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Double Gamow-Teller matrix elements in the germanium region

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The matrix elements involved in the double-beta-decay process for the nuclei ^{76}Ge and ^{82}Se are calculated in terms of the variational wave functions resulting from realistic effective interactions operating in the unrestricted $(2p_{1/2}, 2p_{3/2}, 1f_{5/2}, 1g_{9/2})^{\pi,\nu}$ configuration space.

The double beta decay[1]— the process involving a transition of the nucleus with neutron and proton number (N,Z) to the nucleus $(N-2,Z+2)$ when the single beta decay to the nucleus $(N-1,Z+1)$ is either highly inhibited or energetically disallowed—is characterized by two modes, one involving the emission of two antineutrinos along with two electrons (the 2ν mode) and the other involving only the emission of two electrons (the 0ν mode). As pointed out by Haxton, Stephenson, and Strottman,[1] the calculation of the decay rates associated with these modes has important ramifications *vis-á-vis* the constraints on the Majorana mass of the neutrino.

A number of calculations have been performed in the past with a view to predict the matrix elements mediating the $2\nu\beta\beta$ decay in the medium-mass nuclei ^{76}Ge and ^{82}Kr. In view of the intractability of the shell model calculations in the model space involving the orbitals $2p_{1/2}$, $2p_{3/2}$, $1f_{5/2}$, and $1g_{9/2}$ lying between $N=28$ and 50, Haxton *et al.*[1] employed in their pioneering work a weak-coupling approximation; the procedure involved the diagonalization of the proton-neutron interaction in a *restricted* subset of states resulting from the shell model calculations performed separately for valence protons and neutrons. The single-particle energies (SPE's) as well as the overall strength of the two-body interaction given by Kuo were empirically adjusted to optimize the agreement between the calculated and observed level energies of a number of nuclei involving the closed shells with $Z=28$ and $N=50$. The transition $^{76}\mathrm{Ge}(0_1^+)\rightarrow{}^{76}\mathrm{Se}(0_1^+)$ was also studied by Tomoda *et al.*[2] in the framework of the Hartree-Fock-Bogolubov (HFB) method (involving number as well as angular momentum projection) in conjunction with the modified surface-delta interaction operating in the same space as the one employed by Haxton *et al.*[1]

The structure of the nuclei in the Ge region is quite complex;[3] this is primarily due to the fact that the shell model orbits constituting the underlying configuration space *do not* exhibit pronounced subshell closures between the magic numbers 28 and 50. Experimental studies involving in-beam γ-ray spectroscopy have yielded a vast amount of data concerning the electromagnetic properties as well as level energies in doubly even Ge and Se isotopes during the past decade. Although the availability of these data permits a rigorous and detailed critique of the ingredients of the microscopic framework that seeks to provide a description of these isotopes, none of the calculations of the double-β-decay matrix element performed so far satisfy this criterion.

The available data in Ge and Se isotopes are characterized by several anomalous features that signal an interplay of the deformation and pairing degrees of freedom. As emphasized by Zamick and Auerbach[4] as well as by Grotz and Klapdor,[5] the double-β-decay matrix element is quite sensitive towards small variations of empirical choices of the input parameters such as Nilsson deformations and the pairing gaps embodying various collective modes. Therefore, for the calculation of the double-β-decay matrix element to be of some reliability, it is essential that one first obtains detailed acceptable agreement with the available data by invoking a calculational framework that permits a consistent treatment of the pairing and deformation-producing components of a *realistic* interaction operating in a reasonably large valence space.

The calculation of the double-β-decay matrix element discussed in the present work satisfies the criterion just mentioned. We have recently shown[6] that the variation-after-projection (VAP) wave functions (based on the HFB ansatz) resulting from Kuo's renormalized interaction[7] for the Ge region provide a consistent quantitative description of the observed features in a large number of nuclei with $A=60$–80. We discuss here an application of these variational wave functions *vis-á-vis* the double-β-decay transitions $^{76}\mathrm{Ge}(0_1^+)\rightarrow{}^{76}\mathrm{Se}(0_1^+)$ and $^{82}\mathrm{Se}(0_1^+)\rightarrow{}^{82}\mathrm{Kr}(0_1^+)$.

In what follows we sketch briefly an outline of the VAP prescription as it applies to the calculation of the double-β-decay matrix element. The axially symmetric HFB state with $K=0$ can be written as

$$|\Phi_0\rangle=\prod_{im}(u_i^m+v_i^m b_{im}^\dagger b_{i\bar{m}}^\dagger)|O\rangle \ , \tag{1}$$

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

$$b_{im}^\dagger=\sum_j c_{ji}^m a_{jm}^\dagger,\quad b_{i\bar{m}}^\dagger=\sum_j(-1)^{j-m}c_{ji}^m a_{j-m}^\dagger \ . \tag{2}$$

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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 different states with the same m.

The states of good angular momentum projected from the HFB intrinsic states $|\Phi\rangle$ can be written as

$$|JK\rangle = P_{MK}^{J}|\Phi_K\rangle = \left[\frac{(2J+1)}{8\pi^2}\right]\int D_{MK}^{J}(\Omega)R(\Omega)|\Phi_K\rangle d\Omega \ , \quad (3)$$

where $R(\Omega)$ and $D_{KK}^{J}(\Omega)$ are the rotation operator and the rotation matrix, respectively.

The energy of the states with angular momentum J is given as

$$E_J = \langle\Phi_0|HP_{00}^{J}|\Phi_0\rangle / \langle\Phi_0|P_{00}^{J}|\Phi_0\rangle \ , \quad (4)$$

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 the projected energy given by Eq. (4). One first generates the self-consistent intrinsic state $\Phi(\beta)$ by carrying out the HFB calculation with the Hamiltonian $(H-\beta Q_0^2)$. The *optimum* intrinsic state for the $J=0$ ground state for *each* nucleus involved in the double β transitions is then selected by ensuring the following condition be satisfied:

$$\delta[\langle\Phi(\beta)|HP_{00}^{J=0}|\Phi(\beta)\rangle / \langle\Phi(\beta)|P_{00}^{J=0}|\Phi(\beta)\rangle] = 0 \ . \quad (5)$$

Following the work of Haxton, Stephenson, and Strottman,[1] the double-β-decay process is expressible, in the absence of the isospin admixtures, in terms of the Gamow-Teller matrix elements connecting the initial state of the nucleus (N,Z) to the final state of the nucleus $(N-2,Z+2)$ provided the closure approximation is invoked:

$$\langle M_{\mathrm{GT}\beta\beta}\rangle = \langle J_f^+, K=0|\tfrac{1}{2}\sum_{i,j}\sigma(i)\cdot\sigma(j)\tau_+(i)\tau_+(j)|J_i^+, K=0\rangle \ . \quad (6)$$

Employing the projected wave functions, one obtains the following expression for the double-β-decay matrix elements:

$$\langle M_{\mathrm{GT}\beta\beta}\rangle = (n_{N-2,Z+2}^{J_f=0} n_{N,Z}^{J_i=0})^{-1/2}\int_0^{\pi/2} n_{(N,Z),(N-2,Z+2)}(\theta)\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\sigma_1\cdot\sigma_2|\gamma\delta\rangle \times\sum_{\epsilon\eta}(1+F_{N,Z}^{(\pi)}f_{N-2,Z+2}^{(\pi)*})_{\epsilon\alpha}^{-1}(f_{N-2,Z+2}^{(\pi)*})_{\epsilon\beta} \times(1+F_{N,Z}^{(\nu)}f_{N-2,Z+2}^{(\nu)*})_{\gamma\eta}^{-1}(F_{N,Z}^{(\nu)*})_{\eta\delta} \ , \quad (7)$$

where

$$n^J = \int_0^{\pi/2}\{\det[1+F^{(\pi)}(\theta)f^{\pi\dagger}]\}^{1/2}\{\det[1+F^{(\nu)}(\theta)f^{\nu\dagger}]\}^{1/2} d_{00}^{J}(\theta)\sin\theta\, d\theta \ , \quad (8)$$

$$n_{(N,Z),(N-2,Z+2)}(\theta) = \{\det[1+F_{N,Z}^{(\pi)}(\theta)f_{N-2,Z+2}^{\pi\dagger}]\}^{1/2}\{\det[1+F_{N,Z}^{(\nu)}(\theta)f_{N-2,Z+2}^{\nu\dagger}]\}^{1/2} \ , \quad (9)$$

$$[F_{N,Z}(\theta)]_{\alpha\beta} = \sum_{m'_\alpha, m'_\beta} d_{m_\alpha, m'_\alpha}^{j_\alpha}(\theta) d_{m_\beta, m'_\beta}^{j_\beta}(\theta)(f_{N,Z})_{j_\alpha m'_\alpha, j_\beta m'_\beta} \ , \quad (10)$$

and

$$(f_{N,Z})_{\alpha\beta} = \sum_i c_{j_\alpha i}^{m_\alpha}(N,Z) c_{j_\beta i}^{m_\beta}(N,Z)(v_i^{m_\alpha}(N,Z)/v_i^{m_\beta}(N,Z))\delta_{m_\alpha,-m_\beta} \ . \quad (11)$$

TABLE I. The matrix elements $\langle M_{\mathrm{GT}\beta\beta}\rangle$ associated with the double-β-decay transition $^{76}\mathrm{Ge}(0_1^+)\rightarrow{}^{76}\mathrm{Se}(0_1^+)$ calculated with different choices for the single-particle energy of the $1g_{9/2}$ orbit. The quadrupole moments of the variational intrinsic states involved in the transition have also been given. Here $\langle Q_0^2\rangle^{\pi}(\langle Q_0^2\rangle^{\nu})$ gives the contribution of the protons (neutrons) to the total intrinsic quadrupole moment of the variational intrinsic state associated with the ground states.

		^{76}Ge			^{76}Se		
$\epsilon(1g_{9/2})$	$\langle Q_0^2\rangle$	$\langle Q_0^2\rangle^{\pi}$	$\langle Q_0^2\rangle^{\nu}$	$\langle Q_0^2\rangle$	$\langle Q_0^2\rangle^{\pi}$	$\langle Q_0^2\rangle^{\nu}$	$\langle M_{\mathrm{GT}\beta\beta}\rangle$
2.5	27.3	11.6	15.7	35.7	15.3	20.4	3.27
3.0	27.0	11.7	15.3	34.8	15.1	19.7	3.19
3.5	26.5	11.8	14.7	33.6	14.8	18.8	2.82
4.0	25.7	11.8	13.9	31.9	14.4	17.4	1.75
4.5	24.7	11.7	13.0	29.6	14.0	15.6	1.65

TABLE II. The matrix elements $\langle M_{GT\beta\beta} \rangle$ associated with the double-β-decay transition ^{82}Se(0_1^+)$\rightarrow$^{82}Kr(0_1^+).

	^{82}Se			^{82}Kr			
$\epsilon(1g_{9/2})$	$\langle Q_0^2 \rangle$	$\langle Q_0^2 \rangle^\pi$	$\langle Q_0^2 \rangle^\nu$	$\langle Q_0^2 \rangle$	$\langle Q_0^2 \rangle^\pi$	$\langle Q_0^2 \rangle^\nu$	$\langle M_{GT\beta\beta} \rangle$
2.5	14.0	9.1	4.9	28.9	16.8	12.1	2.73
3.0	15.0	9.6	5.4	27.9	15.9	12.0	2.67
3.5	16.3	10.2	6.1	26.1	14.3	11.8	2.70
4.0	17.5	10.9	6.6	23.7	12.4	11.3	2.60
4.5	19.1	11.9	7.2	21.5	10.9	10.6	2.22

In the calculations presented here we treat the doubly closed shell nucleus ^{56}Ni as an inert core. The relevant effective two-body interaction that we use is a renormalized G matrix due to Kuo;[7] the use of this effective interaction is expected to compensate to some extent for the additional configuration mixing within the $(2p_{1/2},2p_{3/2},1f_{5/2},1g_{9/2})^{\pi,\nu}$ space that is expected to result from an explicit consideration of the extended space involving higher shells. In addition to explaining the observed $B(E2,J_i \rightarrow J_f)$ systematics,[6,8] yrast spectra as well as the gyromagnetic factors[9] associated with a large number of Ge, Se, and Kr isotopes, this interaction has also described successfully the observed anomalous sequence of the high-spin yrast spectra in ^{60}Ni in the exact shell model framework.[10] The SPE's we have employed are (in MeV) $\epsilon(2p_{3/2})=0.0$, $\epsilon(1f_{5/2})=0.78$, and $\epsilon(2p_{1/2})=1.08$. In view of the sensitivity of the $M_{GT\beta\beta}$ values towards the $1g_{9/2}$ SPE, we have tried to illustrate the range within which a reasonable variation of this parameter can alter the theoretical predictions.

The matrix elements $M_{GT\beta\beta}$ are calculated as follows. Using the results of the variational calculation—and these are summarized by the amplitudes (u_i^m, v_i^m) and the expansion coefficients c_{ij}^m—we first set up the matrices $F^{(\pi,\nu)}$ and $f^{(\pi,\nu)}$ given by Eqs. (10) and (11) for the nuclei ^{76}Ge, ^{76,82}Se, and ^{82}Kr for 20 Gaussian quadrature points in the range $(0,\pi/2)$. Finally, the relevant double-β-decay matrix elements are calculated from Eq. (7).

We first discuss here the double-β-decay matrix elements associated with the transition ^{76}Ge(0_1^+) $\rightarrow$^{76}Se(0_1^+). (See Table I.) The VAP study of doubly even Ge, Se, and Kr isotopes has earlier revealed that the available experimental information in these nuclei is consistent with the value $\epsilon(1g_{9/2})=3.5$ MeV provided Kuo's renormalized interaction is employed. With this choice of the $1g_{9/2}$ SPE we obtain $M_{GT\beta\beta}[^{76}\text{Ge}(0_1^+)\rightarrow{}^{76}\text{Se}(0_1^+)]=2.82$. The present estimate is a factor of two larger than the one obtained earlier by Haxton *et al.*;[1] it is also considerably larger than the value predicted by Tomoda *et al.*[2] It may be mentioned here that although the random-phase-approximation (RPA) and the projected Bardeen-Cooper-Schrieffer (PBCS) methods employed by Grotz and Klapdor[5] yielded $M_{GT\beta\beta}=5.54$ and 7.05, respectively, subsequent inclusion of the spin-isospin as well as the quadrupole-quadrupole terms in the nucleonic and the Δ-nucleon hole space (along with the contribution due to higher-order phonons) finally led to $M_{GT\beta\beta}=1.93$—a value that is only about 35 percent lower than the present estimate.

We next move on to the transition ^{82}Se(0_1^+) $\rightarrow$^{82}Kr(0_1^+). (See Table II.) In this case the choice $\epsilon(1g_{9/2})=3.5$ MeV dictated by the successful VAP description of the available experimental data suggests $M_{GT\beta\beta}=2.70$—a value that is almost three times as large as the one obtained earlier by Haxton *et al.*[1] This striking difference is not entirely unexpected since the increased number of interacting proton-neutron pairs—a feature that is instrumental *vis-á-vis* the occurrence of enhanced configuration mixing—is expected to affect the efficacy of the shell model calculations involving truncated basis.

It is interesting to note that in contrast to the situation in the case of the ^{82}Se(0_1^+)$\rightarrow$^{82}Kr(0_1^+) transition where $M_{GT\beta\beta}$ does not vary significantly, the matrix element associated with the ^{76}Ge(0_1^+)$\rightarrow$^{76}Se(0_1^+) transition is reduced by almost a factor of two when the $1g_{9/2}$ SPE is varied from 2.5 to 4.5 MeV. This feature is related to the differing trends of the variation of the intrinsic deformation of the parent and the daughter nuclei as a function of the $1g_{9/2}$ energy; whereas the increase in the intrinsic deformation of ^{82}Se is offset by the reduction in the intrinsic deformation of ^{82}Kr in the case of the ^{82}Se(0_1^+) $\rightarrow$^{82}Kr(0_1^+) transition, the pair ^{76}Ge-^{76}Se displays a simultaneous decrease of the intrinsic quadrupole moments.

Summarizing, we have discussed here the calculation of the matrix elements involved in the transitions ^{76}Ge(0_1^+)$\rightarrow$^{76}Se(0_1^+) and ^{82}Se(0_1^+)$\rightarrow$^{82}Kr(0_1^+). We obtain the following estimates for these matrix elements:

$$M_{GT\beta\beta}[^{76}\text{Ge}(0_1^+)\rightarrow{}^{76}\text{Se}(0_1^+)]=2.82\ ,$$

$$M_{GT\beta\beta}[^{82}\text{Se}(0_1^+)\rightarrow{}^{82}\text{Kr}(0_1^+)]=2.70\ .$$

These predictions—which are nearly of the same magnitude as the ones obtained in some earlier investigations[1,2]—can be looked upon as essential implications of an underlying microscopic description involving variational methods in conjunction with realistic interactions that has already turned out to be quite successful in interpreting and correlating the available experimental information in the Ge region.

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