Shell-Model Analysis of the ^{136}Xe Double Beta Decay Nuclear Matrix Elements

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Neutrinoless double beta decay, if observed, could distinguish whether the neutrino is a Dirac or a Majorana particle, and it could be used to determine the absolute scale of the neutrino masses. ^{136}Xe is one of the most promising candidates for observing this rare event. However, until recently there were no positive results for the allowed and less rare two-neutrino double beta decay mode. The small nuclear matrix element associated with the long half-life represents a challenge for nuclear structure models used for its calculation. We report a new shell-model analysis of the two-neutrino double beta decay of ^{136}Xe, which takes into account all relevant nuclear orbitals necessary to fully describe the associated Gamow-Teller strength. We further use the new model to analyze the main contributions to the neutrinoless double beta decay matrix element, and show that they are also diminished.

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Neutrinoless double beta ($0\nu\beta\beta$) decay can only occur by violating the conservation of the total lepton number, and if observed it would unravel physics beyond the standard model (SM) of particle physics and would represent a major milestone in the study of the fundamental properties of neutrinos [1]. Recent results from neutrino oscillation experiments have demonstrated that neutrinos have mass and that the neutrino can oscillate from one flavor to another [2–4]. In addition, they show that the neutrinoless double beta decay process could be used to determine the absolute scale of the neutrino masses, and can distinguish if neutrinos are Dirac or Majorana particles [5]. A key ingredient for extracting the absolute neutrino masses from $0\nu\beta\beta$ decay experiments is a precise knowledge of the nuclear matrix elements (NME) for this process. There is a large experimental effort in the United States and worldwide to investigate the double beta decay of some even-even nuclei [1]. Experimental data for two-neutrino double-beta decay ($2\nu\beta\beta$) to the ground state (g.s.) and excited states already exist for a group of nuclei [6]. There are no confirmed experimental data so far for neutrinoless double-beta decay. The prediction, analysis, and interpretation of experimental results, present and expected, are very much dependent on precise nuclear structure calculations of corresponding transition probabilities.

Although many experimental efforts such as MAJORANA and GERDA [1], are investigating the $\beta\beta$ decay of ^{76}Ge there are very encouraging results related to the $\beta\beta$ decay of ^{136}Xe. For a long time only lower limits for the $2\nu\beta\beta$ half-life were available. Recently, the EXO-200 collaboration reported a precise measurement of this half-life of $2.11 \pm 0.04(\mathrm{stat}) \pm 0.21(\mathrm{syst}) \times 10^{21}$ yr [7,8], and a NME of 0.019 ± 0.002 MeV^{-1} [7,8] extracted using the phase-space factor $G^{2\nu}$ [see Eq. (1)] from Ref. [9]. This large half-life would imply a relatively smaller background for the associated $0\nu\beta\beta$ measurement and EXO. A larger version of EXO-200 designed for reaching this goal, is under consideration [1]. The lower limit for the $0\nu\beta\beta$ half-life reported by EXO-200 is 1.6×10^{25} yr [8]. In addition, the KamLAND-Zen Collaboration reported a $2\nu\beta\beta$ half-life of $2.38 \pm 0.02(\mathrm{stat}) \pm 0.14(\mathrm{syst}) \times 10^{21}$ yr and a lower limit for the $0\nu\beta\beta$ half-life of 5.7×10^{24} yr [10].

Since most of the $\beta\beta$ decay emitters are open-shell nuclei, many calculations of the NME have been performed within the pnQRPA approach and its extensions [11–13]. However, the pnQRPA calculations of the more common two-neutrino double beta decay half-lives, which were measured for about 10 cases [6], are very sensitive to the variation of the g_{pp} parameter (the strength of the particle-particle interactions in the 1^+ channel) [14,15], and this drawback persists in spite of various improvements brought by its extensions, including higher-order QRPA approaches [13]. Although the QRPA methods do not seem to be suited to predict the $2\nu\beta\beta$ decay half-lives, they use the measured $2\nu\beta\beta$ decay half-lives to calibrate the g_{pp} parameters, then use them to calculate the $0\nu\beta\beta$ decay NME [12]. Another method that was recently used to calculate NMEs for most $0\nu\beta\beta$ decay cases of interest is the interacting boson model (IBM-2) [16]. However, a reliable IBM-2 approach for $2\nu\beta\beta$ decay is not yet available.

Recent progress in computer power, numerical algorithms, and improved nucleon-nucleon effective interactions, made possible large-scale configuration-interaction (CI) calculations (also known as shell-model calculations) of the $2\nu\beta\beta$ [17–20] and $0\nu\beta\beta$ decay NME [21,22].

The main advantage of the large-scale shell-model calculations is that they take into account all of the many-body correlations for the orbitals near the Fermi surface. Also, they are less dependent on the effective interaction used, as long as they are based on realistic nucleon-nucleon interactions with minimal adjustments to the single-particle energies and some two-body matrix elements so they reproduce general spectroscopy of the nuclei involved in the decay [22]. Their main drawback is the limitation imposed by the exploding CI dimensions even for limited increase in the size of the valence space used. The most important success of the large-scale shell-model calculations was the correct prediction of the $2\nu\beta\beta$ decay half-life for ^{48}Ca [17,23]. In addition, the CI calculations do not have to adjust any additional parameters; i.e., given the effective interaction and the Gamow-Teller (GT) quenching factor extracted from the overall spectroscopy in the respective mass region, they are able to accurately predict the $2\nu\beta\beta$ decay half-life of ^{48}Ca.

CI methods provide realistic many-body wave functions (w.f.) for many nuclei from ^{16}O to ^{100}Sn and beyond. These wave functions can describe observables related to specific experiments, e.g., for nuclear astrophysics and electroweak interactions with the nucleus. The minimal valence space required for ^{136}Xe involves the $0g_{7/2}1d_{5/2}1d_{3/2}2s_{1/2}0h_{11/2}$ orbitals for protons and neutrons (the $jj55$ model space). There are no spurious center-of-mass (c.m.) states in the $jj55$ model space since the c.m. operator $\vec{R}$ does not connect any of the orbitals. The key is to obtain effective interactions (EI) that can provide energies and wave functions in the $jj55$ model space that are at a similar level of accuracy as those obtained for the sd shell [24] and for the pf shell [25]. The CI $\beta\beta$ decay NME have been reported [18,21,26] with continuous improvements of the EI. These calculations indicate a significant sensitivity of the results to the improving EI. For example, the quenching factor used to describe $2\nu\beta\beta$ NME varies from 0.74 [18] to 0.45 [26], and the $0\nu\beta\beta$ NME varies by a factor of about 3 between Ref. [18] and the more recent Ref. [21]. One of the drawbacks of model spaces such as $jj55$ is that in order to maintain center-of-mass purity they do not include the spin-orbit partners of orbitals such as $0g_{7/2}$ and $0h_{11/2}$. The known effect is that the Ikeda sum rule is not satisfied, indicating that some the Gamow-Teller strength, which is so important for both types of NME, is missing from this model space. For example, in $jj55$, the total sum of the Gamow-Teller strength for ^{136}Xe is 52, compared to the value of 84 expected from the Ikeda sum rule (see also Table I below).

In this Letter we investigate the effects of the missing $0g_{9/2}$ and $0h_{9/2}$ orbitals in $jj55$. This expanded model space that includes seven orbitals for protons and neutrons will be called $jj77$. We consider a hierarchy of approximations in the $jj77$ model space. The two-body matrix elements with good J and T were obtained from the code CENS [27]. The procedure discussed below was used to obtain a Hamiltonian for the $jj77$ model space that we will refer to as $jj77a$. In the first step, the short-range part of the N^{3}LO potential [28] was integrated out using the $V_{\mathrm{low}\,k}$ method [29]. The relative two-body matrix elements were evaluated in a harmonic-oscillator basis with $\hbar\omega = 7.874$ (a value appropriate for ^{132}Sn). In the second step the interaction was renormalized into the $jj77$ model space assuming a ^{100}Sn closed core. The $0g_{9/2}$ orbital was treated as a hole state, while the others are treated as particle states. For the energy denominators we take all orbits in the $jj77$ space to be degenerate, with the other orbitals spaced in units of $\hbar\omega$ above and below. The core-polarization calculation used the $\hat{Q}$-box method included all non-folded diagrams through second-order in the interaction, and sums the folded diagrams to infinite order [30]. Particle-hole excitations up through $4\hbar\omega$ were included. Matrix elements obtained in the proton-neutron basis were transformed to a good-T basis by using the neutron-neutron matrix elements for the $T = 1$ components.

TABLE I. Matrix elements in MeV^{-1} for 2ν decay calculated using the standard quenching factor 0.74 for the Gamow-Teller operator using different number of excitations from $jj55$ to the larger model space. The last column gives the calculated Ikeda sum rule for ^{136}Xe.

$n(0^+)$	$n(1^+)$	$M^{2\nu}$	Ikeda
0	0	0.062	52
0	1	0.091	84
1	1	0.037	84
1	2	0.020	84

The single-particle matrix elements were obtained starting with the $jj55$ model space for a ^{132}Sn closed core. The five single-particle energies for $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ were adjusted to reproduce the experimental values for neutron holes related to the spectrum of ^{131}Sn as given in [31]. The results obtained for the single-particle energies of protons related to the spectrum of ^{133}Sb are in reasonable agreement with experiment [31] except that the $1d_{5/2}$ energy is too high by 1.2 MeV and the $1h_{11/2}$ energy is too high by 2.4 MeV. Reduction of the diagonal two-body matrix elements by 0.3 MeV for these two orbitals improves the agreement with experiment with minimal overall change to the Hamiltonian. The theoretical and experimental spectra for nuclei with up to six protons added and/or four neutrons removed from ^{132}Sn agree within an rms deviation of a few hundred keV. The results are similar to those shown and discussed in the review by Coraggio *et al.* [32]. The adjustment of the single-particle energies to experiment implicitly includes the effects due to three-body interactions of one valence nucleon with two nucleons in the ^{132}Sn core. The three-body interaction of two-valence nucleons with one nucleon in the core is neglected, but it is small, on the order of 100 keV [33].

The two-hole spectrum for ^{130}Sn and the two-particle spectrum for ^{134}Te are in best overall agreement with experiment if the $T = 1$ matrix elements are multiplied by 0.9. The results (experiment vs theory) are (1.28, 1.34) MeV for ^{130}Sn and (1.22, 1.35) MeV for ^{134}Te. For application to the larger $jj77$ model space, the single-neutron hole energy for $0g_{9/2}$ was placed six MeV below the $0g_{7/2}$ energy in ^{131}Sn, and the single-proton particle energy for $0h_{9/2}$ was placed six MeV above the $0h_{11/2}$ energy in ^{133}Sb. Using this interaction, we calculated the excitation energies of the 2^+, 3^+, and 4^+ states of ^{136}Xe and ^{136}Ba and found deviations from the experimental values smaller than 200 keV for both $n = 0$ and $n = 1$ (definition of n is given below).

The $2\nu\beta\beta$ half-life for the transition from the 0^+ g.s. of ^{136}Xe to the 0^+ g.s. of ^{136}Ba can be calculated [9] using

$$[T_{1/2}^{2\nu}]^{-1} = G^{2\nu}|M_{\rm GT}^{2\nu}(0^+)|^2, \tag{1}$$

where $G^{2\nu}$ is a phase space factor, and $M_{\rm GT}^{2\nu}(0^+)$ is the $2\nu\beta\beta$ matrix element given by the double Gamow-Teller sum

$$M_{\rm GT}^{2\nu}(0^+) = \sum_k \frac{\langle 0_f^+\|\sigma\tau^-\|1_k^+\rangle\langle 1_k^+\|\sigma\tau^-\|0_i^+\rangle}{E_k + E_0}. \tag{2}$$

Here, E_k is the excitation energy of the 1_k^+ state of ^{136}Cs and $E_0 = (1/2)Q_{\beta\beta}(0^+) + \Delta M = 1.31$ MeV, where we used the recently reported [34] Q value $Q_{\beta\beta}(0^+) = 2.458$ MeV corresponding to the $\beta\beta$ decays to the g.s. of ^{136}Ba; ΔM is the ^{136}Cs-^{136}Xe mass difference. For the $2\nu\beta\beta$ of ^{136}Xe a $G^{2\nu}$ of 1.279×10^{-18} yr^{-1} MeV^2 [9] was used to extract [7,8] the $M_{\rm GT}^{2\nu}(0^+)$ of 0.019 MeV^{-1}. Newer values of $G^{2\nu}$ were recently proposed [35]. They depend on the fourth power of the axial coupling constant g_A, which may be quenched in heavy nuclei. For $g_A = 1.254$ [9], the new value [35] of $G^{2\nu}$ is 0.925×10^{-18} yr^{-1} MeV^2, corresponding to a $M_{\rm GT}^{2\nu}(0^+)$ of 0.023 MeV^{-1}.

In Ref. [20] we fully diagonalized 250 1^+ states in the intermediate nucleus to calculate the $2\nu\beta\beta$ decay NME for ^{48}Ca. This procedure can be used for somewhat heavier nuclei using the J-scheme shell-model code NUSHELLX [36], but for cases with very large dimensions one needs an alternative method. Here we used a novel improvement [37] of the known strength-function approach [17], which is very efficient for cases with large dimensions. such as $jj55$ and $jj77$. For example, to calculate the NME for the decays of ^{128}Te in $jj55$ and ^{136}Xe in $jj77$ ($n = 1$ for 0^+ and $n = 2$ for 1^+ in Table I) one needs to solve problems with m-scheme dimensions of up to the order of up to ten billions.

The result when restricting the $jj77$ model space to $jj55$ is given on the first line in Table I. As already mentioned, the Ikeda sum rule is only 52 rather then 84, indicating that not all GT strength is available in the $jj55$ space. Although the excitation energies of the GT strength distribution are reasonably well reproduced, the GT operator $\sigma\tau$ has to be multiplied by a quenching factor due to correlations beyond the $jj77$ model space. In one major harmonic-oscillator shell calculations, such as the sd or pf, this quenching factor was determined to be 0.74–0.77 (see, e.g., Refs. [38,39]), which is consistent with that obtained in second-order perturbation theory [40,41]. Here we use 0.74. Ref. [26] suggests that one should use a lower quenching factor in the $jj55$ model space, 0.45, to get an NME consistent with the recent experimental data. Indeed, our matrix element in the $jj55$ model space becomes 0.022 MeV^{-1} when 0.45 is used.

However, it would be important to check if the missing spin-orbit partners are responsible for the larger result; the relative phases in Eq. (2) could lead to large cancellations. Here we consider the larger $jj77$ model space, where we can allow a few particles (n) to be excited from the $0g_{9/2}$ orbital or into the $0h_{9/2}$ orbital, relative to $jj55$. Table I also presents the NME for different combinations of the allowed n for the initial and final 0^+ states and the intermediate 1^+ states. One can see that when n is 1 for the 0^+ states and 2 for the 1^+ states, the NME decreases almost to the experimental value without the need of artificially reducing the quenching factor. In addition, the Ikeda sum rule is always satisfied in the larger model space.

One should mention that in the $jj77$ model space the wave functions could have c.m. spurious components. We checked our initial and final 0^+ g.s. w.f. and we found negligible (less than 3 keV) spurious contribution to expectation values of the c.m. Hamiltonian. We did not check the amount of c.m. spuriously in the intermediate 1^+ states, but it's unlikely to be large because the strength function method [37] performs a small number of Lanczos iterations (about 30) starting with a door-way state obtained by applying the GT operator on the largely nonspuroius 0^+ state. As a further check we compared the GT strength (BGT) for the transition from the g.s. of ^{136}Xe to the first 1^+ state in ^{136}Cs with recent experimental data [42]. Table I of Ref. [42] provides a BGT of 0.149(21) for the first 1^+ state at 0.59 MeV, but we learned [43] that this will be updated to 0.24(7). Our BGT is 0.51 in the $jj55$ model space, but 0.34 in the largest $jj77$ model space, much closer to the experimental value. Although we cannot verify if the calculations are converged, we can conclude that including all spin-orbit partners is essential for a good description of the $2\nu\beta\beta$ for ^{136}Xe.

Having tuned our nuclear structure techniques for the description of the two-neutrino double-beta decay, we calculate the NME necessary for the analysis of the neutrinoless double-beta decay half-life ^{136}Xe [22,44]. Considering the most important mechanisms that could be responsible for $0\nu\beta\beta$ decay [45], one can write the $0\nu\beta\beta$ half-life as

TABLE II. Matrix elements for 0ν decay using two SRC models [13], CD-Bonn (SRC1), and Argonne (SRC2). The upper values of the neutrino physics parameters η_j^{up} in units of 10^{-7} are calculated using the $G^{0\nu}$ from Refs. [9,35].

		$M_\nu^{0\nu}$	$M_N^{0\nu}$	$M_{\lambda'}^{0\nu}$	$M_{\tilde{q}}^{0\nu}$
$n=0$	SRC1	2.21	143.0	1106	206.8
	SRC2	2.06	98.79	849.0	197.2
$n=1$	SRC1	1.46	128.0	1007	157.8
	$\lvert\eta_j^{up}\rvert$ [9]	8.19	0.093	0.012	0.075
	$\lvert\eta_j^{up}\rvert$ [35]	9.02	0.103	0.013	0.083

$$[T_{1/2}^{0\nu}]^{-1} = G^{0\nu}|\eta_{\nu L}M_\nu^{0\nu} + \eta_N M_N^{0\nu} + \eta_{\lambda'}M_{\lambda'}^{0\nu} + \eta_{\tilde{q}}M_{\tilde{q}}^{0\nu}|^2, \quad (3)$$

where $M_j^{0\nu}$ NME and η_j are neutrino physics parameters for light neutrino exchange ($j=\nu$), heavy neutrino exchange ($j=N$), gluino exchange ($j=\lambda'$), and squark-neutrino mechanism ($j=N$) as described in Refs. [44,45]. $G^{0\nu}$ is a phase space factor tabulated in several publications. One widely used value [9] is 43.7×10^{-15} yr^{-1}. A recent publication [35] proposes 36.05×10^{-15} yr^{-1}, which is about 20% lower. The results for the NME calculated in the closure approximation are presented in Table II using the $n=0$ and $n=1$ 0^+, w.f. (see Table I). Two recent short-range correlation (SRC) parameterizations are used [13,22]. No quenching of the bare transition operator was used [22,46]. The $M_\nu^{0\nu}$ for the $jj55$ model space ($n=0$) is consistent with other recent shell-model results [21]. The NME for the other three mechanisms calculated within a shell-model approach are reported here for the first time. The NME in the largest space ($n=1$) are 10%–30% lower. These results suggest that the inclusion of the spin-orbit partners, which proved to be significant for a good description of the $2\nu\beta\beta$ NME, are also important for a reliable description of the $0\nu\beta\beta$ NME. In addition, they indicate that the net effect is a decrease of the NME, which seems to be in agreement with recent QRPA calculations [47], rather than the increase relative to the $jj55$ value found in [48], suggesting a trend towards the larger results reported by other QRPA, IBM-2, Projected Hartree-Fock Bogoliubov [49], and generator coordinate method [50] calculations. We performed similar calculations of the NME for the transition of the ^{134}Te g.s. to the ^{134}Xe g.s., for which $n=2$ can be included. When $n=2$ is included the $T=1$ (pairing) part of the Hamiltonian needs to be reduced by 20% in order to describe the energies of ^{130}Sn and ^{134}Te. We found that the $M_\nu^{0\nu}$ NME is somewhat closer to the $jj55$ value but still smaller, while the $2\nu\beta\beta$ NME remains about the same. These results for the nearby semi-magic ^{134}Te suggest that the NME for ^{136}Xe might not change significantly when $n>1$ truncations are considered for the 0^+ states, provided that the effective interaction is adjusted to describe the spectroscopy of the nuclei involved. Table II also presents upper limits for the neutrino physics parameters $|\eta_j^{up}|$ under the assumption of single mechanism dominance. They were obtained from Eq. (3) using the lower limit for the half-life 1.6×10^{25} yr from Ref. [8] and the two phase space factors of Refs. [9,35]. Using the upper limits for $|\eta_{\nu L}| = m_{\beta\beta}/m_e$ one can extract an upper limit for the effective neutrino mass $m_{\beta\beta}$ of 0.42–0.46 eV.

In conclusion, we reported a new shell-model analysis of the two-neutrino double beta decay of ^{136}Xe that takes into account all relevant nuclear orbitals necessary for a good description of the Gamow-Teller strength. We show that this extension of the valence space can account for the small NME without recourse to an artificially small quenching factor. We also show that it could lead to smaller NME for the most interesting neutrinoless double beta decay mode.

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