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Two-neutrino double-beta decay matrix elements for ground and excited states of ^{76}Ge and ^{82}Se nuclei

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Here we present the theoretical results for the Gamow-Teller two-neutrino double-beta decay (DBD) matrix elements for $0_1^+ \rightarrow 0_1^+$ and 2_1^+ transitions in the case of ^{76}Ge to ^{76}Se and ^{82}Se to ^{82}Kr nuclei. The calculations have been done in the framework of the variation after projection on the Hartree-Fock-Bogoliubov model with $2p_{1/2}$, $2p_{3/2}$, $1f_{5/2}$, and $1g_{9/2}$ valence space employing the modified Kuo-Brown interactions. The value of DBD half-lives result in excellent agreement for ground state (g.s.) to g.s. excitations of ^{76}Ge and ^{82}Se nuclei. Our results are in contrast with existing theoretical calculations for g.s. to 2^+ excited state and are much closer to the experimental limits.

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In recent years the investigations of double-beta decay (DBD) yields are becoming very important and have engaged many theoretical nuclear and particle physicists. The interest in the problem has been boosted mainly due to the experimental results [1–8] from active sources bringing the confidence levels (C.L.) of the DBD half-life measurements to very large values. Recently for the case of ^{76}Ge, new techniques enabled the C.L. to reach 95%. The importance of DBD lies in the fact that it can put a limit on the neutrino mass and the related fundamental questions like the Dirac or Majorana nature of neutrinos, and the mixing angle between the vector bosons mediating right- and left-handed weak interactions. The extraction of the value of DBD half-lives mainly depends on the nuclear matrix elements, which are essentially dependent on the nuclear models and its ingredients.

^{76}Ge, ^{82}Se, and some other nuclei have been observed to undergo the two-neutrino DBD that is described as a second-order process in the effective weak interaction. DBD is a process in which an atomic nucleus with Z protons decays to another one with two more (or less) protons and with same mass number A, by emitting two electrons and usually other light particles.

A systematic study for calculation of nuclear matrix elements involves first looking for the applicability of the microscopic model whose most important inputs are two-body interactions. Before really looking for the new mechanisms for obtaining a correct value of the matrix element, one must study other electromagnetic properties with this microscopic model and get satisfactory results with the experiments. One must be sure of the reasonable validity of the model before expecting it to provide us with a reliable value for the DBD matrix element.

Earlier nuclear structure calculations for the two-neutrino DBD matrix elements of ^{76}Ge and ^{82}Se were performed by Haxton and Stephenson [9] with the weak coupling shell model in $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, and $1g_{9/2}$ valence space by using the modified Kuo [10] effective interaction. Tomoda and co-workers [11] and Sharma, Mukherjee, and Rath [12] have studied the g.s. to g.s. decays in the framework of the Hartree-Fock-Bogoliubov (HFB) method by employing the different effective interaction in the same valence space. Estimates of nuclear matrix elements with these interactions for ^{76}Ge and ^{82}Se nuclei are large with the present level of confidence and do not give the matching results for half-lives of these decays. There are other groups [13,14] who have performed the calculations for g.s. to g.s. decay in the quasiparticle random phase approximation (QRPA) formalism with large valence space by using effective interactions derived from realistic nucleon-nucleon (NN) potentials (Paris and Bonn potentials). Here the Gamow-Teller matrix elements ($M_{\rm GT}^{2\nu}$) are very sensitive to particle-particle strength parameter $g_{\rm pp}$, and, normally, in the vicinity of its physical value, $g_{\rm pp}=1.0$, the solution becomes unstable. Stout and Kuo [14] have shown that when one treats the BCS self-energy correctly, in a self-consistent way, the QRPA $M_{\rm GT}^{2\nu}$ matrix element are quite stable for $g_{\rm PP}=1.0$.

Recently, the experimental measurements of 2ν double-beta decay have been reported for the excitations from the ground state of ^{100}Mo to the excited 2_1^+ and other states in ^{100}Ru by a Tokyo and Moscow group [5]. Experimental results of 2ν $\beta\beta$ decays for the first excited $0^+, 2^+$ states have been reported by the Moscow-Heidelberg group [4] in the case of a $^{76}\text{Ge} \rightarrow {}^{76}\text{Se}$ transition and they also expect the 2ν decay transition to be occurring for the 2_1^+ excited state of ^{82}Se with a Q value of 1479.5 keV. The half-lives for the excited state transitions are expected to be longer than for the ground state transitions. This is mainly due to the suppression of the phase space factor and the small Q value of the transition, rather than that for final ground state.

However, the experimental investigations for double-beta decay transitions to excited states are still at a preliminary stage. To compare these experimental data the theoretical activity has started and results for ^{100}Mo and ^{136}Xe have been calculated in the framework of the QRPA [15,16]. Haxton and Stephenson have reported earlier the results [9] for ^{48}Ca and ^{76}Ge excited state decays, but in the case of ^{76}Ge

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their estimate for the $0^+\rightarrow 2_1^+$ transition greatly exceeds the obtained experimental limit [4].

The two-neutrino half-life for the g.s. to g.s. transitions can be written [11] as

$$[T_{1/2}^{2\nu}(0_1^+\rightarrow 0_1^+)]^{-1}=F_{2\nu}|M_{2\nu}|^2 \tag{1}$$

where $F_{2\nu}$ is the lepton phase space integral and $M_{2\nu}$ is the nuclear matrix element usually approximated by

$$M_{2\nu}=\frac{2M_{\mathrm{GT}}^{2\nu}}{\frac{1}{2}W_0+\langle E_N\rangle-E_I}, \tag{2}$$

where $M_{\mathrm{GT}}^{2\nu}$ is the Gamow-Teller matrix element given by

$$M_{\mathrm{GT}}^{2\nu}=\left\langle J_f^+\left|\frac{1}{2}\sum_{ij}\sigma(i)\cdot\sigma(j)\tau_+(i)\tau_+(j)\right|J_i^+\right\rangle, \tag{3}$$

E_N-E_I is the typical nuclear excitation energy due to the Gamow-Teller operator $\sigma\tau_+$, and W_0 is the total energy released

$$W_0=Q_{\beta\beta}-2m_e=E_I-E_F. \tag{4}$$

In a similar way one can write the half-life for $0_1^+\rightarrow 2_1^+$ of 2ν $\beta\beta$ decay as

$$[T_{1/2}^{2\nu}(0_1^+\rightarrow 2_1^+)]^{-1}=F_{2\nu}^2|M_{2\nu}|^2. \tag{5}$$

In the closure approximation the nuclear matrix elements for the $0_1^+\rightarrow 2_1^+$ transition is given by

$$M_{2\nu}^2=\frac{2M_{\mathrm{GT}}^{2\nu}}{(\frac{1}{2}W_0+\langle E_N\rangle-E_I)^3}. \tag{6}$$

To calculate the above nuclear matrix element, we need to know the respective wave functions and energies which can be obtained from the model-space effective interaction.

In the present work we have obtained the variation after projection (VAP) wave functions (based upon the HFB ansatz). The doubly closed ^{56}Ni is treated as an inert core. We have also taken the same model space and single particle energies as used by Tomoda and co-workers [11], but the effective two-body interaction matrix element due to Kuo were modified following the approach of McGrory, Wildenthal, and Halbert [17] as well as Sharma and Bhatt [18]. These modifications were essential for description of some experimental observations in transition charge densities of the germanium nuclei. The interaction matrix elements of $\langle(0f_{5/2})^2|V|(0f_{5/2})^2\rangle$ for $J=0^+$ to 5^+ were made more attractive, the $\langle(1p_{3/2})^2|V|(1p_{3/2})^2\rangle$ for $J=0^+$ to 3^+ were made more repulsive, and the quantitative change in keV is expressed by the number associated with Kuo and Brown (KB), e.g., KB250 stands for the modification of Kuo interactions with above interaction matrix elements changed by 250 keV.

A brief outline of the VAP prescription used in the calculation of double-beta decay matrix element is as following. The axially symmetric HFB state with $K=0$ can be written as

$$|\phi_0\rangle=\prod_{im}(U_i^m+V_i^m b_{im}^\dagger b_{i\bar{m}}^\dagger)|0\rangle, \tag{7}$$

where the creation operators $b_{im}^\dagger$ can be expressed as

$$b_{im}^\dagger=\sum_j C_{ji}^m a_{jm}^\dagger, \tag{8a}$$

$$b_{i\bar{m}}^\dagger=\sum_j(-1)^{j-m}C_{ji}^m a_{j-m}^\dagger, \tag{8b}$$

Here the operator $a_{jm}^\dagger$ creates a particle in the orbit $|jm\rangle$ and C_{ji}^m are the expansion coefficients. The index j labels the single particle states $2p_{1/2}$, $2p_{3/2}$, $1f_{5/2}$, and $1g_{9/2}$, and the index i is employed to distinguish between states with the same m.

The energy of the projected states is given by

$$E_J=\langle\phi_0|HP_{00}^J|\phi_0\rangle/\langle\phi_0|P_{00}^J|\phi_0\rangle, \tag{9}$$

where H is the shell model Hamiltonian. The VAP procedure involves the selection of an appropriate intrinsic state for the ground states through a minimization of projected energy given by Eq. (10). We first generated the self-consistent intrinsic state $\phi(\beta)$ by the HFB calculation with the Hamiltonian $(H-\beta Q_0^2)$. The optimum intrinsic state for the ground state for each nuclei involved in the double-beta transition is then selected by ensuring the following condition be satisfied:

$$\delta[\langle\phi(\beta)|HP_{00}^{J=0}|\phi(\beta)\rangle/\langle\phi(\beta)|P_{00}^{J=0}|\phi(\beta)\rangle]=0. \tag{10}$$

Employing the VAP wave functions, one can obtain the following expression for the double-beta decay matrix elements:

$$\langle M_{\mathrm{GT}}^{2\nu}\rangle=(n_{N-2,Z+2}^{J_f}n_{N,Z}^{J_i})^{-1/2}\int_0^{\pi/2}n_{(N,Z),(N-2,Z+2)}(\theta)\frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\sigma_1\cdot\sigma_2|\gamma\delta\rangle\sum_{\epsilon\eta}(1+F_{N,Z}^{(\pi)}f_{N-2,Z+2}^{(\pi)*})_{\epsilon\alpha}^{-1}$$
$$\times(f_{N-2,Z+2}^{(\pi)*})_{\epsilon\beta}(1+F_{N,Z}^{(\nu)}f_{N-2,Z+2}^{(\nu)*})_{\nu\eta}^{-1}(F_{N,Z}^{(\nu)*})_{\eta\delta}\sin\theta\,d\theta, \tag{11}$$

where

$$n^J=\int_0^{\pi/2}\{\det[1+F^{(\pi)}(\theta)f^{(\pi)\dagger}]\}^{1/2}\{\det[1+F^{(\nu)}(\theta)f^{(\nu)\dagger}]\}^{1/2}d_{MK}^J(\theta)\sin\theta\,d\theta, \tag{12}$$

$$n_{(N,Z)(N-2,Z+2)}(\theta)=\{\det[1+F^{(\pi)}_{N,Z}(\theta)f^{(\pi)\dagger}_{N-2,Z+2}]\}^{1/2}\{[1+F^{(\nu)}_{N,Z}f^{(\nu)\dagger}_{N-2,Z+2}]\}^{1/2}, \tag{13}$$

$$[F_{N,Z}(\theta)]_{\alpha\beta}=\sum_{m'_\alpha,m'_\beta} d^{j_\alpha}_{m_\alpha m'_\alpha}(\theta)d^{j}_{m_\beta m'_\beta}(\theta)(f_{N,Z})_{j_\alpha m_{\alpha'},j_\beta m'_\beta},$$

and

$$(f_{N,Z})_{\alpha\beta}=\sum_i C^{m_\alpha}_{j_\alpha,i}(N,Z)C^{m_\beta}_{j_\beta,i}(N,Z)V^{m_\alpha}_i(N,Z)/U^{m_\beta}_i(N,Z)\,\delta_{m_{\alpha'},-m_\beta} \tag{14}$$

where α denotes the quantum number (j_α, m_α).

Since two-body interaction matrix elements used in the calculation of the double-beta decay matrix elements are the most important inputs to the nuclear model calculations, we present a brief evolution of these two-body interactions in the f-p region. From the literature we notice that the use of the two-body interactions has been of considerable interest to those who have made many theoretical attempts in this region to describe the energy spectrum, multipole moments, and transition probabilities for more than two decades. The realistic interaction for the f-p and f-p-g shell nuclei was constructed by Kuo and Brown (KB) [10] and, as usual, was put to the test successfully for the spectra of some nuclei near shell closure. Then, exhaustive spectroscopic shell model calculations for Ca nuclei by McGrory *et al.* (MWH) [17] revealed that these interactions have to be modified slightly, suggesting that effective interactions for $f_{7/2}$ with other orbits of the space are too strong. The next attempt made in modifying these effective interactions in the f-p region was made by Sharma and Bhatt [18] to examine the intrinsic structure of even-even nuclei of Ti, Cr, and Fe. Based on these results and the Nilsson structure of the orbits, they suggested, in line with MWH, that interaction matrix elements for the particles in $(f_{7/2})^2$ should be made more attractive and the interaction of the $f_{7/2}$ with other orbits should be made repulsive. The variation of these interaction matrix elements have been attempted by them for 200 and 400 keV.

With the above developments about the evolution of two-body interactions in f-p shell nuclei in mind and also the anomalous observations in the electroexcitation of the Ge nuclei by Bazantay *et al.* [19], where it has been observed theoretically with the IBM calculations that $f_{5/2}$ orbitals have a very crucial role to play in these nuclei, we have made the changes in the f-p-g valence space KB interactions. It has been observed [20] that the spectrum, transition probabilities for even-even Ge and Se nuclei, as well as the transition charge densities for the germanium nuclei for $0^+ \rightarrow 2^+$ excitations give quite good agreement with the experimental results when we change the two-body interaction matrix elements of the KB interaction, making the $(f_{5/2})^2$ interaction matrix elements attractive and the $(p_{3/2})^2$ interaction matrix elements repulsive. With the experience [20,21] of working on the transition charge density in f-p-g shell nuclei, we can now say that these changes in the effective interactions lead us to the right direction by taking the proper role of $f_{5/2}$ and $p_{3/2}$ orbitals into consideration.

As shown in Fig. 1 HFB results of energy spectrum for ^{76}Ge, ^{76,82}Se, and ^{82}Kr nuclei are in good agreement with the experiments. Our results for the two-neutrino Gamow-Teller matrix elements and half-lives for g.s. transitions in the case of ^{76}Ge$\rightarrow$^{76}Se and ^{82}Se$\rightarrow$^{82}Kr are presented in Table I. These results for matrix elements and half-lives of ^{76}Ge and ^{82}Se decays show that we get the same magnitudes

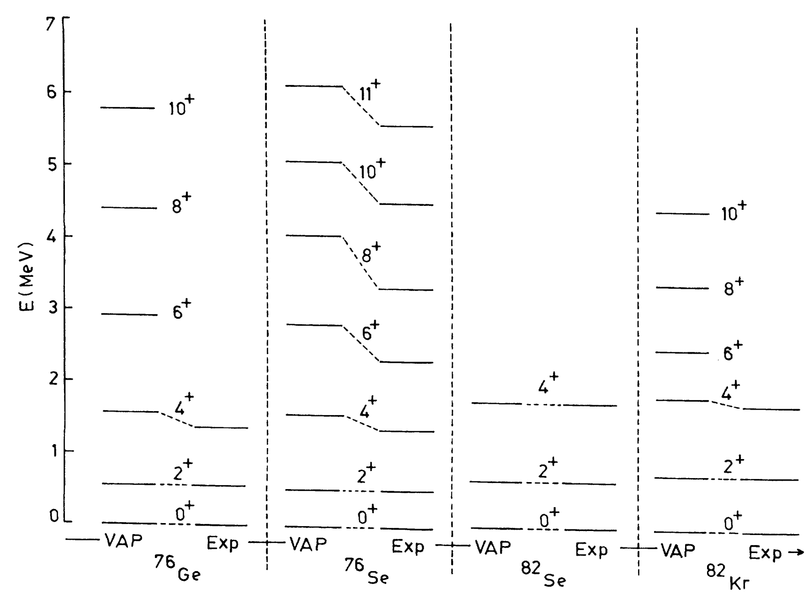

FIG. 1. Comparison of experimental as well as the calculated yrast spectra for ^{76}Ge, ^{76,82}Se, and ^{82}Kr nuclei.

TABLE I. $2\nu\ \beta\beta$ decay matrix elements and half-lives for g.s. to g.s. and g.s. to quadrupole excitations calculated by VAP. Also presented are the latest available experimental results.

	^{76}Ge$\rightarrow$^{76}Se			^{82}Se$\rightarrow$^{82}Kr		
		$T_{1/2}^{2\nu}$ (yr)			$T_{1/2}^{2\nu}$ (yr)	
Transition	$\langle M_{\mathrm{GT}}^{2\nu}\rangle$	Theor.	Expt.	$\langle M_{\mathrm{GT}}^{2\nu}\rangle$	Theor.	Expt.
$0^+\rightarrow 0^+$	0.879	1.32×10^{21}	$1.42\pm 0.2\times 10^{21}$ [a]	0.452	1.48×10^{20}	$1.1^{+0.8}_{-0.3}\times 10^{20}$ [b]
$0^+\rightarrow 2^+$	1.04	5.79×10^{23}	$>6.3\times 10^{20}$ [a]	0.598	5.52×10^{21}	
		1.18×10^{30} [c]				

[a] Reference [4].
[b] Reference [7].
[c] Reference [9].

for KB300 as the ones obtained in the recent experiments. The same is true in the case of ^{82}Se$\rightarrow$^{82}Kr but here the experimental result for the half-life has a lower confidence level. So our results corresponding to the KB300 interaction can also act as a prediction and help the experimental studies.

In the second row of Table I we present the results for excited states for the same decay processes. We believe that if DBD matrix elements corresponding to KB300 are in good agreement with experiment for g.s. to g.s. excitations then these values should be the ones expected for the excited states from experiments. The order of magnitudes for ^{76}Ge decay is closer to the experimental limit in comparison to the only available theoretical result [9].

We summarize by saying that the HFB model equations are used to set the matrices for the nuclei ^{76}Ge, ^{76,82}Se, and ^{82}Kr with the KB300 interaction, a modified version of Kuo, and are solved for amplitudes and expansion coefficients. The wave functions obtained in the VAP framework with KB300 have been successfully used for the testing of the model for static properties of ^{76}Ge, ^{76,82}Se, and ^{82}Kr nuclei, as well as for the electron scattering data for quadrupole excitations of Ge nuclei providing an answer to some observed anomalies features. Furthermore, we are getting the good agreement for DBD matrix elements for $0^+\rightarrow 0^+$ transitions and half-lives of ^{76}Ge and ^{82}Se decays with the ones obtained in the recent experiments. One important observation from the comparison of the g.s. to g.s. and g.s. to excited 2^+ states is that the order of magnitudes of the DBD matrix elements for g.s. to g.s. transitions are not much different from the g.s. to excited states. The half-life results presented here shall be of help for the experimentalists looking for the DBD to excited states.

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