Nonperturbative renormalization of the neutrinoless double-β operator in p-shell nuclei

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Abstract

We use Lee-Suzuki mappings and related techniques to construct effective two-body p-shell interactions and neutrinoless double-beta operators that exactly reproduce the results of large no-core-shell-model calculations of (fictitious) double-beta decay in nuclei with mass number $A = 6$. We then apply the effective operators to the (also fictitious) decay of nuclei with $A = 7$, 8, and 10, again comparing with no-core calculations in much larger spaces. The results with the effective two-body operators are generally good. In some cases, however, they differ non-negligibly from the full no-core results, suggesting that three-body corrections to the decay operator in heavier nuclei may be important. An application of our procedure and related ideas to fp-shell nuclei such as ^{76}Ge should be feasible within coupled-cluster theory.

I. INTRODUCTION

Particle physicists hope to learn about the overall neutrino-mass scale by observing neutrinoless double-beta ($0\nu\beta\beta$) decay [1]. To extract a mass from a lifetime, however, one must know the value of the nuclear matrix element that governs the decay. For that reason, theorists have worked hard over the last 20 years to better calculate the matrix elements.

One of the best frameworks for the job at present is the nuclear shell model. Good calculations (e.g. Refs. [2, 3]) use model spaces of dimension 10^7 or larger by including the full valence shell. Even these calculations, however, omit most of the relevant many-particle Hilbert space by requiring that most particles remain frozen in an inert core and prohibiting even active particles from sampling levels above the valence shell. These approximations induce error that can in principle be accounted for through the use of an effective Hamiltonian and decay operator. The literature contains a number of schemes for constructing effective operators [4, 5]. In practice, however, such techniques are generally restricted to the effective Hamiltonian, and even there the application is usually through a perturbative scheme whose weaknesses must be compensated for by fitting to spectra. The decay operator is usually not corrected at all, except at short distances (and sometimes through an overall phenomenological multiplication factor). How much are calculated matrix-element corrupted as a result? How might one do better?

To begin to answer these questions, we look at the $0\nu\beta\beta$ matrix element in nuclei with mass number A between 6 and 10. Such nuclei, of course, do not undergo $\beta\beta$ decay, but one can calculate the matrix elements nonetheless. Moreover, in these nuclei we can carry out fairly complete no-core shell-model (NCSM) [6] calculations and map their results onto valence-shell (p-shell) calculations to construct effective operators that reproduce the full matrix elements exactly. We can then bypass perturbation theory, which is often unreliable (and was applied inconclusively to $\beta\beta$ decay in Ref. [7]), and test nonperturbative approximations to the full effective operator. Reference [8, 9] carried out this program for charge-conserving electromagnetic transition operators, the leading pieces of which are one-body. Here, the lowest-order effective decay operator acts on two bodies, and we examine the restriction to this leading term. We define effective operators that reproduce the exact matrix element for the artificial decay of states in ^{6}He to those in ^{6}Be. Are these operators significantly different from their bare counterparts? Can they also reproduce $0\nu\beta\beta$ matrix

elements in heavier nuclei, or are three- and higher-body effective operators necessary as well? The answers will provide a good idea of how much work awaits us in the heavier nuclei that actually undergo $\beta\beta$ decay.

In Sec. II below, we describe the concepts and methods we employ. Section III presents our results, and Sec. IV discusses their implications for matrix elements in the heavier nuclei that are used in $\beta\beta$ experiments.

II. METHODS

In the closure approximation (which is good for neutrinoless decay) and with the usual assumption that the nuclear weak current is adequately represented by a one-body operator, the $0\nu\beta\beta$ matrix element is a sum of three terms:

$$\mathcal{M}_{fi} \equiv \langle f | \sum_{ab} M^{GT}_{ab} + M^{F}_{ab} + M^{T}_{ab} \, | i \rangle \ , \tag{1}$$

the last of which is a very small tensor piece [10] that will be ignored here. The other two M's are given by [10, 11]

$$\begin{aligned} M^{GT}_{ab} &= H_{GT}(r_{ab}) \, \boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b \\ M^{F}_{ab} &= H_{F}(r_{ab}) \, , \end{aligned} \tag{2}$$

with the labels a and b indicating nucleons both here and in Eq. (1), r_{ab} representing inter-nucleon distance, and the "neutrino potentials" H defined by

$$H_K(r) = \frac{2R}{\pi r} \int_0^\infty \frac{h_K(q) \sin qr}{q + \bar{\omega}} \, dq \, , \quad K = GT, F \, . \tag{3}$$

The $h_K(q)$ in Eq. (3) contain the vector and axial-vector coupling constants, form factors that account for the finite size of the nucleon, and the effects of forbidden currents (weak magnetism and the induced pseudoscalar term). The quantity $\bar{\omega}$ is an average intermediate-nucleus excitation energy to which the H_K are not very sensitive. The authors of Ref. [12] recently applied chiral effective-field theory to derive two-body corrections to the weak current and thus three-body corrections to the operators in Eq. (2). From our point of view, these corrections modify the bare $0\nu\beta\beta$ operator and are subject to the same nuclear-structure renormalization that we apply to the two-body operators in Eq. (2). We neglect the chiral corrections here to keep matters simple.

The matrix element $\mathcal{M}_{fi}$ is often small because of cancellations among contributions at different internucleon distances r_{ab}. Instead of looking only at the matrix element, therefore, we also examine the internucleon matrix-element distribution $C(r)$, defined e.g. in Ref. [13], so that

$$\int_0^\infty C(r)\, dr = \mathcal{M}_{fi}\,. \tag{4}$$

Our starting point for calculating matrix elements is the NCSM. We use different starting interactions — the CD Bonn potential [14] and the N^{3}LO chiral effective-field-theory interaction [15] — and model spaces that allow between six and ten $\hbar\omega$ of excitation energy outside the p shell (i.e. the NCSM parameter $N_{\max}$ is between 6 and 10). We first apply standard Lee-Suzuki techniques [16–18] to the Bonn potential and the Similarity Renormalization Group (SRG) [19, 20] to the chiral potential to construct interactions appropriate for those model spaces. In principle the double-beta decay operator should be treated in the same way. Preliminary studies [21] show, however, that the renormalization is slight and confined to short distances as expected, and instead of carrying it out here we simulate short-range effects through an effective Jastrow function from Ref. [22].

Many of the isotopes we discuss are very weakly bound or unbound in reality, and our representation of them in the oscillator-based NCSM distorts their structure. For our purposes, however, the poor representation is not important; we want to examine the effect of moving to a much smaller model space, and take the large-space calculations to be the "exact" results we want to reproduce.

Our small model space consists of all but four particles residing anywhere in the $0p$ shell and the rest forming an inert $0s$-shell core. As in Refs. [8, 9], we first equate the effective neutron $p_{3/2}$ and $p_{1/2}$ single-particle energies to the two lowest-energy eigenvalues produced by the full calculation in ^{5}He, and the effective proton energies to the corresponding eigenvalues in ^{5}Li. Then in the $A = 6$ nuclei we use the Lee-Suzuki procedure to map the two lowest $J^\pi = 0^+$ states, the lowest 1^+ state, and the two lowest 2^+ states (all with $T = 1$) onto corresponding orthogonal p-shell states. In doing so we assume isospin conservation in our small-space calculation; breaking isospin would require only the additional straightforward step of carrying out separate calculations in He and Be.

We implement the Lee-Suzuki mapping, which comes as close as possible to making the p-shell energy eigenstates the projections of the corresponding full-space states without

spoiling orthogonality, as follows. We let P project onto the d-dimensional small space, let $Q \equiv 1 - P$, and denote by $|p\rangle$, $|p'\rangle$, $|p_1\rangle$, etc., states for that are contained entirely in the small space (with an analogous convention defining $|q\rangle$, $|q'\rangle$, etc.). The d orthogonal small-space states $|\tilde{k}\rangle$ corresponding to d selected full-space eigenstates $|k\rangle$ are defined by

$$|\tilde{k}\rangle \equiv M^{-\frac{1}{2}} \left(P + \omega^\dagger\right) |k\rangle \ , \tag{5}$$

with

$$\langle q| \, \omega \, |p\rangle = \sum_{k=0}^{d-1} \langle q|k\rangle \, \langle \underline{\mathrm{k}}|p\rangle \ . \tag{6}$$

and

$$M = P + \omega^\dagger\omega = P \left(1 + \omega^\dagger\omega\right) P \, . \tag{7}$$

In Eq. (6) the $\langle \underline{\mathrm{k}}|p\rangle$ are defined as the elements of the inverse of the matrix with the d^2 elements $\langle p|k\rangle$. With these definitions the effective operator $O_{\rm eff}$ in the dimension-d small space that gives the same matrix elements as (the $T_z = 0$ analogue of) the decay operator O in the full space, is

$$O_{\rm eff} = M^{-\frac{1}{2}}(P + \omega^\dagger)O(P + \omega)M^{-\frac{1}{2}} \, . \tag{8}$$

The matrix elements of this operator can be written without reference to any vectors $|q\rangle$ or any of the eigenstates $|k\rangle$ beyond the d that are mapped, as

$$\langle p| \, O_{\rm eff} \, |p'\rangle = \tag{9}$$
$$\sum_{p_1,p_2,k,k'=0}^{d-1} \langle p| \, M^{-\frac{1}{2}} \, |p_1\rangle \, \langle p_1|\underline{\mathrm{k}}\rangle \, \langle k| \, O \, |k'\rangle \, \langle \underline{\mathrm{k}}'|p_2\rangle \, \langle p_2| \, M^{-\frac{1}{2}} \, |p'\rangle \ ,$$

where the elements of M can be written in the same fashion as

$$\langle p| \, M \, |p'\rangle = \sum_{k=0}^{d-1} \langle p|\underline{\mathrm{k}}\rangle \, \langle \underline{\mathrm{k}}|p'\rangle \ . \tag{10}$$

With the $T_z = 0$ $O_{\rm eff}$ in place, we then simply use isospin algebra to obtain the matrix elements of the real $T_z = 2$ effective decay operator, for which p represents two protons and p' two neutrons. To get the effective interaction we carry out a similar procedure but also include the $T = 0$ states in ^{6}Li to obtain a complete set of matrix elements.

The Lee-Suzuki mapping actually is only one of many that are possible. As noted above, the Lee-Suzuki procedure makes the small-space eigenvectors as close as possible to projections of the full eigenvectors without sacrificing orthogonality. In other words, it constructs

the orthonormal set $\{|\tilde{k}\rangle\}$ that minimizes the quantity [23]

$$\sum_{k=0}^{d-1} \left(\langle k| - \langle\tilde{k}|\right)\left(|k\rangle - |\tilde{k}\rangle\right) . \tag{11}$$

This prescription seems particularly appropriate for a comprehensive description of the spectrum, but in double-beta decay we are not equally interested in all states. One alternative, known as the Contractor Renormalization (CORE) mapping [24], is to make the small-space ground state $|\tilde{0}\rangle$ proportional to $P|0\rangle$, the projection of the full ground state, and then construct the other $|\tilde{k}\rangle$ from the set $P|k\rangle$ through Graham-Schmidt orthogonalization. But in fact any unitary transformation of the $|\tilde{k}\rangle$'s generated by the Lee-Suzuki procedure defines a valid mapping. In our case, we can generate an arbitrary time-reversal-preserving transformation by rotating the two small-space 0^+ states in $A = 6$ by an arbitrary angle α and the two 2^+ states by another angle β. We will try to see whether there are values of these angles that are particularly suited for double-beta decay.

III. RESULTS

We now test the performance of our Lee-Suzuki effective operator in heavier nuclei. Figure 1 presents our results for the decays ^{7,8,10}He$\rightarrow^{7,8,10}$Be when we use the SRG-evolved chiral N^{3}LO ([15]) interaction in a $6\hbar\omega$ full space. The black (solid) curves in each of the panels denote the full $N_{max} = 6$ $0\nu\beta\beta$ distributions $C(r)$. These curves are what the effective operators are supposed to reproduce. The red (dashed) curves denote the results obtained with the bare $0\nu\beta\beta$ operator in the p shell, with wave functions produced by the effective p-shell interaction, which in turn comes from the Lee-Suzuki procedure for $A = 5$ and 6 discussed above. The blue (dot-dashed) curves are the results with the effective operator, used in conjunction with the wave functions from the same effective interaction.

The use of the effective decay operator clearly improves the agreement between the p-shell $C(r)$ and the full one in all three panels. One problem, however, is that $C(r)$ is not itself measurable; its integral is what we want. And it turns out that oscillations can make apparent poor agreement between curves much better in the integral, and good agreement worse. Table I compares the matrix elements themselves for the three decays represented by the figure.

The effective operator produces a clear improvement in the integrated matrix element

in A= 7 and (particularly) 8, but by A= 10 the bare operator does pretty well and the effective operator not as well. The reason is apparent from the bottom panel of Fig. 1: the effective-operator curve, while a better approximation than the bare curve, is not as good when integrated because because it is above the full curve until about $r \sim 4$ fm. The bare curve strays from the full curve at both the peak and dip but in opposite directions; it thus

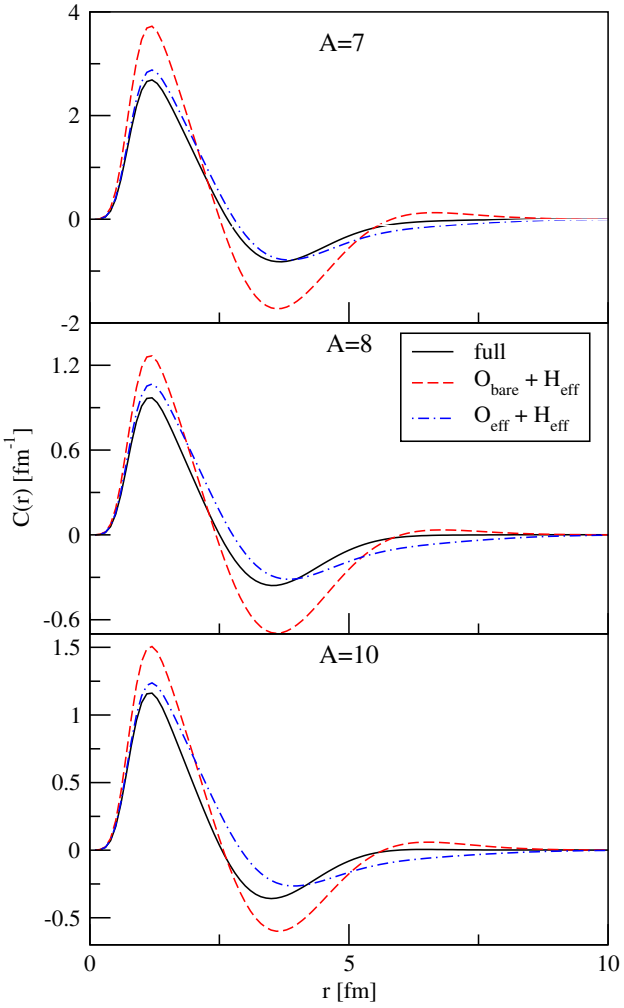

FIG. 1. (Color online) The curves $C(r)$, the integrals of which give the matrix elements for neutrinoless double-beta decay. The solid (black) lines are the results of the full ($N_{max} = 6$) calculations with the SRG-evolved N^{3}LO potential, the dashed (red) lines are the results of the p-shell calculation with the effective two-body Hamiltonian and the bare decay operator, and the dot-dashed (blue) lines are the results with the effective Hamiltonian and the effective decay operator. The top panel is for the decay ^{7}He $\rightarrow$ ^{7}Be, the middle panel for ^{8}He $\rightarrow$ ^{8}Be, and the bottom panel for ^{10}He $\rightarrow$ ^{10}Be.

TABLE I. Matix elements $\mathcal{M}_{fi}$ produced by the distributions $C(r)$ in Fig. 1.

	7	8	10
full	1.76	0.48	0.79
bare	1.49	0.18	0.91
effective	1.90	0.59	1.23

supplies a good approximation when integrated.

Is this behavior a fluke? Does it depend on the shell-model interaction or the size of the full model space? To address the questions we repeated our calculations with different interactions and model spaces. In $A = 7$, the effective operator is always a decided improvement but in $A = 8$ and 10 the results are more ambiguous. Figure 2 and Tab. II present results of calculations in a $N_{max} = 8$ space with the CD-Bonn interaction, conditioned as described in section II for $A = 8$ and 10. (We do not show $A = 7$, and the size of the problem in ^{10}Be limits us to $N_{max} = 6$ in $A = 10$.) Once again the effective operator appears to be an improvement in both cases, but now, as Tab. II shows, the effective-operator curve for

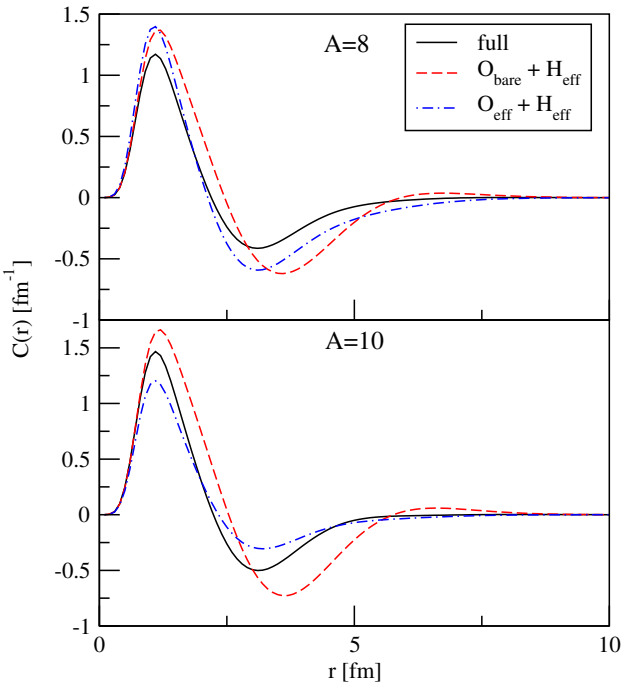

FIG. 2. (Color online) Same as Fig. 1 but for for ^{8}He $\rightarrow$ ^{8}Be and ^{10}He $\rightarrow$ ^{10}Be only and with the CD-Bonn interaction conditioned for $N_{max} = 8$ in $A = 8$ and $N_{max} = 6$ in $A = 10$.

TABLE II. Matix elements $\mathcal{M}_{fi}$ produced by the distributions $C(r)$ in Fig. 2.

	8	10
full	-0.41	-0.67
bare	-0.48	-0.80
effective	-0.03	-0.68

$A = 8$ cancels itself *too much* in the integral. And in $A = 10$ the effective operator does better than the figure indicates it should.

One might expect the procedure to work better when the full model space is smaller, and/or when the full results differ less from the bare p-shell prediction but neither of those are entirely the case either. Figure 3 and Tab. III show results of calculations in which we

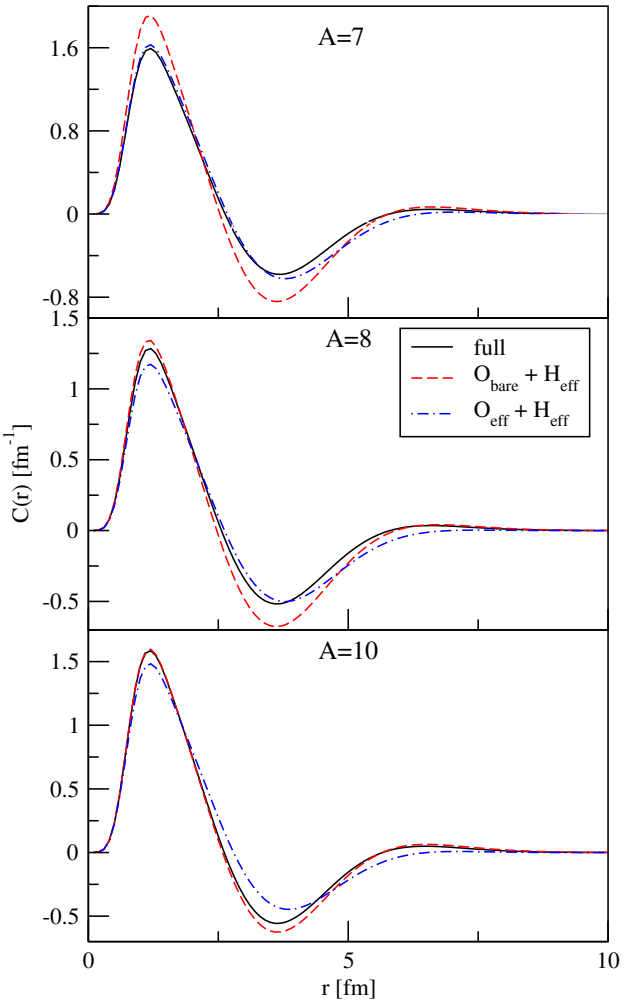

FIG. 3. (Color online) Same as Fig. 1 but carried out in a small model space with $N_{max} = 2$.

TABLE III. Matix elements $\mathcal{M}_{fi}$ produced by the distributions $C(r)$ in Fig. 3.

	7	8	10
full	-1.06	0.70	1.10
bare	-0.90	0.37	0.99
effective	-0.92	0.45	1.14

use the SRG-evolved interaction in a severely truncated space: $\mathrm{N}_{max} = 2$. Because we are using the same effective interaction as before, we have reduced the amounts of the wave functions that lie outside the p shell. Now all curves are close to each other everywhere, but the effective operator, as expected, is an improvement in $A = 7$ and 8. In $A = 10$, however, the bare operator is nearly perfect and the effective operator worse (though now, as Tab. III shows, it is accidentally better in the integral).

It seems, then, that except in this last example the effective decay operator is a decided improvement, but also that the oscillations in $C(r)$ can sometimes negate its advantages. The natural way to do better is by adding three-body terms to the effective interaction and decay operator. We will not do so in this preliminary study, but can look into whether the discrepancy at the two-body level is due mainly to the defects in the decay operator or in the interaction. If we were to carry out the Lee-Suzuki procedure in $A = 8$ and 10, the p-shell ground states would resemble the normalized p-shell projections of the full ground states. We can therefore use these normalized projections as proxies for the states that would be produced by the complete A-body Lee-Suzuki p-shell Hamiltonian. Figure 4 shows the resulting $C(r)$ with both the bare and two-body effective operators, alongside the curves already displayed in Fig. 1. The performance of the bare operator improves noticeably, so that it is about as good as that of the two-body effective operator in conjunction with the two-body effective Hamiltonian; its integral is $\mathcal{M}_{fi} = 0.63$. And interestingly, performance gets worse when the effective two-body operator is used instead ($\mathcal{M}_{fi} = 0.74$). The first result indicates that three-and-more-body terms in the Hamiltonian affect the matrix element, and the second that such terms in the decay operator do as well.

Figure 4 has one other curve, produced by the bare operator in conjunction with the phenomenological Cohen-Kurath potential [25]. We can't really expect this empirical potential to reproduce the results of an NCSM calculation in a nucleus that isn't in reality

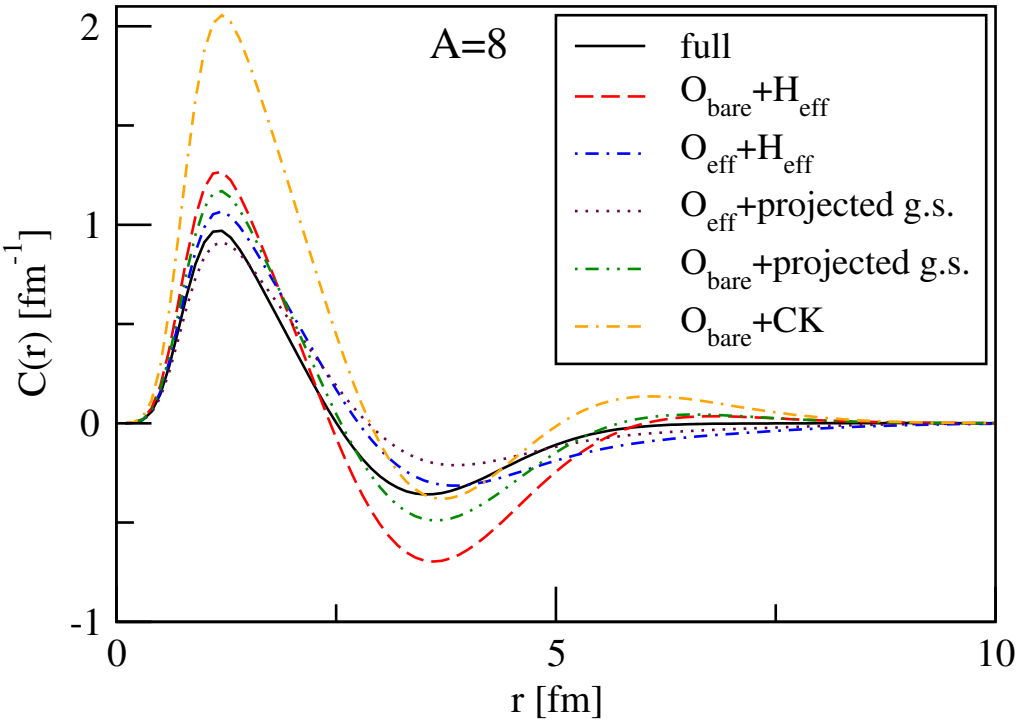

FIG. 4. (Color online) $C(r)$ for ^{8}He $\rightarrow^8$Be: the solid (black), dashed (red) and dot-dashed (blue) lines are as in Fig. 1. The dotted (maroon) and the dot-dot-dashed (green) curves result from using the normalized $p-$shell projections of the full ground states with the effective and the bare decay operator respectively. The dot-dashed-dashed (orange) curve is the result with bare decay operator and the Cohen-Kurath (CK) interaction [25].

even stable, but it is nevertheless interesting to see how different its results are.

As mentioned in the introduction, the Lee-Suzuki mapping is only one of an infinite number of possible mappings. We tested for better-performing mappings in $A = 6$ by rotating the Lee-Suzuki p-shell basis vectors by arbitrary real angles. Though we didn't exhaustively explore all such possibilities, we found it difficult to improve on the Lee-Suzuki results. With the SRG interaction in $\mathrm{N_{max}} = 6$, rotation of the two 2+ vectors by 15° improved the effective operator $C(r)$'s marginally, but nowhere did we see a dramatic improvement.

IV. DISCUSSION

We have shown that a nonperturbative renormalization of the effective decay operator improves the shell-model's ability to reproduce $0\nu\beta\beta$ matrix elements from ab initio calcu-

lations. What do these results imply for the heavier nuclei we really care about? There is some reason to hope that a two-body effective operator will perform even better there than it did here. Both QRPA and shell-model calculations in these nuclei show that the curves $C(r)$ produced by the bare operator nearly vanish beyond about 3 fm; there are no oscillations of consequence in those curves [11]. For that reason, the performance of the effective operator may not be degraded by the cancellations that play such a large role here. In any event, the effective two-body operator is clearly worth determining.

There are several possible routes to that end. Ref. [26] reports coupled-cluster calculations in ^{6}He, the first in a nucleus with two valence nucleons. Coupled-cluster techniques scale well to intermediate-mass nuclei and it should be possible to treat the nuclei ^{58}Ni, ^{58}Cu, and ^{58}Zn with two nucleons in the $f_{5/2}pg_{9/2}$ shell (along with the simpler nuclei with one nucleon in that shell). Such calculations will play the same role as the NCSM calculations here, allowing the extraction of a two-body effective Hamiltonian and decay operator, which can then be used in a shell-model calculation of the decay of e.g. ^{76}Ge. If the Hamiltonian proves inadequate, a better phenomenological one can be substituted, though at the obvious cost of consistency. Other techniques, including many-body perturbation theory with soft renormalization-group-produced interactions [27] and the in-medium similarity renormalization group [28] offer a path to effective operators as well.

For a truly accurate calculation we probably will need three-body decay operators. All the methods mentioned above can produce these in principle, but at least a few years of development are required. In the meantime, we can examine the question of whether two- and three-body decay operators will be sufficient (or whether horribly complicated four-body operators will be required) by extending the p-shell tests we report here. Work in that direction is underway.

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