M_{GT} varies even though at each point we have reproduced the same eight interaction matrix elements as well as possible. The reason is that the result of Ref. [7], which is best approximated by the Yukawa force with range 0.4 fm, is small because of a close cancellation between components in the final wave function with neutron angular momenta 0 and 2; a small change in the wave function can weaken the cancellation significantly. In any event, the important feature of Fig. 2 is that the OEM approximation is always smaller than the true M_{GT}, and behaves more or less randomly as the range is changed, even crossing zero for a range of about 2 fm.

We conclude our discussion of the $f_{7/2}$ model by fixing the range of the force (somewhat arbitrarily) at 0.55 fm and multiplying the strength of the potential in the $J=1, T=0$ channel by a factor g_{pp}. This procedure mimics very closely the variation [6] of the particle-particle strength that is typically carried out in QRPA studies. Figure 3 shows the exact and OEM results for g_{pp} between -2 and 2. The exact matrix element changes significantly over this interval (though more slowly than in the QRPA calculations, at least partly because of the small model space we use here), while the OEM results are nearly constant. This "stability," touted in a recent application of the OEM in conjunction with the QRPA [3], is not real, and the claim that the steep variation of QRPA matrix elements with g_{pp} has something to do with the way intermediate states are handled is clearly wrong. Taken together, the arguments presented here so far make it difficult to trust the OEM in any context.

The uncontrolled approximations in the OEM are in fact unnecessary; there exists a well-tested, exact, and efficient algorithm for evaluating the fully interacting nuclear Green's function appearing in double-beta decay. The technique is based on a general method of inverting linear operators discussed, for instance, by Haydock [10]. The specific method we employ starts from the tridiagonal Lanczos matrix and has been tested extensively by one of us in calculations of nuclear anapole moments, electric dipole moments, etc. [11]. (Similar techniques were used for the double-beta decay of ^{48}Ca in Refs. [12,13]. Reference [14] contains additional information on Lanczos-generated strength functions.) The method is iterative and the convergence is so rapid that the computer time required to evaluate the Green's function is a small percentage of that needed for calculating the initial and final ground-state nuclear wave functions (which itself, unfortunately, is still too long to make complete shell-model calculations in heavy nuclei feasible). We will illustrate the procedure in an unrestricted fp-shell calculation of the transition ^{48}Ca$\rightarrow$^{48}Ti, using both a modified Kuo interaction and a Serber-Yukawa force. Although interactions that better reproduce fp-shell ob-

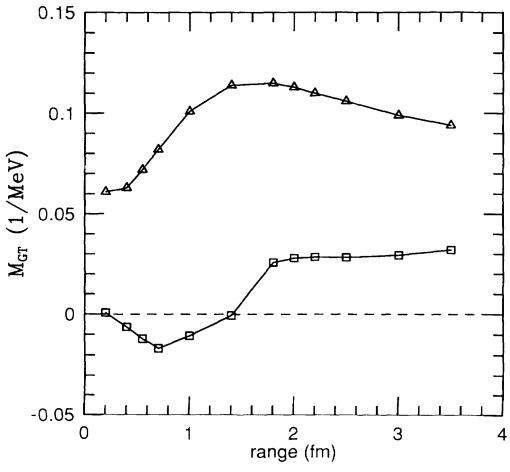

FIG. 2. The exact and OEM two-neutrino matrix elements for the decay ^{48}Ca$\rightarrow$^{48}Ti in the $f_{7/2}$ shell for Yukawa forces of varying range. The triangles are the exact result and the squares the OEM approximation.

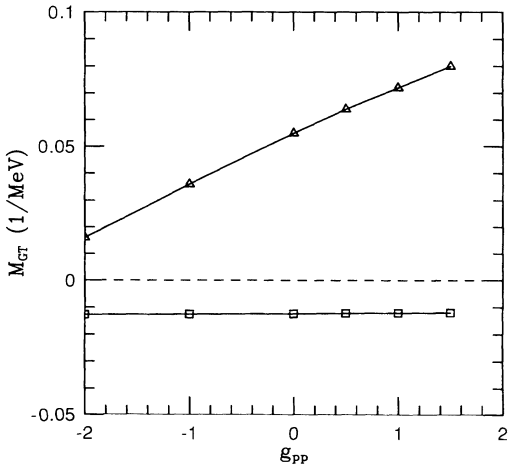

FIG. 3. The exact and OEM two-neutrino matrix elements for the decay ^{48}Ca$\rightarrow$^{48}Ti in the $f_{7/2}$ shell with a Yukawa force of fixed range with varying g_{pp} (defined in the text). The triangles are the exact result and the squares the OEM approximation.

servables are available [12,15], these choices allow interesting comparisons to be made. The modified Kuo interaction is the same one that was used in the closure calculations of Ref. [8]; the Serber-Yukawa force contains only central terms, allowing us to compare exact results to those of the OEM. These complete $0\hbar\omega$ calculations have the virtue of preserving exactly the Gamow-Teller sum rules governing the single-beta strength.

Consider a Hamiltonian H, defined over a finite Hilbert space of dimension N, and a starting normalized vector $|v_1\rangle$ in that space. We begin to construct a basis for representing H by

$$H|v_1\rangle=\alpha_1|v_1\rangle+\beta_1|v_2\rangle\ , \tag{7}$$

where $|v_2\rangle$ is a normalized vector representing that part of $H|v_1\rangle$ orthogonal to $|v_1\rangle$. Proceeding, we have

$$\begin{aligned} H|v_2\rangle&=\beta_1|v_1\rangle+\alpha_2|v_2\rangle+\beta_2|v_3\rangle\ ,\\ H|v_3\rangle&=\beta_2|v_2\rangle+\alpha_3|v_3\rangle+\beta_3|v_4\rangle\ ,\\ &\vdots \end{aligned} \tag{8}$$

and so on. The term $\beta_1|v_1\rangle$ must appear in the first line above because H is Hermitian. Furthermore, $|v_1\rangle$ does not appear in the second line above because everything that connects to $H|v_1\rangle$ other than $|v_1\rangle$ is defined as $|v_2\rangle$. Similarly, $H|v_4\rangle$ will contain nothing proportional to $|v_1\rangle$ or $|v_2\rangle$. Thus H is cast in the tridiagonal form

$$H=\begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 & \\ \beta_1 & \alpha_2 & \beta_2 & 0 & \cdots \\ 0 & \beta_2 & \alpha_3 & \beta_3 & \\ 0 & 0 & \beta_3 & \alpha_4 & \\ & \vdots & & & \end{pmatrix}\ . \tag{9}$$

If this procedure were continued for N steps, the full H would then be in tridiagonal form. The power of the algorithm, however, derives from the information in the Lanczos matrix when the procedure is truncated after n iterations, $n \ll N$. If $\{\psi_{E_i},\ i=1,\ldots,N\}$ are the exact eigenfunctions of H, then

$$\langle v_1|H^\lambda|v_1\rangle-\sum_{i=1}^{N}|\langle v_1|\psi_{E_i}\rangle|^2E_i^\lambda\equiv\sum_{i=1}^{N}f(E_i)E_i^\lambda\ . \tag{10}$$

The distribution $\{f(E_i),\ i=1,\ldots,N\}$ can be thought of as a set of N weights $f(E_i)$ and measures E_i (the eigenvalues) fully characterizing the distribution of $|v_1\rangle$ in energy, i.e., the f's determine a complete set of moments. The truncated Lanczos matrix, when diagonalized, provides the information needed to construct a distribution $\{g(\tilde{E}_i),\ i=1,\ldots,n\}$ which has the same $2n-1$ lowest moments in E as the exact distribution $\{f(E_i)\}$. In other words, the Lanczos algorithm at each iteration provides a solution to the classical moments problem [16]. As Whitehead has emphasized [16,17], the speed and numerical stability of this algorithm is a very special property of the Lanczos method, and leads to surprisingly efficient procedures for evaluating response functions.

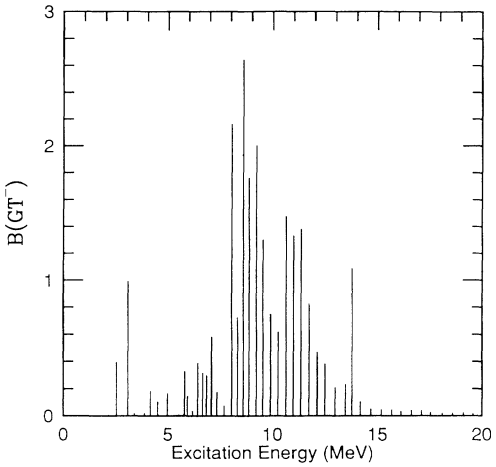

FIG. 4. The distribution of β^- strength in ^{48}Sc from ^{48}Ca resulting from the modified Kuo-Brown force.

If we choose

$$|v_1\rangle=\hat{O}_{\rm GT}|0_I^+\rangle\equiv\sum_{i=1}^{A}\sqrt{3}\sigma_z(j)\tau_-(j)|0_I^+\rangle\ , \tag{11}$$

where, in this application, $|0_I^+\rangle$ is the ^{48}Ca shell-model ground state, we can use the Lanczos algorithm to determine, iteratively, the resulting Gamow-Teller distribution in ^{48}Sc. The results for our more realistic interaction are given in Fig. 4, and the analogous results for $\sqrt{3}\sigma_z(j)\tau_+(j)$ acting on the ^{48}Ti ground state are presented in Fig. 5. The latter strength function differs somewhat from those of recent calculations [12,15], because of the more accurately determined forces used there.

The action of the full Green's function on a vector can also be represented as an expansion involving the Lanczos vectors $|v_i\rangle$ and the entries in the tridiagonal matrix. This can be accomplished by rewriting Eq. (7) in terms of the operator $1/(E_0-H)$, rather than H, or by using Haydock's [10] recursion relations for the Lanczos repre-

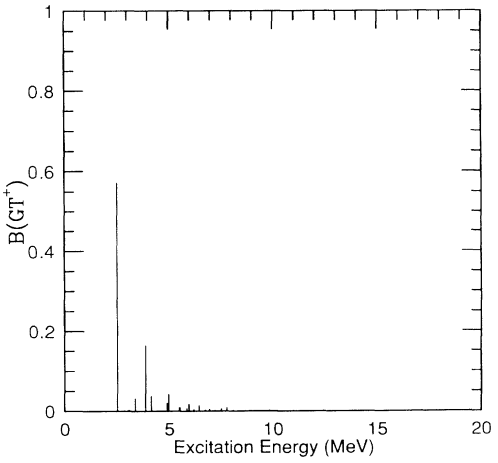

FIG. 5. The distribution of β^+ strength in ^{48}Sc from ^{48}Ti resulting from the modified Kuo-Brown force.

sentation of H. One finds

$$\frac{1}{E_0-H}|v_1\rangle=g_1(E_0)|v_1\rangle+g_2(E_0)|v_2\rangle+\cdots, \tag{12}$$

where the $|v_i\rangle$ are the Lanczos vectors and the $g_i(E_0)$ continued fractions formed from the entries in the tridiagonal Lanczos matrix. For example,

$$g_1(E_0)=\cfrac{1}{E_0-\alpha_1-\cfrac{\beta_1^2}{E_0-\alpha_2-\cfrac{\beta_2^2}{E_0-\alpha_3-\cfrac{\beta_3^2}{\ddots}}}}. \tag{13}$$

As iterations proceed, the coefficients $g_i(E_0)$ are updated, and additional Lanczos vectors $|v_i\rangle$ contribute to the expansion. In practice, the convergence is very rapid. In our double-beta decay applications, machine accuracy was achieved in 12 iterations. For comparison, the Lanczos diagonalizations we performed to determine the ^{48}Ti and ^{48}Ca ground states required ~ 100 iterations.

We can write the two-neutrino matrix element Eq. (1) in the form

$$M_{\mathrm{GT}}=-\frac{1}{2}\left\langle 0_f^+\left|\sum_{i=1}^{A}\sqrt{3}\sigma_z(i)\tau_-(i)\frac{1}{E_0-H}\right.\right.$$
$$\left.\left.\times\sum_{j=1}^{A}\sqrt{3}\sigma_z(j)\tau_-(j)\right|0_i^+\right\rangle \tag{14}$$

with E_0 given by $E_I-\Delta$. Thus we choose $|v_1\rangle$ as in Eq. (11) and evaluate Eq. (12) iteratively, in effect completing the sum over a complete set of fp-shell 1^+ states in ^{48}Sc. The result for the 2ν matrix element with the more realistic Kuo-Brown force is $M_{\mathrm{GT}}=-0.0539$/MeV, corresponding to a half-life of 1.18×10^{20} years. (Perhaps this number and those of Refs. [12,15] are sufficiently close to the experimental lower bound to inspire renewed effort to observe ^{48}Ca double-beta decay.) The matrix element obtained from the simple Serber-Yukawa force is $M_{\mathrm{GT}}=0.0428$/MeV. The OEM, applied to the same force, yields -0.0115/MeV, a factor of more than three smaller than the correct result and with the wrong sign. Once again, here in a "realistic" model space, the OEM fails badly.

In conclusion, we have shown in a series of calculations ranging from the simplest schematic models to a complete fp-shell diagonalization that the OEM is systematically unable to reproduce exact results. The failure is inherent in the uncontrolled approximations that lead to Eqs. (3) and (4). In all of the tests, including the most sophisticated, the OEM result is significantly smaller in magnitude than the correct matrix element, and often has the wrong sign. We have also pointed out the existence of an elegant and efficient algorithm that generates Green's functions to arbitrary accuracy. The technique would seem to obviate the need for any work to improve approximate methods like the OEM. Instead, effort might be more profitably applied, in conjunction with the Green's function method outlined here, to improving the interactions and model spaces used to generate ground state wave functions in the parent and daughter nuclei.

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