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Accurate shell-model nuclear matrix elements for neutrinoless double- β decay

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We investigate a novel method of accurate calculation of the neutrinoless double- β decay shell-model nuclear matrix elements for the experimentally relevant case of ^{76}Ge . We demonstrate that with the new method the nuclear matrix elements have perfect convergence properties and, using only the first 100 intermediate states of each spin, the matrix elements can be calculated with better than 1% accuracy. Based on the analysis of neutrinoless double- β decays of ^{48}Ca , ^{82}Se , and ^{76}Ge isotopes, we propose a new method to estimate the optimal values of the average closure energies at which the closure approximation gives the most accurate nuclear matrix elements. We also analyze the nuclear matrix elements for the heavy-neutrino-exchange mechanism, and we show that our method can be used to quench contributions from different intermediate spin states.

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Observation of neutrinoless double- β ($0\nu\beta\beta$) decay will have profound implications in modern physics. It will prove that neutrino and antineutrino are identical particles (Majorana fermions), provide evidence for lepton-number violation, and help to determine the absolute scale of neutrino masses. In other words, it will change our understanding of Nature significantly.

In this Rapid Communication, we analyze the $0\nu\beta\beta$ decay of ^{76}Ge in a shell-model approach. From an experimental point of view, ^{76}Ge is one of the most promising and important $0\nu\beta\beta$ decay candidates. The most sensitive limits on $0\nu\beta\beta$ -decay half-lives have been obtained from germanium-based experiments: the Heidelberg-Moscow experiment [1], the International Germanium experiment [2], and the GERDA-I experiment [3]. ^{76}Ge is the only isotope for which an observational claim has been made (though it was not accepted by the double-beta decay community) [4, 5]. GERDA-II [6] and MAJORANA DEMONSTRATOR [7], the second generation of the germanium-based experiments, are in progress.

Interpretation of the experimental results and planning of new experiments require an accurate analysis of the $0\nu\beta\beta$ decay process and the corresponding nuclear matrix elements (NME). Various theoretical models have been used for the NME calculations, including the Quasi-particle Random Phase Approximation (QRPA) [8–10], the Interacting Shell Model (ISM) [11, 12], the Interacting Boson Model (IBM-2) [13], the Generator Coordinate Method (GCM) [14], and the Projected Hartree-Fock Bogoliubov model (PHFB) [15].

A $0\nu\beta\beta$ decay process can be presented as a transition from the ground state of an initial nucleus to an arbitrary state of the intermediate nucleus and then transition to the ground state of the final nucleus. In an exact approach one needs to calculate all the intermediate states which can be a very demanding task. To avoid this computational challenge the closure approximation is usually introduced [16]. In the closure approximation the energies of the intermediate states are replaced with a constant value (closure energy), which allows the use of completeness to remove the sum over the intermedi-

ate states so that no information about the intermediate states is required.

In this Rapid Communication, we present calculations of the NME for $0\nu\beta\beta$ decay of ^{76}Ge in the shell-model approach beyond closure approximation. Going beyond closure requires knowledge of a large number of the intermediate nuclear states. In the case of ^{76}Ge , the intermediate nucleus ^{76}As , being considered in a realistic model space, has about 1.5×10^8 states. Shell-model calculations for such a large number of nuclear states are practically impossible. To avoid the unmanageable computational costs, we use the mixed method [17, 18] in which the intermediate states are ordered according to their energies and a state cutoff parameter N is introduced, so that all the intermediate states below the cutoff parameter are taken into account exactly, i.e. in a non-closure manner. The states which are above the cutoff are included within the closure approximation. Defined in such a way, the mixed NME depend on both the state cutoff parameter N and the closure energy. The mixed method was carefully tested on the fictitious cases of ^{44}Ca and ^{46}Ca , where all the intermediate states can be obtained, and then on the realistic case of ^{48}Ca , where it is possible to get the first 500 intermediate states for each spin and parity J^π [17]. It was shown that the mixed NME converge much faster with increasing the state cutoff parameter N compared to the nonclosure matrix elements. It was also shown that the mixed NME have very weak dependence on the closure energy, which makes this method more accurate compared to the closure approximation. Finally, the mixed method was successfully used to calculate the $0\nu\beta\beta$ decay of ^{82}Se where the first 250 intermediate states for each J^π were calculated [18]. It was shown that in order to achieve a 1% accuracy in the $0\nu\beta\beta$ NME it is possible to consider only a small number of intermediate states: one needs about 20 intermediate states for each J^π for the $0\nu\beta\beta$ decay of ^{48}Ca and about 60 states for the $0\nu\beta\beta$ decay of ^{82}Se , while the corresponding total number of the intermediate states for these cases are about 10^5 and 10^7 . For ^{76}Ge , about 100 intermediate states of nucleus ^{76}As for each J^π is required to provide a 1% accuracy for the $0\nu\beta\beta$ matrix

elements. In calculations we use the shell model code NuShellX@MSU [19], the $jj44$ model space, which consist of the nucleus ^{56}Ni as a core and the $f_{5/2}$, $p_{3/2}$, $p_{1/2}$, and $g_{9/2}$ single-particles orbitals, and the JUN45 effective interaction [20].

We demonstrate that the mixed method allows us to obtain practically exact values for the $0\nu\beta\beta$ NME in the sense of going beyond the closure approximation. There are still uncertainties associated, for example, with the way the shell model treats the short-range correlations (SRC), the restriction of the model space, and the effective interaction. However, since we know the exact (beyond closure) NME we can compare them with the closure NME and find optimal values for the average closure energies at which the closure approximation provides the most accurate NME. We have also calculated the optimal closure energies for the $0\nu\beta\beta$ decays of ^{48}Ca , ^{82}Se , and ^{76}Ge isotopes. One can expect a 7-10% growth in the absolute values of the closure NME using our optimal closure energies instead of the commonly accepted ones [21]. We also discuss contributions of the heavy neutrino-exchange mechanism to the $0\nu\beta\beta$ decay rate of ^{76}Ge [8, 11, 22].

Assuming the light neutrino-exchange mechanism, the decay rate of a $0\nu\beta\beta$ decay process can be written as [8]

$$\left[T_{1/2}^{0\nu}\right]^{-1} = G^{0\nu} |M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta} \rangle}{m_e}\right)^2, \quad (1)$$

where $G^{0\nu}$ is the phase-space factor [23], $M^{0\nu}$ is the nuclear matrix element, m_e is the electron mass, and $\langle m_{\beta\beta} \rangle$ is the effective neutrino mass, which depends on the neutrino masses m_k and the elements of neutrino mixing matrix U_{ek} [8]. The nuclear matrix element $M^{0\nu}$ is usually presented as a sum of three terms: Gamow-Teller ($M_{GT}^{0\nu}$), Fermi ($M_F^{0\nu}$), and tensor ($M_T^{0\nu}$) nuclear matrix elements (see, for example, Refs. [17, 18, 24]).

In the case of $0\nu\beta\beta$ decay of ^{76}Ge , the matrix elements can be presented as an amplitude for the transitional process where the ground state $|i\rangle$ of the initial nucleus ^{76}Ge changes into an intermediate state $|\kappa\rangle$ of the nucleus ^{76}As and then to the ground state $|f\rangle$ of the final nucleus ^{76}Se ,

$$M_\alpha^{0\nu} = \sum_\kappa \sum_{1234} \langle 13 | \mathcal{O}_\alpha | 24 \rangle \langle f | \hat{c}_3^\dagger \hat{c}_4 | \kappa \rangle \langle \kappa | \hat{c}_1^\dagger \hat{c}_2 | i \rangle. \quad (2)$$

Here the sum over κ spans all the intermediate states $|\kappa\rangle$, indices 1,2,3, and 4 correspond to the single-particle quantum numbers, label α describes different terms in the total NME (1): Gamow-Teller ($\alpha = GT$), Fermi ($\alpha = F$), and tensor ($\alpha = T$). The operators \mathcal{O}_α carry all the details of a $0\nu\beta\beta$ decay process, they explicitly depend on the intermediate-state energy E_κ , $\mathcal{O}_\alpha = \mathcal{O}_\alpha(E_0 + E_\kappa)$, through the energy denominators in perturbation theory. The actual form of the \mathcal{O}_α operators can be found in Ref. [17]. Here, we would like only to emphasize the energy dependence of these operators. The constant $E_0 = [E_{gs}(^{76}\text{As}) - E_{gs}(^{76}\text{Ge})] Q_{\beta\beta}/2 \approx 1.943 \text{ MeV}$.

Exact calculation of the NME (2) can be problematic due to the sum over a large number of intermediate states. One way to proceed in this situation is to use the *closure* approximation, in which the energies of intermediate states are replaced by a constant value so that $\mathcal{O}_\alpha(E_0 + E_\kappa) \rightarrow \tilde{\mathcal{O}}_\alpha \equiv \mathcal{O}_\alpha(\langle E \rangle)$, where $\langle E \rangle$ is the closure energy. Values of $\langle E \rangle$ from Ref. [21] are frequently used.

To go beyond the closure approximation, a *nonclosure* approach can be considered. In this approach, the sum over intermediate states κ in Eq. (2) is restricted by a finite cutoff parameter N . Success of the nonclosure approach is defined by the convergence properties of NME as a function of N . The nonclosure approach cannot be directly used for the heavier cases, such as $0\nu\beta\beta$ decay of ^{82}Se and ^{76}Ge , where only a few hundred intermediate states of each spin J can be calculated.

In the *mixed* method, the intermediate states below the cutoff parameter N are taken into account within the nonclosure approach, while the states above the N are included within the closure approach. For more details see Refs. [17, 18].

The nonclosure approach allows us to calculate the $0\nu\beta\beta$ decay NME for fixed spin and parity J^π of the intermediate states $|\kappa\rangle$,

$$M_\alpha^{0\nu}(J) = \sum_{\kappa, J_\kappa=J} \langle 13 | \mathcal{O}_\alpha | 24 \rangle \langle f | \hat{c}_3^\dagger \hat{c}_4 | \kappa \rangle \langle \kappa | \hat{c}_1^\dagger \hat{c}_2 | i \rangle, \quad (3)$$

where the sum over κ spans all the intermediate states with given spin and parity J^π . This J decomposition can be obtained only within a nonclosure approach.

We also analyze the nuclear matrix elements for the right-handed heavy-neutrino exchange mechanism, whose corresponding contribution to the total decay rate can be written as

$$\left[T_{1/2}^{0\nu}\right]_{\text{heavy}}^{-1} = G^{0\nu} |M_N^{0\nu}|^2 |\eta_{NR}|^2, \quad (4)$$

where the heavy neutrino-exchange matrix elements $M_N^{0\nu}$ have the structure similar to the light neutrino-exchange NME, while the parameter η_{NR} depends on the heavy neutrino masses (for more details see, for example, Ref. [11]). One difference between the heavy and light neutrino-exchange mechanisms is that the heavy neutrino-exchange NME do not depend on the energy of intermediate states. Thus for the heavy neutrino-exchange mechanism the closure approach provides the exact matrix elements.

First, we studied the convergence properties of the $0\nu\beta\beta$ decay NME of ^{76}Ge . $N = 100$ is the maximum number of states we are able to calculate in ^{76}As with an computational effort of about $500000 \text{ CPU} \times \text{hour}$. In the mixed method, the states above the cutoff parameter N are included within the closure approximation which makes the mixed NME dependent on the closure energy $\langle E \rangle$. However this dependence is not strong. For $N = 0$ (the closure approximation), it results in a 10% uncertainty in the total NME [24]. When the cutoff parameter

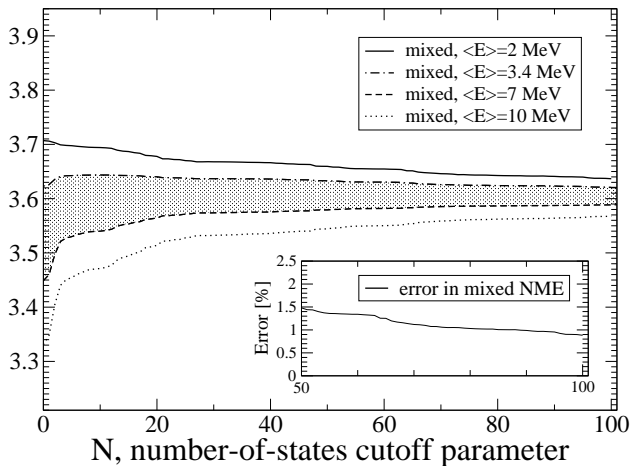


FIG. 1: Dependence of mixed NME (light-neutrino exchange) on the cutoff parameter N calculated for different average closure energies $\langle E \rangle$. The main panel: $\langle E \rangle = 2$ MeV (solid

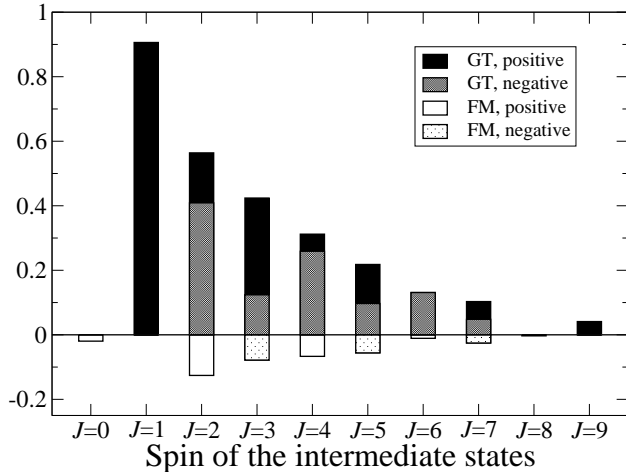


FIG. 2: J decomposition: contributions of the intermediate states $|\kappa\rangle$ with certain spin and parity J^π to the nonclosure Gamow-Teller (dark colors) and Fermi (light colors) matrix elements for the $0\nu\beta\beta$ decay of ^{76}Ge (light-neutrino exchange). Solid black and white bars correspond to the positive-parity states, while shaded bars represent the states with negative parity. The CD-Bonn SRC parametrization was used.

increases this dependence weakens relatively fast. Figure 1 shows the convergence properties of the mixed NME in an enhanced form and how these properties change when the closure energy varies. The solid, dash-dotted, dashed, and dotted lines in the figure present the mixed NME calculated with $\langle E \rangle$ equals to 2, 3.4, 7, and 10 MeV, respectively. If we restrict the range of possible closure energies to be from 3.4 MeV to 7.0 MeV (which is quite reasonable since one curve approaches the final NME from above and the other approaches it from below, so the true NME should be confined somewhere in be-

tween) then the corresponding shaded area on the main panel gives us the uncertainty in the mixed NME. We can see how the uncertainty goes down when the cutoff parameter N increases. The corresponding relative error in the mixed matrix elements is presented by the insert in Figure 1. It shows that it is sufficient to use only the first 100 nuclear states for each J^π of ^{76}As to obtain the $0\nu\beta\beta$ decay NME of ^{76}Ge within a 1% accuracy.

Figure 2 presents the J decomposition (see Eq. (3)) of the nonclosure NME. All the Gamow-Teller matrix elements are positive and all the Fermi matrix elements are negative. If we neglect the tensor NME (which are actually small), then the total height of each bar corresponds to the total nuclear matrix element calculated for each spin J in Eq. (3). We can see that all the spins contribute coherently to the total NME. The contribution of $J = 1$ is dominating, but it provides only about 30% of the total value. If we include only the $J = 1$ intermediate states then we will lose about 70% of the total matrix element and about 91% of the decay rate. Table I summarizes the results for the light-neutrino-exchange NME $0\nu\beta\beta$ decay of ^{76}Ge calculated for different SRC parametrization sets [24]. The mixed total matrix element is about 7% percent greater than the total closure NME. This increase is consistent with similar calculations [17, 18, 25].

TABLE I: Mixed and closure (the last column) NME for the $0\nu\beta\beta$ decay of ^{76}Ge (light-neutrino exchange) calculated with different SRC parametrizations schemes [24]. The closure NME were calculated for a standard closure energy of $\langle E \rangle = 9.41$ MeV [21].

SRC	$M_{GT}^{0\nu}$	$M_F^{0\nu}$	$M_T^{0\nu}$	$M_{total}^{0\nu}$	$M_{closure}^{0\nu}$
None	3.06	-0.63	-0.01	3.45	3.24
Miller-Spencer	2.45	-0.44	-0.01	2.72	2.55
CD-Bonn	3.15	-0.67	-0.01	3.57	3.35
AV18	2.98	-0.62	-0.01	3.37	3.15

It should be noted that the $jj44$ model space is incomplete because the $f_{7/2}$ and $g_{7/2}$ orbitals are missing. As a result the Ikeda sum rule is not satisfied and some contributions from the Gamow-Teller NME with $J^\pi = 6^+, 8^+$ and from the Fermi NME $J^\pi = 1^-$ are missing. Looking at Fig. 2, it seems safe to suggest that the missing contributions are not very large. However, this deficiency is reflected in the two-neutrino NME, which requires a quenching factor of about 0.64, smaller than the usual 0.74, to describe the experimental data (see also Table 2 of Ref. [26]). Although the spin-isospin operators entering the $0\nu\beta\beta$ decay NME are different from pure Gamow-Teller, some authors (see e.g. Ref. [27]) advocate using appropriate quenching factors for contributions coming from different spins of the intermediate states. The most important are those from $J^\pi = 1^+$ states, which represent about 30% of the total NME, and from $J^\pi = 2^-$ states [27], which represents about 15% of the total NME.

It would be interesting to investigate whether quenching factors obtained from other processes, such as $2\nu\beta\beta$ decay and charge-exchange reactions, quench the corresponding contributions to the $0\nu\beta\beta$ decay NME. For example, if one uses a quenching factor of 0.64^2 for the contribution from the $J^\pi = 1^+$ states and 0.40^2 for the contribution of the $J^\pi = 2^-$ [27], one gets for CD-Bonn SRC a NME of 2.369 rather than 3.572 (see Table I). One can view this as a lower limit NME within our approach.

Since we can calculate both the beyond-closure NME and the closure NME, it is possible to find such optimal values for the closure energies at which the closure approach provides the most accurate NME (see e.g. the lines crossing on Fig. 5 of Ref. [18]). One interesting observation is that the optimal energies calculated for the $0\nu\beta\beta$ decay of ^{82}Se [18] and ^{76}Ge with the same JUN45 effective interaction and the same $jj44$ model space practically coincide: they both equal about $\langle E \rangle \approx 3.5$ MeV, although the two cases describe quite different nuclei. It would then be interesting to find a method to estimate the optimal closure energies rather than using estimates from other methods, such as those of Ref. [21]. Figure 3 presents the optimal closure energies calculated for the fictitious $0\nu\beta\beta$ decays of ^{44}Ca (diamonds) and ^{46}Ca (squares) and for the realistic $0\nu\beta\beta$ decays of ^{48}Ca (circles), ^{76}Ge (triangle up), and ^{82}Se (triangle down). All calcium isotopes were calculated in the pf model space using several realistic interactions. The ^{76}Ge and ^{82}Se isotopes were considered in the same $jj44$ model space and with the same JUN45 interaction. The optimal closure energies are significantly lower than the standard closure energies (7.72 MeV for Ca, 9.41 MeV for Ge MeV and 10.08 for Se [21]), which explains a 7–10% growth in absolute values of the nonclosure NME compared to the closure values. We conjecture that the optimal energies depend on the effective interaction and possibly on the model space. We found the optimal closure energies for the three different interactions in the pf model space: GXPF1A [28], FPD6 [29], and KB3G [30]. However, it seems that the energies do not depend much on the specific nucleus: all the calcium isotopes calculated with the same interaction, and both ^{76}Ge and ^{82}Se isotopes calculated with the same model space and with the same interaction give similar optimal closure energies. This opens an interesting opportunity: one could calculate the optimal closure energy in a realistic model space with an effective interaction for a nearby less computationally demanding isotope (for example, ^{44}Ca), after which one can use it for the realistic case (for example, ^{48}Ca). This scheme offers a consistent way of “calculating” the closure energies that has never been discussed before.

We also calculated the heavy-neutrino-exchange mechanism NME (see e.g. Ref. [11] for more details) for the $0\nu\beta\beta$ of ^{76}Ge , and we get a value of 202 for CD-Bonn SRC and 126 for AV18 SRC. Their J^π decompositions will be published elsewhere [31].

Summarizing, we calculated the $0\nu\beta\beta$ decay NME of ^{76}Ge using for the first time a realistic shell-model ap-

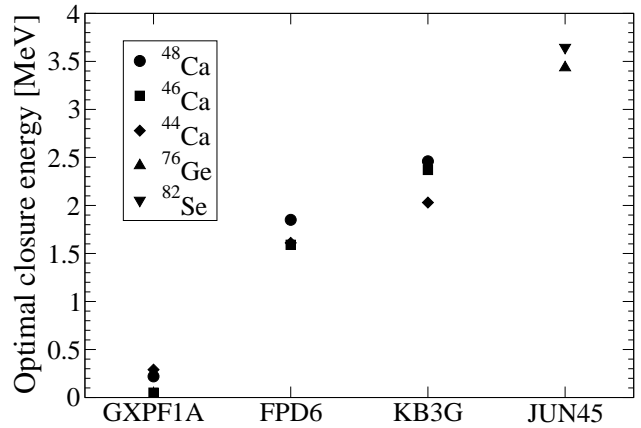


FIG. 3: Optimal closure energies $\langle E \rangle$ calculated for different isotopes and effective interactions: fictitious $0\nu\beta\beta$ decays ^{44}Ca (diamonds) and ^{46}Ca (squares) and real decays ^{48}Ca (circles), ^{76}Ge (triangle up), and ^{82}Se (triangle down). The different effective interactions considered are: GXPF1A, FPD6, KB3G for Ca and JUN45 for Ge and Se isotopes.

proach beyond closure approximation. We demonstrated that the mixed NME converge very fast compared to the nonclosure matrix elements and we found a 7-10% increase in the total NME compared to the closure values.

For the light-neutrino-exchange mechanism we predict $M^{0\nu} = 3.5 \pm 0.1$ for $0\nu\beta\beta$ decay of ^{76}Ge , where the average value and the error were estimated considering the NME calculated with CD-Bonn and AV18 SRC parametrization sets. These values should be compared with the corresponding calculations performed within different approaches: 2.96 (ISM-1 [32]), 3.77 (ISM-2 [34]), 4.6 (EDF [14]), 2.28-4.17 (QRPA-Jy [33]), and 5.42 (IBM-2 [13]). For the heavy-neutrino-exchange NME for ^{76}Ge , we get a value of 202 for CD-Bonn SRC and 126 for AV18 SRC. The corresponding QRPA results are 412 and 265 [8], and the IBM-2 results are 163 and 107 [13].

We proposed a new method of calculating the optimal closure energies at which the closure approach gives the most accurate NME. We argue that these optimal closure energies depend on the interaction and model space and have a weak dependence on the actual isotopes. It offers the opportunity to estimate the beyond closure $0\nu\beta\beta$ NME without actually calculating the intermediate states.

We calculated for the first time a decomposition of the shell-model NME in light- and heavy-neutrino-exchange mechanisms for different spins of intermediate states. We found that for the light-neutrino exchange NME the contribution of the $J^\pi = 1^+$ states is about 30% and that of the $J^\pi = 2^-$ states is about 15%. The shell-model J decomposition that we obtained provides a unique opportunity to selectively quench different contributions to the total NME, which in the case of ^{76}Ge could lead to a decrease of the total matrix elements by about 30%. Although the QRPA approach can provide a J decom-

position, its methodology of choosing the g_{pp} parameter to describe the $2\nu\beta\beta$ half-life [25] makes the selective quenching ambiguous.

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