

Effective operators for double- β decay

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We use a solvable model to examine double- β decay, focusing on the neutrinoless mode. After examining the ways in which the neutrino propagator affects the corresponding matrix element, we address the problem of finite model-space size in shell-model calculations by projecting our exact wave functions onto a smaller subspace. We then test both traditional and more recent prescriptions for constructing effective operators in small model spaces, concluding that the usual treatment of double- β -decay operators in realistic calculations is unable to fully account for the neglected parts of the model space. We also test the quality of the quasiparticle random phase approximation and examine a recent proposal within that framework to use two-neutrino decay to fix parameters in the Hamiltonian. The procedure eliminates the dependence of neutrinoless decay on some unfixed parameters and reduces the dependence on model-space size, though it does not eliminate the latter completely.

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I. INTRODUCTION

Next-generation double- β -decay experiments will provide data on the mass of the lightest neutrino [1]. But to interpret the data accurately we will need to better understand the nuclear physics that influences the decay rate. The problem of calculating double- β -decay matrix elements has occupied nuclear theorists for a long time. The latest in a long history of neutrinoless-decay calculations are thought to approximate exact results to within factors of 3 or 4, but that estimate is not much more than an informed guess. In short, the calculations need to be improved.

Almost all current calculations are performed either in the quasiparticle random phase approximation (QRPA) or the shell model. The two methods differ in the types of correlations they take into account. The QRPA can include the cumulative effects of small numbers of particles or holes far above or below the Fermi surface, but the correlations are of a specific type. The shell model is restricted to configurations with low excitation, but correlates them in all possible ways. The QRPA calculations indicate that nearly empty orbits relatively far from the Fermi surface play a significant role in the nuclear ground states, implying that the shell model is leaving something out. We are not referring here to the short-range correlations coming from the nucleon hard core, the representation of which requires very high-lying excitations. QRPA correlations are longer range, connected to orbits just 10 or 20 MeV away from the Fermi surface; the shell model usually cannot include even these. Within the levels it does include, however, the shell model indicates that QRPA correlations are too simple. We need either to add the effects of more complicated correlations to the QRPA or to include

effects of additional single-particle levels in the shell model (or perhaps do both).

The way to correct for the finite shell-model space is to construct effective Hamiltonians and transition operators. Unfortunately, the equations that determine effective operators are hard to solve and perturbative approximations often do not work. Phenomenology is the usual substitute. Thus, the effective Hamiltonians computed within perturbation theory usually include only two-body terms that are then renormalized to fit ground-state energies and other observables. Effective transition operators are often taken to have the same form as the bare operators but are multiplied by effective coupling constants. Such prescriptions can work well when there are lots of data to which parameters can be fit, but for the two-body operator governing neutrinoless double- β beta decay, which has not yet been observed at all, the use of the bare operator with or without simple multiplicative renormalization is suspect. Yet such is the state of the art in shell-model calculations of double- β decay. To improve these calculations, we should focus on a better determination of the effective decay operator.

Here we use a solvable model based on the algebra $SO(5)$ to test some of the assumptions that go into calculations of double- β decay in ^{76}Ge , one of the most promising isotopes for experiment. We diagonalize the model Hamiltonian and calculate the rates of both two-neutrino (2ν) and neutrinoless (0ν) decay in a space consisting of a degenerate $pf_{g_{9/2}}$ valence shell, and a higher-energy degenerate $sd_{g_{7/2}}$ shell. In this quite realistic model space (albeit with unrealistically simple correlations), we can compare the behavior of the two kinds of decays, which depend differently on radial wave functions, as we vary couplings in the Hamiltonian. We can also project the full wave function onto states in which all nucleons are in the lower shell and test procedures for constructing effective interactions and operators. Though technically we are calculating Fermi decay, we allow isospin to be

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violated so that our calculation mimics many of the aspects of Gamow-Teller decay. We find, for example, that an effective two-body operator that reproduces decay rates exactly in nuclei with just a few valence nucleons, while better than the bare operator, is far from perfect when applied to a nucleus such as ^{76}Ge that has many valence particles. The more phenomenological prescription of multiplying the bare operator by an effective coupling requires different renormalization factors for 2ν and 0ν decay. Such results, while perhaps unsurprising, contradict common practice.

We also examine some related ideas. A recently proposed technique for constructing effective operators nonperturbatively through a Lanczos approximation to the many-body Green's function usually proves efficient but appears to offer little advantage over the Lanczos methods already used in shell-model calculations for double- β decay. A recent proposal for adjusting the Hamiltonian in the QRPA to fit measured 2ν decay, though it eliminates the dependence on some of the parameters in the Hamiltonian and reduces the dependence on model-space size, does not work as well in this model as in more realistic calculations. The QRPA itself, ironically, reproduces exact solutions extremely accurately here.

The rest of this paper is divided as follows: In Sec. II we discuss the model. Though it has been used before in 2ν decay [2], ours is the first application to 0ν decay, the operator for which is not built from $\text{SO}(5)$ generators and therefore takes some effort to manipulate. Section III tests common prescriptions for constructing effective operators in a truncated model space against exact solutions in the full model space. In Sec. IV we examine the proposal of Ref. [3] to renormalize the Hamiltonian in the QRPA. Section V is a conclusion. The Appendix contains explicit formulas for matrix elements of double- β decay operators in the model.

II. $\text{SO}(5)$ MODEL

We consider the nuclei ^{76}Ge and ^{76}Se in a “small” shell-model space containing 12 protons and 24 neutrons (for Ge) in a degenerate $pf g_{9/2}$ valence shell, and in a “large” space containing the small space together with all possible excitations of the nucleons into a degenerate version of the next shell ($sd g_{7/2}$), which is an energy ϵ above the $pf g_{9/2}$ shell. We usually use one of two different values of ϵ so that either about 20% of the particles are in the upper levels, or about 6%. Both values of the splitting, probably, are unrealistically small for the kind of long-range correlations we have in mind, but our correlations are unrealistically simple and we compensate in part by lowering ϵ (for one test we will use a very large ϵ that results in 1% of the particles in the upper levels). The single-particle wave functions come from a harmonic oscillator with length parameter $b=2.12$ fm.

The Hamiltonian, constructed from the generators of $\text{SO}(5) \times \text{SO}(5)$ [one $\text{SO}(5)$ for each degenerate set of levels], is [4]

$$H = \epsilon \hat{N}_2 - G \sum_{a,b=1}^2 (S_{pp}^{\dagger a} S_{pp}^b + S_{nn}^{\dagger a} S_{nn}^b + g_{pp} S_{pn}^{\dagger a} S_{pn}^b - g_{ph} \mathbf{T}_a \cdot \mathbf{T}_b), \quad (1)$$

where $a, b=1, 2$ label the shells (lower and upper), ϵ is the energy difference between the shells, \hat{N}_2 is the number op-

erator for the upper shell, \mathbf{T}_a is total isospin operator for shell a , and

$$\begin{aligned} S_{pp}^{\dagger a} &= \frac{1}{2} \sum_{\alpha \in a} \hat{j}_\alpha [\pi_\alpha^\dagger \pi_\alpha^\dagger]_0^0, \\ S_{nn}^{\dagger a} &= \frac{1}{2} \sum_{\alpha \in a} \hat{j}_\alpha [\nu_\alpha^\dagger \nu_\alpha^\dagger]_0^0, \\ S_{pn}^{\dagger a} &= \frac{1}{\sqrt{2}} \sum_{\alpha \in a} \hat{j}_\alpha [\pi_\alpha^\dagger \nu_\alpha^\dagger]_0^0. \end{aligned} \quad (2)$$

Here π_α^\dagger (ν_α^\dagger) creates a proton (neutron) in level α with angular momentum j_α , $\hat{j} \equiv \sqrt{2j+1}$, and the square brackets indicate angular-momentum coupling. The algebra of $\text{SO}(5)$ contains the three pair-creation operators above (for a given set a of levels), three corresponding destruction operators, the three components of the isospin \mathbf{T}_a , and the number operator \hat{N}_a . Since H contains only generators of $\text{SO}(5) \times \text{SO}(5)$, its lowest-lying eigenstates will consist of configurations in which the nucleons are entirely bound in isovector S pairs of the type in Eq. (2).

The Hamiltonian in Eq. (1) is not the most complicated that could be built from generators of $\text{SO}(5) \times \text{SO}(5)$. One could, for instance, assign different strengths to the pairing forces in the two levels, or make the proton pairing stronger than the neutron pairing. Even without the last complication, the Hamiltonian violates isospin (T) conservation unless $g_{pp}=1$. In our application of this model, we will make an analogy between double-Fermi decay, the 2ν version of which vanishes when isospin is exactly conserved, and double-Gamow-Teller decay in a more general model, which vanishes when Wigner $\text{SU}(4)$ is exactly conserved. Of course, $\text{SU}(4)$ is more badly violated than isospin, which is nearly a good quantum number, but in our simplified model, we will let isospin be badly violated to mock up the violation of $\text{SU}(4)$ in more realistic calculations.¹ When T is violated, the space of fully paired states in the two sets of levels $pf g_{9/2}$ and $sd g_{7/2}$ has dimension 1042 for ^{76}Ge and 1347 for the daughter nucleus ^{76}Se .

We will calculate the ground-state to ground-state transition matrix elements of two operators: the 2ν double-Fermi operator and the 0ν double-Fermi operator (both obtained from the closure approximation). These operators have the form

$$\mathcal{M}_\kappa = \sum_{i,j} \mathcal{O}_\kappa(i,j) \tau_i^\dagger \tau_j^\dagger, \quad (3)$$

where i, j refer to particles and τ^\dagger changes a neutron into a proton. The space/spin parts of the operators are

$$\mathcal{O}_{2\nu}(i,j) = 1 \quad (4)$$

and

¹ $\text{SU}(5)$ is violated primarily at the mean-field level, while in our calculations isospin is violated only in the two-body interaction.

$$\mathcal{O}_{0\nu}(i,j) = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (5)$$

The label κ in Eq. (3) refers to the kind of decay. The denominator in Eq. (5) reflects the propagation of a virtual neutrino inside the nucleus. We have neglected the average nuclear excitation and short-range correlations in writing $\mathcal{O}_{0\nu}$. We will also evaluate an operator that includes those effects:

$$\mathcal{O}'_{0\nu}(i,j) = \frac{f(|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (6)$$

where [5,6]

$$f(r) \equiv e^{-1.5\bar{E}r/\hbar c} [1 - e^{-\gamma_1 r^2} (1 - \gamma_2 r^2)]^2, \quad (7)$$

with $\gamma_1 = 1.1 \text{ fm}^{-2}$, $\gamma_2 = 0.68 \text{ fm}^{-2}$, and \bar{E} taken somewhat arbitrarily to be 15 MeV.

The fully paired basis states can be labeled $|\mathcal{N}_1, T_1, M_1; \mathcal{N}_2, T_2, M_2\rangle$, where \mathcal{N}_1 refers to the number of pairs in level set 1 (the $pf_{g_{9/2}}$ shell), T_1 to the isospin of those \mathcal{N}_1 pairs (with $\mathcal{N}_1 - T_1$ even), M_1 to the isospin projection of those pairs, etc., and $M_1 + M_2 = 1/2(Z - N)$. The Hamiltonian, Eq. (1), and 2ν decay operator, Eq. (4), are products of generators and one can evaluate their matrix elements, which depend only on the quantum numbers of the pairs, following, e.g., Ref. [7]. But the 0ν operators, Eqs. (5) and (6), contain position-dependent factors that do not belong to the algebra. Their matrix elements will depend on the wave functions of the single-particle states that make up our basis and require more effort to evaluate. We have computed them by applying the generalized Wigner-Eckart theorem [7], which for matrix elements of an operator \mathcal{M} between fully paired states in SO(5) is

$$\begin{aligned} & \langle \Omega_a, \mathcal{N}_a, T_a, M_a | \mathcal{M}_{N_0, T_0, M_0}^{(\omega_1, \omega_2)} | \Omega_a, \mathcal{N}'_a, T'_a, M'_a \rangle \\ &= \langle (\Omega_a, 0) | \mathcal{M}^{(\omega_1, \omega_2)} | (\Omega_a, 0) \rangle \\ & \times \langle (\Omega_a, 0) \mathcal{N}'_a T'_a; (\omega_1, \omega_2) \mathcal{N}_0 T_0 | (\Omega_a, 0) \mathcal{N}_a T_a \rangle \\ & \times \langle T'_a M'_a; T_0 M_0 | T_a M_a \rangle. \end{aligned} \quad (8)$$

Here the extra “quantum number” Ω_a , omitted in the labeling scheme discussed in the previous paragraph, is the half the total degeneracy of the level set a ,

$$\Omega_a = \frac{1}{2} \sum_{\alpha \in a} j_{\alpha}^2, \quad a = 1, 2, \quad (9)$$

and labels the representations ($\omega_1 = \Omega_a, \omega_2 = 0$) of SO(5) in which all particles are fully paired. More general representations, such as that characterizing the operator in Eq. (8), require two nonzero labels ω_1 and ω_2 . The first factor on the right-hand side of that equation is a reduced matrix element that depends only on Ω_a and the operator quantum numbers ω_1 and ω_2 . All the dependence on the initial and final number of particles in the system, the initial and final isospin and isospin projection, and the isospin and particle-number quantum numbers of the operator appear in the double-barred SO(5) “reduced Clebsch-Gordan” coefficient (which is independent of the isospin-projection quantum numbers) and an ordinary isospin Clebsch-Gordan coefficient.

The work of Ref. [7] allows us to decompose the operators $\mathcal{M}_{0\nu}$ and $\mathcal{M}'_{0\nu}$ into operators with good SO(5) \times SO(5) quantum numbers, lists some of the SO(5) Clebsch-Gordan coefficients we need, and contains enough information to allow us to construct (laboriously) those it does not list: the coefficients for isospin-changing components of operators belonging to the SO(5) representations (2,0) and (2,2). Here we show expressions for matrix elements of double-charge-changing two-body operators in the “small space” — all particles in the degenerate $pf_{g_{9/2}}$ levels — the states of which we write in the form $|\mathcal{N}, T, M\rangle$, where all quantum numbers refer to the first set of levels ($a=1$) because the second set is empty. We focus on these matrix elements because they are the most complicated and because they will determine the behavior of the effective decay operators when we truncate the wave function to the small space (other matrix elements needed for the full calculation are in the Appendix). Defining summed particle-particle and particle-hole-like matrix elements of an arbitrary two-body operator \mathcal{M}_{κ} that changes charge by two units (acting, for generality of notation, in either of the two sets of levels) as

$$\begin{aligned} \mathcal{F}_{\kappa}^{pp}[a,b] &\equiv \sum_{\alpha \in a, \beta \in b} \hat{j}_{\alpha} \hat{j}_{\beta} \langle [\alpha\alpha]^0 | \mathcal{O}_{\kappa} | [\beta\beta]^0 \rangle, \\ \mathcal{F}_{\kappa}^{ph}[a,b] &\equiv \sum_{\alpha \in a, \beta \in b} \sum_J \hat{J}^2 \langle [\alpha\beta]^J | \mathcal{O}_{\kappa} | [\alpha\beta]^J \rangle, \end{aligned} \quad (10)$$

where, as before, a and b refer to degenerate sets of levels and the matrix elements are antisymmetrized, we have when all the particles are in the lowest set

$$\begin{aligned} \langle \mathcal{N}, T \pm 2, M \pm 2 | \mathcal{M}_{\kappa} | \mathcal{N}, T, M \rangle &= \frac{\sqrt{T_{>}(T_{>} - 1)(2\Omega - \mathcal{N} + T_{>} + 1)(2\Omega - \mathcal{N} - T_{<})(\mathcal{N} + T_{>} + 1)(\mathcal{N} - T_{<})}}{8(2T_{>} - 1)\Omega(\Omega - 1)(2\Omega + 1)} \\ & \times \langle T \pm 2, M \pm 2; 1 - 1 | T_{>} - 1, M + 1 \rangle \langle T, M; 1, 1 | T_{>} - 1, M + 1 \rangle \{ 2\mathcal{F}_{\kappa}^{ph}[1,1] - (2\Omega - 1)\mathcal{F}_{\kappa}^{pp}[1,1] \}, \end{aligned} \quad (11)$$

and

$$\begin{aligned} \langle \mathcal{N}, T, M+2 | \mathcal{M}_\kappa | \mathcal{N}, T, M \rangle &= \frac{\sqrt{T(T+1)}}{4\sqrt{6(2T-1)(2T+3)\Omega(\Omega-1)(2\Omega+1)}} \langle T M; 2 2 | T M+2 \rangle \\ &\times \{ [\mathcal{N}(\mathcal{N}-2\Omega) - 3(2\Omega+1) + (4\Omega+1)T(T+1)] 2\mathcal{F}_\kappa^{ph}[1,1] \\ &- [(2\Omega-1)\mathcal{N}(\mathcal{N}-2\Omega) - 3\Omega(2\Omega+1) + (2\Omega+3)T(T+1)] \mathcal{F}_\kappa^{pp}[1,1] \}. \end{aligned} \quad (12)$$

Here $\Omega \equiv \Omega_1$, and $T_>$ ($T_<$) is the largest (smallest) of the isospins in the bra and ket of Eq. (11). The eigenstates of the Hamiltonian, Eq. (1), have good particle number \mathcal{N} and isospin projection M , but are mixtures of states with different isospins T . The same is true of the projection of the wave functions onto the small space, so both the equations above are important.

The most important fact about Eqs. (11) and (12) is that they depend on the two-body matrix elements of the operator through only two quantities, $\mathcal{F}^{pp}[1,1]$ and $\mathcal{F}^{ph}[1,1]$, the particle-particle and particle-hole (with some factors of \hat{j} removed) matrix elements summed over all orbits in the lower shell. The action of any two-body operator that changes charge by two units on fully paired states in that shell can therefore be constructed by specifying just two parameters. This simplicity reflects the nature of the underlying correlations. The interaction cannot create particle-hole excitations involving different orbits.

III. MATRIX ELEMENTS, TRUNCATION OF WAVE FUNCTIONS, AND EFFECTIVE OPERATORS

Before addressing the issues of effective decay operators in the small space, we examine the behavior of the matrix elements

$$M_\kappa \equiv \langle 0_f | \mathcal{M}_\kappa | 0_i \rangle \quad (13)$$

of the operators $\mathcal{M}_{2\nu}$, $\mathcal{M}_{0\nu}$, and $\mathcal{M}'_{0\nu}$, connecting the ground states of ^{76}Ge and ^{76}Se . The matrix elements are plotted in Fig. 1 for fixed G , $\epsilon=10G$ (resulting in about 20% of the nucleons occupying the upper set of levels), and two values of g_{ph} . We vary g_{pp} , which measures the strength of proton-neutron pairing (the graphs look qualitatively the same when we change ϵ to $20G$ and about 6% of the particles are in the upper set). To compare the behavior of the three matrix elements with g_{pp} , we have scaled the 0ν matrix elements so that they are equal to the 2ν elements at $g_{pp}=0$. At $g_{pp}=1$ isospin is conserved and the 2ν matrix element crosses zero. In realistic calculations the analog of g_{pp} in the $J^\pi=1^+$ channel is close to 1; indeed, early QRPA calculations gave matrix elements that were much too large precisely because they neglected the particle-particle interaction. The 0ν matrix elements cross zero only for larger g_{pp} , much larger when $g_{ph}=1$, and are therefore less sensitive than the 2ν elements to that parameter when it is at a realistic value. This reduced sensitivity is another aspect of our model that mirrors more complicated calculations. The two versions of the 0ν matrix ele-

ment are nearly proportional; the short-range correlations and average excitation energy shrink the matrix element by a factor of about 1.5, almost independently of g_{pp} .

The different behavior of the 2ν and 0ν matrix elements with g_{pp} is explored in Fig. 2, which shows the pair-separation transition density

$$P(r) \equiv \langle 0_f | \sum_{i,j} \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \tau_i^+ \tau_j^+ | 0_i \rangle \quad (14)$$

(r is the magnitude of the internucleon separation) at several values of g_{pp} . The density $P(r)$ is defined so that

$$\int P(r) dr = M_{2\nu}, \quad (15)$$

$$\int \frac{P(r)}{r} dr = M_{0\nu}, \quad (16)$$

etc. The figure shows that as g_{pp} increases $P(r)$ decreases and then changes sign at large r , while remaining positive at small r . At $g_{pp}=1$ the integral of $P(r)$ is zero but the $1/r$ -weighted integral is still positive because small values of r are most important. Thus, the matrix elements of $\mathcal{M}_{0\nu}$ and $\mathcal{M}'_{0\nu}$ cross zero at larger g_{pp} than that of $\mathcal{M}_{2\nu}$.

The reason that $P(r)$ is most affected by g_{pp} at large r is the following: At $g_{pp}=0$ only one pair can participate in the

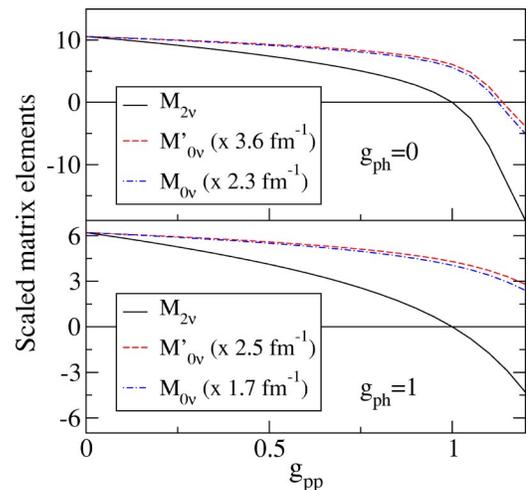


FIG. 1. Double- β -decay matrix elements vs the strength of neutron-proton pairing g_{pp} for two values of the particle-hole coupling g_{ph} . The matrix elements of the two 0ν operators are scaled to that of the 2ν operator at $g_{pp}=0$.

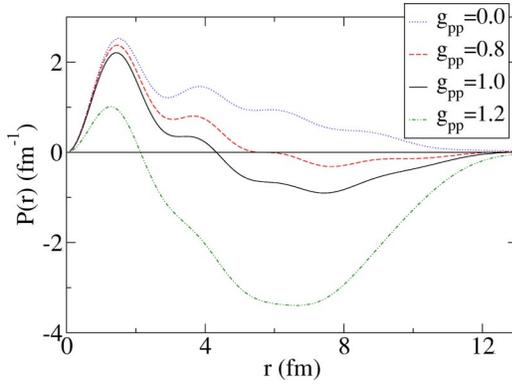


FIG. 2. The transition density $P(r)$ [see Eq. (14)] as a function of internucleon separation r for several values of g_{pp} , with $\epsilon = 10G$ and $g_{ph} = 0$.

ground-state to ground-state decay; since there are no correlated proton-neutron pairs, the decay operator turns two neutrons within a given pair into two protons. As g_{pp} becomes larger the ground states contain neutron-proton pairs, and double- β decay can proceed, e.g., through the transformation of one neutron in a neutron-neutron pair and one in a (separate) proton-neutron pair. These two neutrons are farther apart on average than two in the same correlated pair, so the transition density changes more at large r than at small r , where it stays positive.

We now turn to the question of effective operators in the small space (all nucleons in the $pf g_{9/2}$ shell). The Bloch-Horowitz equation [8]

$$H_{\text{eff}}(E) = PHP + PHQ \frac{1}{E - QH} QHP \quad (17)$$

and approximations thereto are designed to construct an effective Hamiltonian H_{eff} that obeys

$$H_{\text{eff}}(E_k)P|\Psi_k\rangle = PH|\Psi_k\rangle = E_k P|\Psi_k\rangle, \quad (18)$$

where H is the full Hamiltonian, $|\Psi_k\rangle$ is an eigenstate with energy E_k , P projects onto the subspace in which all particles are in the $pf g_{9/2}$ shell, and $Q = 1 - P$. Once the projections of the eigenstates are known, effective transition operators $\mathcal{M}_\kappa^{\text{eff}}$ can be constructed to satisfy

$$\langle \bar{\Psi}_k | \mathcal{M}_\kappa^{\text{eff}} | \bar{\Psi}_l \rangle = \langle \Psi_k | \mathcal{M}_\kappa | \Psi_l \rangle, \quad (19)$$

where

$$|\bar{\Psi}\rangle \equiv \frac{P|\Psi\rangle}{\sqrt{\langle \Psi | P | \Psi \rangle}} \quad (20)$$

is the normalized component of $|\Psi\rangle$ that has all the particles in the lower set of levels. We do not actually have to know H_{eff} to construct $\mathcal{M}_\kappa^{\text{eff}}$; we just need the full wave functions $|\Psi_k\rangle$ and their normalized projections $|\bar{\Psi}_k\rangle$.

Effective operators must in general be sums of 1-body, 2-body, ... up to N -body terms. It is common practice, however, to attempt to incorporate the effects of the excluded space in an effective operator of the same rank (number of

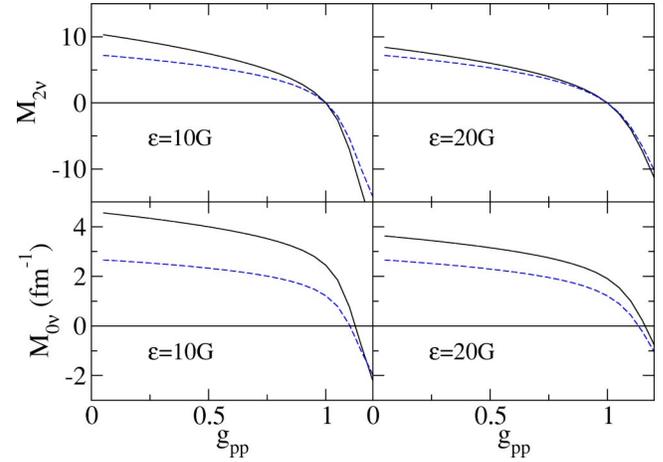


FIG. 3. 2ν (top) and 0ν (bottom) matrix elements vs the strength of neutron-proton pairing g_{pp} for $g_{ph} = 0$. The solid lines are the results in the full model space and the dashed lines are the results obtained by sandwiching the bare operator between normalized projections of the wave functions onto the small model space.

bodies) as the original operator. Thus effective electromagnetic transition operators are often taken to be one-body but of a more general form than the original operator, with “level-dependent effective charges.” In calculations of 2ν double- β decay, people often just multiply the bare operator by a single effective coupling, usually $1/(1.25^2)$, to take into account the observed quenching of spin-dependent transitions. When calculating 0ν decay they either use the bare operator or the same quenched coupling as for 2ν decay. Nothing beyond a simple multiplicative renormalization has ever been attempted.

Although by definition there always exists a multiplicative factor that will work, the trick is to know what it is. Figure 3 shows that the appropriate factor is different in 0ν decay than in 2ν decay. At $g_{pp} = 0.9$, a value yielding a reasonable approximation to the real world within our model, the renormalization factor for 0ν decay must be 1.8 when $\epsilon = 10G$ and 1.5 when $\epsilon = 20G$ ($g_{ph} = 0$). For 2ν decay, these numbers are 1.3 and 1.1 (adding the particle-hole force changes the numbers only a little). These results measure the quality both of calculations that use bare operators and of those that attempt to incorporate the effects of neglected single-particle levels by renormalizing the 2ν and 0ν operators by the same factor.

Figure 4, which shows $P(r)$ at $g_{pp} = 0.5$ for the full ground states $|0\rangle$ and their normalized small-space projections $|\bar{0}\rangle$, sheds some light on the different renormalization factors. Interestingly, the transition density spreads out when projected onto the small space, so that most of the change is at small r and, as a result, the renormalization factor for the 0ν transition is larger than for the 2ν transition. One can understand the spreading by looking at the structure of the correlated pairs in Eq. (2). The one-body piece of the mean-square internucleon distance $\langle (\mathbf{r}_1 - \mathbf{r}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) \rangle$ is uniformly reduced by the cross term $-2\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle$. In the $pf g_{9/2}$ shell \mathbf{r} connects only the $f_{7/2}$ and $g_{9/2}$ levels. Adding the upper shell introduces many more contributions to $\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle$ and so reduces the

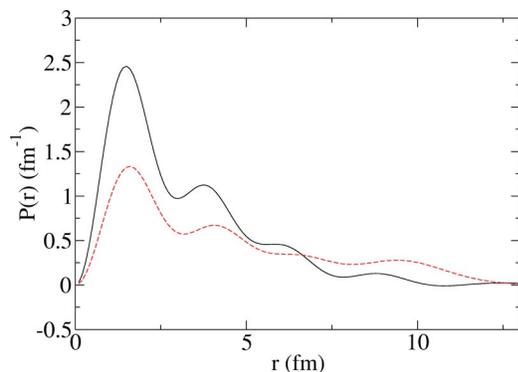


FIG. 4. The transition density $P(r)$ as a function of internucleon separation, at $g_{pp}=0.5$, for the full ground-state wave functions (solid line) and their normalized projections onto the small space (dashed line).

mean-square radius below its value in one shell. Alternatively (and more simply), the 0ν matrix element is more sensitive to occupation of the upper set of levels because the neutrino propagator in Eq. (5) allows the 0ν operator to connect those levels with the more highly occupied levels in the lower shell. The 2ν operator, which lacks radial dependence, does not connect levels from different shells.

If simple renormalization by a constant factor is dangerous, what about applying ideas used in electromagnetic physics to obtain a more general two-body operator? The usual practice there is to assume N nucleons in the valence shell when constructing an effective N -body operator, and then to apply that operator when there are larger numbers of valence particles. We can implement that procedure easily and exactly here, with $N=2$. The ground-state to ground-state transition for two valence neutrons in the small space decaying to two protons does not depend on the parameter $\mathcal{F}_{\kappa,\text{eff}}^{ph}$ of the effective operator in Eq. (19) (i.e., the coefficient of $\mathcal{F}_{\kappa}^{pp}[1,1]$ in Eq. (12) vanishes when $\mathcal{N}=1$ and $T=1$ because the particle-hole piece of the operator does not act on nucleons within the same pair), and so determines the parameter $\mathcal{F}_{\kappa,\text{eff}}^{pp}$. The excited states in both the initial and final nuclei have seniority 2 and are unaffected by the interaction; their structure plus that of the paired ground state determine $\mathcal{F}_{\kappa,\text{eff}}^{ph}$ in a simple way. More precisely, the effective particle-particle and particle-hole parameters for the operator $\mathcal{M}_{\kappa}^{\text{eff}}$ are given by

$$\mathcal{F}_{\kappa,\text{eff}}^{pp} = \mathcal{F}_{\kappa}^{pp}[1,1] \frac{\langle 0_f | \mathcal{M}_{\kappa} | 0_i \rangle}{\langle \bar{0}_f | \mathcal{M}_{\kappa} | \bar{0}_i \rangle} \quad (21)$$

and

$$\mathcal{F}_{\kappa,\text{eff}}^{ph} = \mathcal{F}_{\kappa}^{ph}[1,1] + \frac{1}{2\Omega} (\mathcal{F}_{\kappa,\text{eff}}^{pp} - \mathcal{F}_{\kappa}^{pp}[1,1]), \quad (22)$$

where the wave functions $|0_i\rangle$ ($|\bar{0}_f\rangle$) are the full two-neutron (two-proton) ground-state wave functions, the barred wave functions are their normalized projections onto the small space, and $\Omega \equiv \Omega_1$ characterizes the $pf g_{9/2}$ shell. With these identifications (the $\mathcal{F}[1,1]$'s are "bare" coupling constants),

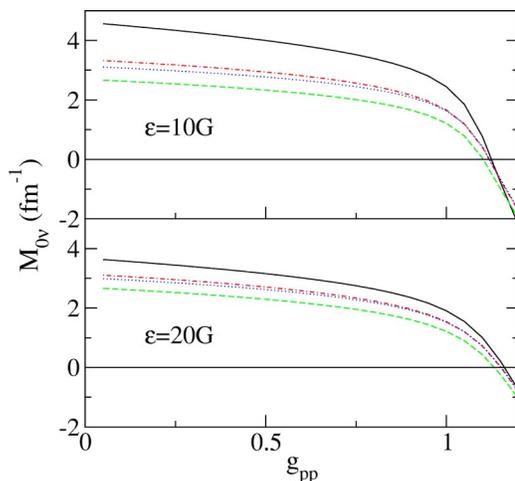


FIG. 5. Matrix elements of 0ν effective operators as a function of g_{pp} . The dashed line corresponds to the bare operator in the small model space, the dotted line to the effective operator that reproduces transitions in the two-valence-nucleon system, and the dot-dashed line to the operator that reproduces ground-state transitions in two- and four-valence-nucleon systems. The solid line is the exact result in the full model space.

the operator $\mathcal{M}_{\kappa}^{\text{eff}}$ reproduces all transitions involving the lowest $\Omega(2\Omega-1)$ states in each nucleus. It is what one would obtain by carrying the usual diagrammatic perturbation theory for the two-valence-nucleon system to all orders.

Of course we really ought to be determining the effective operator for $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$, rather than the two-valence-nucleon transition $^{42}\text{Ca} \rightarrow ^{42}\text{Ti}$. That, however, would amount to solving the problem exactly. But one might decide that it would be better (and feasible) to focus on ground-state to ground-state transitions, in the two-nucleon system and, say, in the four-nucleon system $^{44}\text{Ca} \rightarrow ^{44}\text{Ti}$. Reproducing these two transitions would determine the two parameters $\mathcal{F}_{\kappa,\text{eff}}^{pp}$ and $\mathcal{F}_{\kappa,\text{eff}}^{ph}$, and would have the advantage of incorporating neutron-proton pairing, which we know plays an important role in the heavier systems when g_{pp} is turned on, into the effective operator (through the two-proton two-neutron state in ^{44}Ti).

We display the results of both these prescriptions for the operator $M_{0\nu}$ in Fig. 5. Both procedures improve on the bare operator, particularly when $\epsilon=20G$, where they make up about half the difference between the bare and full results, but neither is perfect.² As expected, the fit to transitions involving two and four nucleons works better than the operator constructed entirely in the two-valence-nucleon system, but not remarkably so. We tried determining the effective operator entirely from four-valence-nucleon systems, but the improvement was minimal. The difference between the exact and approximate results is a measure of the amount higher-body effective operators contribute to the transitions.

One reason that two-valence-nucleon systems are empha-

²For 2ν decay the bare operator gives a better approximation than for 0ν decay (see Fig. 3), but the effective-operator procedures improve on it only slightly.

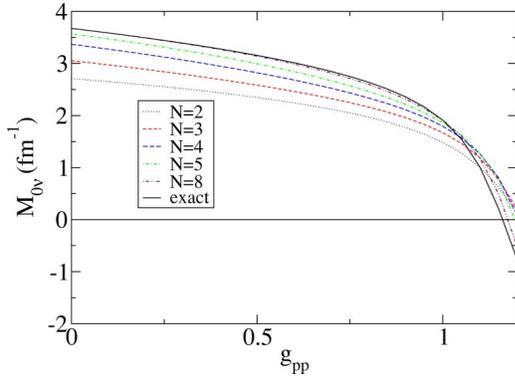


FIG. 6. Approximations to the 0ν matrix element, for $\epsilon=20G$, from a Lanczos representation of the Bloch-Horowitz equation, as described in Ref. [9]. Results are shown when the representation is truncated at different numbers of Lanczos vectors, and compared to the exact results.

sized in the traditional treatment of effective operators is that diagrammatic perturbation theory becomes complicated when more particles are considered. Reference [9] proposed a nonperturbative algorithm, based on the Lanczos representation of Green's functions as continued fractions [10], that can be used for any number of particles. For every state $|\mathcal{N}, T, M\rangle$ in the small space and some guess for the ground-state energy E (in both the initial and final nuclei), we construct the approximation to the large-space vector $(E - QH)^{-1}|\mathcal{N}, T, M\rangle$ and $H_{\text{eff}}(E)$, and then diagonalize the latter in the small space. We then redefine E to be the lowest eigenenergy and repeat the process until E does not change. Finally we construct the Lanczos approximation to the full ground-state wave functions

$$|0\rangle = \mathcal{Z} \left(1 + \frac{1}{E - QH} QH \right) |\bar{0}\rangle, \quad (23)$$

where \mathcal{Z} is a computable normalization factor, and calculate the transition matrix elements. The results for different numbers of Lanczos vectors appear in Fig. 6, where $\epsilon=20G$. Only eight or nine such vectors are required to get excellent results, but the iteration method fails to converge if ϵ is too small (e.g., $10G$). Furthermore, it is hard in our context to see the advantage of this procedure over simply doing a Lanczos diagonalization to obtain the ground-state eigenvectors in the large space with the “starting vector” determined, for example, by diagonalizing H in the small space. Such techniques are already exploited in shell-model calculations, and it is not clear that replacing them with the Bloch-Horowitz equation would be useful. Reference [11] proposed a new perturbative approach to solving that equation, but it has been worked out only in very light systems.

IV. QRPA

The QRPA is the most commonly used method for calculating double- β decay rates. How accurate is it? If it is not so accurate, can its predictions for 0ν decay be improved by

fixing certain parameters in the Hamiltonian to reproduce 2ν decay, as suggested in Ref. [3]? We examine both questions here.

We carry out the QRPA in the usual way (see, e.g., Ref. [5]). We first solve the BCS equations in the initial and final nuclei, obtaining the amplitudes $u_{\alpha_p}^i, v_{\alpha_p}^i, u_{\alpha_n}^i, v_{\alpha_n}^i$ and $u_{\alpha_p}^f, v_{\alpha_p}^f, u_{\alpha_n}^f, v_{\alpha_n}^f$. The corresponding occupation probabilities agree very well with the exact occupation probabilities for all values of the energy splitting ϵ . Next, we solve the usual QRPA equations of motion for both nuclei and use the expressions in Ref. [5] to evaluate the transition matrix elements. (The only difference is that in that paper the matrix element was obtained by averaging results from a calculation purely within the initial nucleus and from one within the final nucleus. Here we use both sets of u 's and v 's in the same expression, inserting an overlap between intermediate states generated by the QRPA from the initial and final ground states.) Since we evaluate only the closure matrix elements we can compare with the exact solutions. The dependence on the level splitting ϵ resides in the BCS amplitudes u, v as well as in the QRPA amplitudes X, Y ; the latter also depend on the interaction strength g_{pp} . The QRPA matrix elements are always evaluated by expanding the transition operator in proton-particle/neutron-hole multipole-multipole form. Since for 2ν decay the transition operator is just $2\tau_1^+ \tau_2^+$, only the 0^+ contribution (in real nuclei, the 1^+ contribution) exists. The neutrino propagator causes all multipoles contribute to 0ν decay.

In our model the interaction acts only in 0^+ intermediate states. For all other multipoles 0ν expressions reduce to their BCS form. The final result can be expressed as

$$\langle 0_f | \mathcal{M}_\kappa | 0_i \rangle_{\text{QRPA}} = (0^+ \text{ part}) + \sum_{\alpha, \beta, J} u_{\alpha_n}^f v_{\beta_p}^f u_{\beta_p}^i v_{\alpha_n}^i \times ([\beta\beta]^J | \mathcal{O}_\kappa | [\alpha\alpha]^J) \left[\hat{j}_{\alpha\beta} \hat{j}_{\beta\alpha} \delta_{J,0} - \frac{\hat{j}^2 \delta_{\alpha,\beta}}{\hat{j}_\alpha^2} \right], \quad (24)$$

where the matrix elements with rounded brackets are unsymmetrized (as usual in the RPA) and “ 0^+ part” refers to the matrix element when only the 0^+ multipole in the particle-hole decomposition of the operator is included. For 2ν decay the rest of the expression vanishes, but for 0ν decay there is a simple contribution from the other multipoles that is independent of the proton-neutron interaction.

The exact and QRPA results for both double- β decay modes are compared in Fig. 7. The agreement is very good over the whole interval $g_{pp}=0-1$. Note that QRPA equations have no solution (the solutions are said to “collapse”) for g_{pp} only slightly above unity. The agreement is equally good for all values of the splitting ϵ .

Previous comparisons between QRPA and exact results for $M_{2\nu}$ in this model [2] have not found such good agreement. The better agreement here is related to the larger degeneracies Ω and the larger number of particles we use to represent shell-model calculations in ^{76}Ge .

Reference [3] suggested a procedure for reducing the dependence of the 0ν rate on the number of single-particle

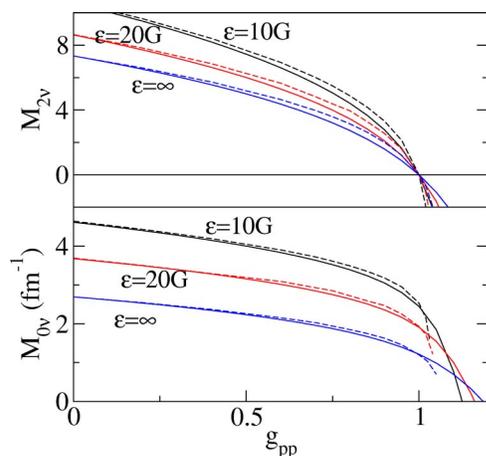


FIG. 7. Comparison of the exact and QRPA values for the 2ν matrix element (top) and 0ν matrix element (bottom) for the indicated values of the spacing ϵ between the degenerate $fp g_{9/2}$ and $sd g_{7/2}$ shells.

states used in the QRPA. Simply put, the method is this: assuming that the strength of the particle-particle interaction, g_{pp} , is the most important parameter, one evaluates both matrix elements $M_{0\nu}$ and $M_{2\nu}$ as a function of that parameter. One can then invert the relation between $M_{2\nu}$ and g_{pp} and express $M_{0\nu}$ directly in terms of $M_{2\nu}$. Reference [3] did this within the QRPA and in a modified version, the renormalized QRPA [12], for ^{76}Ge , ^{100}Mo , ^{130}Te , and ^{136}Xe . It turned out that the effects of single-particle levels far away from the Fermi surface, while noticeable for $M_{0\nu}$ and $M_{2\nu}$ considered separately, became negligible when $M_{0\nu}$ was plotted against $M_{2\nu}$. In other words, knowing $M_{2\nu}$ (from experiment) one could obtain the unknown $M_{0\nu}$, and its value was the same whether the far away single-particle states were included or not in the QRPA, as long as at least two oscillator shells (more than in our small space) were included. The question remains whether the QRPA result, even if insensitive to the model space, is correct.

When we carry out an analogous procedure in the $\text{SO}(5) \times \text{SO}(5)$ model, we find that $M_{0\nu}$ and $M_{2\nu}$ are related as shown in Fig. 8. While the relation between them is a simple one, it is not independent of ϵ , as it would be if the

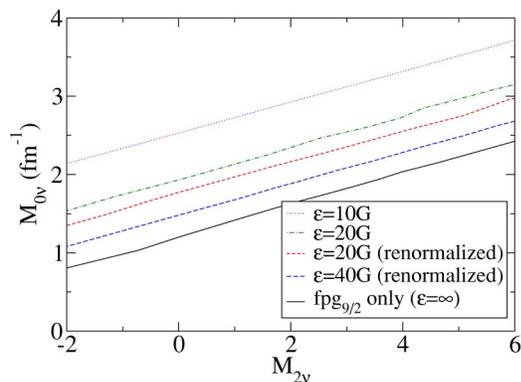


FIG. 8. Dependence of the matrix element $M_{0\nu}(g_{pp})$ on the matrix element $M_{2\nu}(g_{pp})$ for the indicated values of the level spacing ϵ . See text for further explanation.

ideas of Ref. [3] played out perfectly. Instead, the offset in $M_{0\nu}$ depends on ϵ (but is independent of g_{pp}). With increasing ϵ the lines in the figure, for obvious reasons, come closer together. While fixing g_{pp} to the exact (large-space) value of $M_{2\nu}$ improves the small-space prediction of $M_{0\nu}$, it always leaves it smaller than the exact result.

In the realistic calculations the strength of the pairing interaction was adjusted so that the pairing gap was the same in the “large” and “small” spaces. We do the same at $\epsilon = 20G$; the corresponding line moves closer to the $\epsilon = \infty$ limit, but is still significantly different. Finally, in Ref. [3] the proton-proton and neutron-neutron pairing constants were adjusted separately. With a typical value $G \sim 22/A$ MeV and $\hbar\omega = 41/A^{1/3}$ MeV, the value of ϵ corresponding to Ref. [3] is at least $40G$. With that value and a charge-dependent pairing renormalization $G_{nn}/G_{pp} \sim 1.2$ here, the line moves even closer to its limiting value.

The matrix elements in Fig. 8 were obtained without any particle-hole force, i.e., for $g_{ph} = 0$. When the calculation is repeated with $g_{ph} = 1$ both $M_{0\nu}$ and $M_{2\nu}$ are significantly reduced (see Fig. 1). When the parameter g_{pp} is eliminated, however, and $M_{0\nu}$ is expressed as a function of $M_{2\nu}$, the resulting lines are essentially identical to those shown in Fig. 8. In other words, the procedure of Ref. [3] eliminates the dependence of $M_{0\nu}$ on the parameter g_{ph} , at least in this model. This important conclusion should be tested in more realistic QRPA calculations.

Why does the prescription of Ref. [3] fail to fully eliminate model-space dependence in this model? There are several possibilities. As we pointed out earlier, the magnitude of the level splitting ϵ used here is unrealistically small. Using larger ϵ moves the large-space lines closer to those of the small space. Also, the interaction here affects only the 0^+ multipole, while in realistic calculations all multipoles are affected to some degree. In any event, even with its shortcomings the procedure is interesting enough here that we find $M_{0\nu} = aM_{2\nu} + b$ independently of the values of both g_{pp} and g_{ph} , with b decreasing as the level splitting increases. Combined with the accuracy of the QRPA in our model, this implies that the procedure gives a lower limit for the exact value of $M_{0\nu}$ provided that the Hamiltonian is corrected to reproduce the exact value of $M_{2\nu}$.

V. CONCLUSIONS

Our most important findings are that (1) calculated 2ν and 0ν decay rates are affected differently by model-space truncation, (2) familiar procedures for finding effective two-body decay operators to correct for truncation help matters but leave substantial room for improvement, and (3) the procedure of Ref. [3] for eliminating model-space dependence in the QRPA helps but does not work as well in our model as in realistic calculations.

Several issues still need to be investigated. How accurate are the QRPA results of Ref. [3] once the renormalization procedure is applied? Ironically, although the QRPA itself is very accurate in our model, almost certainly more accurate than in reality because the model has very collective modes (the pairs), the renormalization procedure leaves more re-

sidual model-space dependence here than in realistic calculations. We therefore cannot really address the question in our model. Another issue we have not addressed is the effects of very-high momentum states on double- β -decay operators. Such effects are usually simulated by the short-range-correlation function f in Eq. (6), but it is not clear how accurate a result is achieved that way. We are currently examining two-body short-range correlations by summing ladder diagrams similar to those that make up the Brueckner G matrix.

Properly treating more-body effects will be harder, both for short-range correlations and the longer-range correlations we investigated here. Finding a good approximation scheme to incorporate them into shell-model calculations is, in our view, the most important problem in the theoretical treatment of double- β decay. Because only the ground states need to be calculated, much of conventional effective-operator theory is superfluous and the biggest payoff may come from pushing Lanczos-diagonalization methods to the largest model spaces possible, leaving only high-momentum correlations to be absorbed into operators.

ACKNOWLEDGMENTS

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APPENDIX

Here we supplement Eqs. (11) and (12) with relations necessary to evaluate matrix elements of charge-changing two-body operators between states of the form $|\mathcal{N}_1, T_1, M_1; \mathcal{N}_2, T_2, M_2\rangle$, corresponding to particles in both sets of levels. Equations (11) and (12) can be used with $\mathcal{N} = \mathcal{N}_1$ (\mathcal{N}_2), $T = T_1$ (T_2), $M = M_1$ (M_2), and the $[1, 1]$ ($[2, 2]$)

\mathcal{F} 's whenever \mathcal{N}_2 (\mathcal{N}_1), T_2 (T_1), and M_2 (M_1) are the same in the bra as in the ket. When those isospin quantum numbers change, we also need (*with* $M'_1 = M_1 + 1$ and $M'_2 = M_2 + 1$ everywhere below)

$$\begin{aligned} & \langle \mathcal{N}_1, T'_1, M'_1; \mathcal{N}_2, T'_2, M'_2 | \mathcal{M}_\kappa | \mathcal{N}_1, T_1, M_1; \mathcal{N}_2, T_2, M_2 \rangle \\ &= \frac{1}{2} \delta_{T_1, T'_1} \delta_{T_2, T'_2} \frac{\sqrt{T_1(T_1+1)T_2(T_2+1)}}{\Omega_1 \Omega_2} \langle T_1 M_1; 1 1 | T_1 M'_1 \rangle \\ & \quad \times \langle T_2 M_2; 1 1 | T_2 M'_2 \rangle \mathcal{F}_\kappa^{ph}[12], \end{aligned} \quad (\text{A1})$$

where the Kronecker δ 's arise from the condition that $\mathcal{N} - T$ be even. When the operator moves pairs from one set of levels to another, finally, we need

$$\begin{aligned} & \langle \mathcal{N}_1 + 1, T'_1, M'_1; \mathcal{N}_2 - 1, T'_2, M'_2 | \mathcal{M}_\kappa | \mathcal{N}_1, T_1, M_1; \mathcal{N}_2, T_2, M_2 \rangle \\ &= \frac{1}{8\Omega_1 \Omega_2} H_{\mathcal{N}_1, T_1, T'_1}^{\Omega_1} H_{\mathcal{N}_2 - 1, T'_2, T_2}^{\Omega_2} \\ & \quad \times \langle T_1 M_1; 1 1 | T'_1 M'_1 \rangle \langle T'_2 M'_2; 1 - 1 | T_2 M_2 \rangle \mathcal{F}_\kappa^{pp}[12], \end{aligned} \quad (\text{A2})$$

and

$$\begin{aligned} & \langle \mathcal{N}_1 - 1, T'_1, M'_1; \mathcal{N}_2 + 1, T'_2, M'_2 | \mathcal{M}_\kappa | \mathcal{N}_1, T_1, M_1; \mathcal{N}_2, T_2, M_2 \rangle \\ &= \frac{1}{8\Omega_1 \Omega_2} H_{\mathcal{N}_1 - 1, T'_1, T_1}^{\Omega_1} H_{\mathcal{N}_2 + 1, T'_2, T_2}^{\Omega_2} \\ & \quad \times \langle T'_1 M'_1; 1 - 1 | T_1 M_1 \rangle \langle T_2 M_2; 1 1 | T'_2 M'_2 \rangle \mathcal{F}_\kappa^{pp}[12], \end{aligned} \quad (\text{A3})$$

where

$$H_{\mathcal{N}, T, T+1}^\Omega = -\sqrt{\frac{(T+1)(2\Omega - \mathcal{N} - T)(\mathcal{N} + T + 3)}{2T + 3}} \quad (\text{A4})$$

and

$$H_{\mathcal{N}, T, T-1}^\Omega = \sqrt{\frac{T(2\Omega - \mathcal{N} + T + 1)(\mathcal{N} - T + 2)}{2T - 1}}. \quad (\text{A5})$$

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