Novel 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 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 result for the allowed and less rare two-neutrino double beta decay mode. The small nuclear matrix element associated with the small 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 half-life, 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 Standard Model (SM) of particle physics and it 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 they mix [2-4]. In addition, they show that neutrinoless double beta decay process could be used to determine the absolute scale of the neutrino masses, and can distinguish whether neutrino is a Dirac or a Majorana particle [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 US 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 is 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 the precise nuclear structure calculations of corresponding transition probabilities.

Although many experimental efforts in US and worldwide, such as MAJORANA and GERDA [1], are pinpointing to 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 there were available only upper limits for the $2\nu\beta\beta$ half-life. Recently, the EXO-200 collaboration reported [7, 8] a precise measurement of this half life of $2.11 \pm 0.04(stat) \pm 0.21(sys) \times 10^{21}$ yr, corresponding to a NME of $0.019$ MeV$^{-1}$. This large half-life would imply a 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 [9]. The upper limit for the $0\nu\beta\beta$ half-life reported by EXO-200 is $1.6 \times 10^{25}$ yr [8]. In addition, the KamLAND-Zen collaboration reported a $2\nu\beta\beta$ half-life of $2.38 \pm 0.02(stat) \pm 0.14(sys) \times 10^{21}$ yr and a upper-limit for the $0\nu\beta\beta$ half-life of $5.7 \times 10^{24}$ yr [9].

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 [10-12]. However, the pnQRPA calculations of the more common two-neutrino double beta decay observable, 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) [13-14], and this drawback persists in spite of various improvements brought by its extensions, including higher-order QRPA approaches [12]. Although the QRPA methods do not seem to be suited to predict the $2\nu\beta\beta$ decay half-lives, they can use the measured $2\nu\beta\beta$ decay half-lives to calibrate the $g_{pp}$ parameters that are further used to calculate the $0\nu\beta\beta$ decay NME [11]. Another method that was recently used to calculate NMEs for most $0\nu\beta\beta$ decay cases of interest is the Interactive Boson Model (IBA-2) [15]. However, a reliable IBA-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 $2\nu\beta\beta$ [16] and $0\nu\beta\beta$ decay NME [20, 21]. 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 also less dependent on the effective interaction used, as long as these 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 [21]. 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 [16, 22]. 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 reliably 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 the electro-weak interactions with the nucleus. The minimal valence space required for $^{136}$Xe involves the $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ orbitals for protons and neutrons (the $jj55$ model space). There are no spurious center-of-mass (CoM) states in the $jj55$ model space since the CoM operator $\hat{R}$ does not connect any of the orbitals. The key is to obtain effective interactions (EI) that can provide energies and wave functions in $jj55$ model space that are at a similar level of accuracy as those obtained for the $sd$-shell [23] and for the $pf$-shell [24]. The CI $\beta\beta$ decay NME were reported over the years [17, 20, 25] considering continuous improvements of the EI. These calculations indicate a significant sensitivity of the results to the improving EI. For example, the quenching factors used to describe $2\nu\beta\beta$ NME varies from 0.74 to 0.45 [25], and the $0\nu\beta\beta$ NME varies by a factor of about 3 between Ref. [17] and the more recent Ref. [24]. One of the drawbacks of model spaces such as $jj55$ is that in order to maintain center-of-mass purity they do not include all 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 $jj55$ typical Ikeda sum-rule for $^{136}$Xe is 52, while the expected result is 84 (see also Table I below).

In this letter we investigate the effect of extending the model space to $jj77$ by including the effects of the missing $0g_{9/2}$ and $0h_{9/2}$ orbitals. The two-body matrix elements with good $J$ and $T$ were obtained from the code CENS [26]. 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 [27] was integrated out using the $V_{\text{low}}k$ method [28]. 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 other 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 and includes all non-folded diagrams through second-order in the interaction and sums up the folded diagrams to infinite order [29]. 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.

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 [30]. The results obtained for the single-particle energies of protons related to the spectrum of $^{132}$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 adjustment of the single-particle energies to experiment implicitly includes most of the effects due to three-body interactions.

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.

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 [31] using

$$\left[T_{1/2}^{2\nu}\right]^{-1} = G^{2\nu} |M_{2\nu}^{GT}(0^+)|^2,$$  \hspace{1cm} (1)  

where $G^{2\nu}$ is a phase space factor that for the the $2\nu\beta\beta$ of $^{136}$Xe is $1.279 \times 10^{-18}$ yr$^{-1}$ MeV$^{2}$ [31]. $M_{2\nu}^{GT}(0^+)$ is the $2\nu\beta\beta$ matrix element given by the double Gamow-Teller sum

$$M_{2\nu}^{GT}(0^+) = \sum_{k} \frac{\langle 0^+_f | \sigma \tau^- | 1^+_i \rangle \langle 1^+_i | \sigma \tau^- | 0^+_i \rangle}{E_k + E_0}.$$  \hspace{1cm} (2)
Here $E_k$ is the excitation energy of the $1^+_k$ state of $^{136}$Cs and $E_0 = \frac{1}{2} Q_{\beta\beta}(0^+) + \Delta M = 1.31$ MeV, where we used the recently reported$^{[32]}$ $Q$-value $Q_{\beta\beta}(0^+) = 2.458$ MeV corresponding to the $\beta$ decays to the g.s. of $^{136}$Ba; $\Delta M$ is the $^{136}$Cs - $^{136}$Xe mass difference.

In Ref. $^{[19]}$ 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$^{[33]}$, but for cases with large dimension one needs an alternative method. Here we used a novel improvement$^{[34]}$ of the known strength-function approach$^{[16]}$, which is very efficient for large model cases, 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 the order of to ten billion.

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 typical one major-shell calculations, such as the $sd$ or $pf$, this quenching factor was determined to be around 0.74-0.77 (see e.g. Ref. $^{[33, 30]}$) that is consistent with that obtained in second-order perturbation theory$^{[37, 38]}$. Here we use 0.74. Ref. $^{[25]}$ 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 elements 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, but we could only allowed few $n$ particle being excited from the $0g_{9/2}$ orbital or to the $h_{9/2}$ orbital, relative to $jj55$. Table I also presents the NME for different combinations.

TABLE I: Matrix elements in MeV$^{-1}$ for $2\nu$ 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. Last column indicate the calculated Ikeda sum-rule for $^{136}$Xe.

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

Here we use 0.74. Ref. $^{[25]}$ suggests that one should use a lower quenching factor in the $jj55$ model space, but we could only allowed few $n$ particle being excited from the $0g_{9/2}$ orbital or to the $h_{9/2}$ orbital, relative to $jj55$. Table I also presents the NME for different combinations.

TABLE II: Matrix elements for $0\nu$ decay using two SRC models$^{[12]}$, CD-Bonn (SRC1) and Argonne (SRC2). The upper values of the neutrino physics parameters $\eta^\nu_j$ in units of $10^{-7}$ are calculated using the $G^\nu\nu$ from Refs. $^{[31]}$ and $^{[43]}$.

| $n$ | $M^\nu\nu_{\nu\beta\beta}$ | $M^\nu\nu_{\nu\beta\beta}$ | $M^\nu\nu_{\nu\beta\beta}$ | $M^\nu\nu_{\nu\beta\beta}$ |
|-----|------------------------|------------------------|------------------------|------------------------|
| 0   | SRC1       | 2.21                   | 143.0                  | 1106.                  | 206.8                  |
| 1   | SRC2       | 2.06                   | 98.79                  | 849.0                  | 197.2                  |
|     | $\eta^\nu_{\nu\beta\beta}$ | $\eta^\nu_{\nu\beta\beta}$ | $\eta^\nu_{\nu\beta\beta}$ | $\eta^\nu_{\nu\beta\beta}$ |
| 1   | SRC1       | 1.46                   | 128.0                  | 1007.                  | 157.8                  |
| 2   | SRC1       | 8.19                   | 0.093                  | 0.012                  | 0.075                  |
| 3   | SRC1       | 9.02                   | 0.103                  | 0.013                  | 0.083                  |

One should mention that in the $jj77$ model space the wave functions could have CoM 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 CoM Hamiltonian. We did not check the amount of CoM spuriously in the intermediate $1^+$ states, but it’s unlikely to be large because the strength function method$^{[34]}$ performs a small number of Lanczos iterations (about 30) starting with a doorway state obtained by applying the GT operator on the largely nonspurious $0^+$ 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$^{[39]}$. Table I of Ref. $^{[43]}$ provides a BGT of 0.149(21) for the first $1^+$ state at 0.59 MeV, but we learned$^{[40]}$ 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 to getting an accurate description of the two-neutrino double-beta decay we calculate the NME necessary for the analysis of the neutrinoless double-beta decay half-life $^{130}$Xe$^{[21, 41]}$. Considering the most important mechanisms that could be responsible for $0\nu\beta\beta$ decay$^{[42]}$ one can write the $0\nu\beta\beta$ half-life
\[
\left( T_{1/2}^{0\nu} \right)^{-1} = T^{0\nu} \left| \eta_{\nu \nu L} M^{0\nu}_{\nu} + \eta_N M^{0\nu}_{N} + \eta_q M^{0\nu}_{q} \right|^2, \tag{3}
\]

where \( M^{0\nu}_{j} \) NME and \( \eta_j \) neutrino physics parameters for light neutrino exchange \((j = \nu)\), heavy neutrino exchange \((j = N)\), gluino exchange \((j = N')\) and squark-neutrino mechanism \((j = N)\) are described in Refs. \[41\] \[42\]. \( T^{0\nu} \) is a phase space factor tabulated in several publications. One widely used value \[31\] is \( 36.05 \times 10^{-15} \text{ yr}^{-1} \), which is about 20\% lower. The results for the NME calculated in the closure approximation are presented in Table \[\text{II}\] using the upper limits for the neutrino physics parameters \( \eta_{\nu \nu L} \) \[43\]. Two recent short-range correlations (SRC) parametrizations are used \[12\] \[21\]. No quenching of the bare transition operator was used \[21\] \[44\]. The \( M^{0\nu}_{jj} \) for the \( jj55 \) model space \((n = 0)\) is consistent with other recent shell-model results \[20\]. 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, could be also very 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 rather than an increase (an assumption often used to understand the lower shell-model value relative to the results of other methods, such as QRPA, IBA-2, Projected Hartree-Fock Bogoliubov \[43\], and Generator Coordinate Method \[40\]). Table \[\text{II}\] also presents upper limits for the neutrino physics parameters \( \eta^{\nu\nu} \) under the assumption of single mechanism dominance. They were obtained from Eq. \[3\] using the lower limit for the half-life \( 1.6 \times 10^{25} \text{ yr} \) from Ref. \[8\] and the two phase space factors of Refs. \[31\] \[43\]. Using the upper limits for \( \eta_{\nu \nu L} \), 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 \(^{136}\text{Xe}\) 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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