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Nuclear Matrix Elements for Double Beta Decay in the QRPA approach: a critical review

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The excitement which goes with theoretical efforts towards the calculation of NME for DBD is, of course, due to the remarkable achievements of the active experimental groups. It is our pleasure and our honor to thank Profs. Ettore Fiorini and Frank Avignone for their life-long efforts devoted to the experimental exploration of DBD transitions. We wish for both of them many years of new contributions and inspirations.

Abstract. The calculation of nuclear matrix elements (NME) for double beta decay transitions (DBD) relies upon several approximations. The purpose of this note is to review some of these approximations, and their impact upon the NME. We shall present our results, which have been obtained in the framework of the proton-neutron quasiparticle random phase approximation (pnQRPA), and we shall focus on short range correlations, pairing, and symmetry effects.

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1. Introduction

The calculation of NME for DBD transitions has been, and still it is, the target of choice for practitioners in the field of nuclear and nucleon structure. The body of literature is indeed huge and for the sake of brevity we shall only refer hereafter to few review articles [1, 2, 3, 4], and to some recently published papers [5, 6, 7, 8, 9]. The spreading of the theoretical results was so noticeable, even for physicists outside the field, that the credibility of the results was questioned severely, particularly with the claimed discovery of neutrinoless double beta decay [10, 11]. The situation was nearly catastrophic, with i) model predictions, obtained with the same models but varying within factors, and with ii) the proliferation of ad-hoc recipes, introduced to justify day by day changes of the theoretical estimations, sometimes also self-contradictory. To this we may add the almost recursive reference to back of the envelope calculations and hand waving arguments presented as illusive pieces of cakes. Fortunately enough the situation has improved recently, and the spread of the theoretical results is much smaller and therefore the reliability of the theoretical estimations of NME has improved considerably. In this note we would like to review some of the elements which, in our opinion, are crucial in determining the stability of the results, namely: a)the effect of short range correlations, b)the effect of pairing correlations, and c)symmetry violation effects introduced by the model assumptions. For details we shall refer the reader to the work of [5, 6, 7], for short range correlations, and to [12, 13] for pairing correlations. Concerning the issue of symmetry violation effects, which mostly reflect the failure of some of the extensions of the pnQRPA method, we shall refer the reader to refs. [14, 15]. The non-physical effects associated with attempts to go beyond the point of collapse of the pnQRPA approach are notorious, particularly in the case of some ad-hoc methods based on non-consistent corrections of the quasi-particle mean field. As a consequence, the results of some renormalized versions of the pnQRPA should be taken with extreme caution [14, 15].

2. Brief Review of Concepts

In the mass mode of the $0\nu\beta\beta$ decay a light virtual Majorana neutrino is exchanged by the two decaying neutrons of the initial nucleus. The measured $0\nu\beta\beta$-decay half-life is connected with the effective neutrino mass $\langle m_\nu \rangle$ through the relation

$$\left[t_{1/2}^{(0\nu)}(0_{\rm i}^+ \rightarrow 0_{\rm f}^+)\right]^{-1} = G_1^{(0\nu)} \left(\frac{\langle m_\nu \rangle}{m_{\rm e}}\right)^2 \left(M^{(0\nu)}\right)^2 \ , \tag{1}$$

where $G_1^{(0\nu)}$ is the leptonic phase-space factor [1, 2]. The $0\nu\beta\beta$ nuclear matrix element $M^{(0\nu)}$ consists of the Gamow–Teller, Fermi and tensor parts as

$$M^{(0\nu)} = M_{\rm GT}^{(0\nu)} - \left(\frac{g_{\rm V}}{g_{\rm A}}\right)^2 M_{\rm F}^{(0\nu)} + M_{\rm T}^{(0\nu)} \ . \tag{2}$$

Numerical calculations show that the tensor part in (2) is quite small and its contribution can be safely neglected. Most often people use the proton-neutron quasiparticle random-phase approximation (pnQRPA) [2] to treat the structure of double-beta decaying nuclei. Also some recent shell-model results are available [16, 17]. The pnQRPA contains a free parameter, the so-called particle-particle strength parameter, $g_{\rm pp}$, that controls the magnitude of the proton-neutron two-body interactions in the $T = 0$ pairing channel [18, 19]. The fixing of the value of this parameter has been done either by using the data on two-neutrino double beta ($2\nu\beta\beta$) decay or the data on single beta decay [20, 21].

3. Short Range Correlations

The average exchanged momentum is large, of the order of 100 MeV, so that the two neutrons tend to overlap. To prevent this a Jastrow type of correlation function has been introduced, in an ad-hoc manner, into the $0\nu\beta\beta$ calculations [22]. This way of using the Jastrow procedure is a very rudimentary way to introduce short-range correlations into many-nucleon systems. A more sophisticated microscopic approach for the inclusion of short-range correlations is the unitary correlation operator method (UCOM). In the UCOM one obtains the correlated many-particle state from the uncorrelated one by a unitary transformation and thus the norm of the correlated state is conserved and no amplitude is lost in the relative wave function. In [5, 6, 7] it was demonstrated that the Jastrow procedure leads to the excessive reduction of 25% – 40% in the magnitudes of the $0\nu\beta\beta$ nuclear matrix elements. At the same time the UCOM reduces the magnitudes of the matrix elements only by 4% – 16%. A fully consistent use of the UCOM method requires to treat not only the wave functions but the Hamiltonian, as well. Here we present our results of nuclear-structure calculations for the $0\nu\beta\beta$ ground-state-to-ground-state decays of ^{76}Ge, ^{82}Se, ^{96}Zr, ^{100}Mo, ^{116}Cd, ^{128}Te, ^{130}Te, and ^{136}Xe. In the following we shall talk

Table 1. Calculated $0\nu\beta\beta$ nuclear matrix elements, the used $g_{\rm pp}$ and $g_{\rm A}$ values and the resulting half-lives. The Jastrow (J) or UCOM (U) plus the other corrections are included. The half-lives $t_{1/2}^{(0\nu)}$ are expressed in units of $\mathrm{yr}/(\langle m_\nu\rangle[\mathrm{eV}])^2$. See [5, 6, 7] for further details.

Nucleus	$g_{\rm pp}$	$g_{\rm A}$	$M^{(0\nu)}$(J)	$t_{1/2}^{(0\nu)}$(J)	$M^{(0\nu)}$(U)	$t_{1/2}^{(0\nu)}$(U)
^{76}Ge	1.02	1.00	−5.077	4.0×10^{24}	−6.555	2.4×10^{24}
	1.06	1.25	−4.029	2.6×10^{24}	−5.355	1.4×10^{24}
^{82}Se	0.96	1.00	−3.535	1.9×10^{24}	−4.597	1.1×10^{24}
	1.00	1.25	−2.771	1.2×10^{24}	−3.722	6.9×10^{23}
^{96}Zr	1.06	1.00	−3.131	1.2×10^{24}	−4.319	6.1×10^{23}
	1.11	1.25	−2.065	1.1×10^{24}	−3.117	4.7×10^{23}
^{100}Mo	1.07	1.00	−3.526	1.2×10^{24}	−4.849	6.2×10^{23}
	1.09	1.25	−2.737	7.9×10^{23}	−3.931	3.8×10^{23}
^{116}Cd	0.82 (β^- decay)	1.25	−3.981	3.5×10^{23}	−4.928	2.3×10^{23}
	0.97	1.00	−3.681	1.0×10^{24}	−4.682	6.3×10^{23}
	1.01	1.25	−3.034	6.1×10^{23}	−3.935	3.6×10^{23}
^{128}Te	0.86 (β^- decay)	1.25	−4.068	9.5×10^{24}	−5.509	5.2×10^{24}
	0.89	1.00	−4.279	2.1×10^{25}	−5.841	1.1×10^{25}
	0.92	1.25	−3.383	1.4×10^{25}	−4.790	6.9×10^{24}
^{130}Te	0.84	1.00	−4.061	9.5×10^{23}	−5.442	5.3×10^{23}
	0.90	1.25	−2.993	7.0×10^{23}	−4.221	3.5×10^{23}
^{136}Xe	0.74	1.00	−2.864	1.8×10^{24}	−3.719	1.1×10^{24}
	0.83	1.25	−2.053	1.4×10^{24}	−2.802	7.6×10^{23}

about the comparison between Jyvaskylas results [5, 6, 7] and those of Tübingen [8, 9] and the recent shell-model calculations [16, 17]. To obtain physical values of the proton-neutron particle-particle interaction strength, $g_{\rm pp}$, of the pnQRPA, we fit it using the experimental rates of the $2\nu\beta\beta$ decay. The fitting included the experimental errors and the uncertainty $1.0 \le g_{\rm A} \le 1.25$ in the value of the axial-vector coupling constant $g_{\rm A}$. For ^{136}Xe only the experimental lower limit of the $2\nu\beta\beta$ half-life is available. The extracted values of $g_{\rm pp}$ and the corresponding values of $g_{\rm A}$ are listed in Table 1. We also used the available β^- decay data to fix the value of $g_{\rm pp}$. The lowest value of $g_{\rm pp}$, compatible with the β^- decay data, is also included in Table 1. For ^{100}Mo the interval determined by the β^- decay is contained in that of the $2\nu\beta\beta$ decay. From Table 1 one notices that for ^{116}Cd and ^{128}Te the β^- determined interval is in conflict with the one determined through the $2\nu\beta\beta$ data. This discrepancy is especially striking for ^{116}Cd, as was already pointed out in [20]. In Table 1 we also give the values of the nuclear matrix element of (1), calculated either by including the Jastrow or the UCOM short-range correlations on top of the other mentioned corrections. In addition, we include the corresponding half-lives $t_{1/2}^{(0\nu)}$, expressed in units of $\mathrm{yr}/(\langle m_\nu\rangle[\mathrm{eV}])^2$. As seen, the UCOM matrix elements are considerably larger in magnitude than those computed by using the traditional Jastrow approach. Such a big difference between the Jastrow and the UCOM results reflects on the estimated neutrino-mass sensitivities of the presently running and the future double-beta-decay experiments.

4. Pairing Effects

The recently measured neutron pairing correlations in the ^{76}Ge and ^{76}Se nuclei can be used as a guideline to adjust single-particle energies, so that the resulting BCS occupations reproduce the measured pairing data. The proton energies were inspected by using the odd-mass nuclei adjacent to ^{76}Ge and ^{76}Se as spectroscopic tools. The nuclear matrix element of the neutrinoless double beta ($0\nu\beta\beta$) decay of ^{76}Ge is calculated in this fitted single-particle basis by using the proton-neutron quasiparticle random-phase approximation (pnQRPA) in a realistic model space and by adopting effective microscopic two-nucleon interactions. We include the nucleon-nucleon short-range correlations and other relevant corrections at the nucleon level, as explained in the previous section. It is found that the resulting $0\nu\beta\beta$ matrix element is smaller than in the previous pnQRPA calculations, and closer to the recently reported shell-model results [16, 17]. The BCS method gives occupations of the single-particle orbitals and the occupation amplitudes are connected to the energy differences between orbitals. The customary way to determine the single-particle energy difference is to use the Woods–Saxon mean-field potential. Small adjustments of the resulting energies can be made based on the data on energy levels of odd-mass nuclei in the neighborhood of the nucleus where the pnQRPA calculation is performed. Recently a new measurement to determine the single-particle energy spectra has been reported[13]. In [13] the neutron pair correlations in the ^{76}Ge and ^{76}Se nuclei were measured by (p,t) reactions. As a result, the vacancies in the neutron subspace $28 \leq \mathrm{N} \leq 50$, hereafter called the pfg subspace, could be deduced. The adjusted basis exactly reproduces the measured spectroscopic factors in a BCS calculation [12] As a model space we have used the $N = 3$ and $N = 4$ oscillator

Table 2. Single-particle energies in the pfg subspace. Shown are the adjusted energies and their Woods–Saxon counterparts.

	^{76}Ge		^{76}Se	
Orbital	WS [MeV]	Adjusted [MeV]	WS [MeV]	Adjusted [MeV]
$\nu 1p_{3/2}$	−11.52		−12.77	
$\nu 0f_{5/2}$	−10.72	−10.30	−11.98	−11.40
$\nu 1p_{1/2}$	−9.797	−9.550	−10.98	−10.70
$\nu 0g_{9/2}$	−7.030	−9.500	−8.305	−11.00
$\pi 1p_{3/2}$	−9.015		−7.000	
$\pi 0f_{5/2}$	−8.212		−6.288	
$\pi 1p_{1/2}$	−6.789		−5.001	
$\pi 0g_{9/2}$	−5.311	−7.100	−3.371	−5.300

shells and the $0h_{11/2}$ single-particle orbital, both for protons and neutrons. The single-particle energies are obtained from the Coulomb-corrected Woods–Saxon potential. These energies are presented for the pfg subspace in Table 2. The measured neutron vacancies [13] in this sub-space have been summarized in Table 3. As can be seen from this table, the computed vacancies in the Woods–Saxon basis (WS) are far from the measured ones: the $0g_{9/2}$ orbital is much too thinly occupied and the other orbitals are too full. This can be cured by lowering the energy of the $0g_{9/2}$ orbital. Shifting also the $0f_{5/2}$ and $1p_{1/2}$ orbitals slightly, as indicated in Table 2, brings the computed vacancies right on the measured ones. This is indicated in Table 3 by the column corresponding to the adjusted basis (labelled Adj) of Table 2. It is harder to adjust the proton single-particle energies since no data on their spectroscopic factors exist yet. The computed proton vacancies in the Woods–Saxon basis are given in Table 4. One possible way to access the adjusted basis for protons is to compute the spectra of the proton-odd nuclei ^{77}As and ^{77}Br, adjacent to ^{76}Ge and ^{76}Se. For this one can use the quasiparticle-phonon coupling in diagonalizing the residual nuclear Hamiltonian. Comparing the energies of the computed one-quasiparticle states with the available data gives information on the quality of the underlying BCS calculation and thus on the mean-field single-particle energies. The critical proton orbit for the success of the quasiparticle-phonon coupling calculation is $\pi 0g_{9/2}$. The corresponding

Table 3. Measured and calculated neutron vacancies in the pfg subspace. The calculations were done in the Woods–Saxon and adjusted basis.

	^{76}Ge			^{76}Se		
Orbital	Exp.	Adj.	WS	Exp.	Adj.	WS
$\nu 1p_{1/2}$	-	0.717	0.195	-	1.016	0.282
$\nu 1p_{3/2}$	-	0.386	0.162	-	0.584	0.213
$\nu 1p_{1/2} + \nu 1p_{3/2}$	1.13	1.10	0.357	1.59	1.60	0.495
$\nu 0f_{5/2}$	1.44	1.43	0.500	2.17	2.16	0.618
$\nu 0g_{9/2}$	3.52	3.50	5.43	4.20	4.22	7.06

Table 4. Predicted proton vacancies in the pfg subspace. The calculations were done in the Woods–Saxon and adjusted basis.

	^{76}Ge		^{76}Se	
Orbital	Adj.	WS	Adj.	WS
$\pi 1p_{1/2}$	1.82	1.80	1.70	1.62
$\pi 1p_{3/2}$	2.19	1.92	1.75	1.44
$\pi 0f_{5/2}$	4.58	4.43	3.80	3.32
$\pi 0g_{9/2}$	9.28	9.73	8.61	9.49

adjusted energy is indicated in Table 2 and the calculated proton vacancies are given in Table 4. As can be seen from these tables, the proton and neutron energy shifts and the resulting vacancies behave qualitatively in the same way. However, the adjustments on the proton side do not have such drastic effects on the vacancies as on the neutron side. After settling the problem with the single-particle energies we are ready to compute the $2\nu\beta\beta$ and $0\nu\beta\beta$ NME's. As usual, we consider the two extreme values of the axial-vector coupling constant, namely the bare value $g_{\rm A} = 1.25$ and the strongly quenched value $g_{\rm A} = 1.00$. In Table 5 we list the corresponding $g_{\rm pp}$ values as extracted by comparing the measured $2\nu\beta\beta$ half-lives with the computed ones. By using these values of $g_{\rm pp}$ we have calculated the $0\nu\beta\beta$ NME's of (2) and we summarize their values in Table 5. Our computed results of Table 5 can be compared with the results of other

Table 5. Matrix elements of (2) computed in this work for different values of $g_{\rm A}$ and $g_{\rm pp}$. For the short-range correlations both the Jastrow and UCOM prescriptions have been used.

		Jastrow			UCOM		
$g_{\rm A}$	$g_{\rm pp}$	$M^{(0\nu)}_{\rm GT}$	$M^{(0\nu)}_{\rm F}$	$M^{(0\nu)}$	$M^{(0\nu)}_{\rm GT}$	$M^{(0\nu)}_{\rm F}$	$M^{(0\nu)}$
1.25	1.12	2.288	−0.772	2.779	3.385	−1.143	4.112
1.00	1.10	1.700	−0.579	2.279	2.413	−0.818	3.231

recent works in the field. A selection of recent calculations including the Jastrow and/or the UCOM correlator is given in Table 6. The second and third columns of this table give the results of [7] where exactly the same methods as here were applied, the only difference being the use of a different set of single-particle energies, where the neutron $0g_{9/2}$ orbital was shifted a good one MeV to better reproduce the low-energy spectra of ^{77}Ge and ^{77}Se in a BCS calculation. By comparing the results of these two calculations, Tables 5 and 6, one notices a significant reduction in the value of the total $0\nu\beta\beta$ matrix element $M^{(0\nu)}$. The Tübingen results [8, 9] are smaller than the results of [7]. The Jastrow results of the shell model [17] are the smallest in

Table 6. Values of the matrix element $M^{(0\nu)}$ obtained in some other recent works. Here (J) stands for Jastrow and (U) for UCOM.

g_A	(J)[7]	(U)[7]	(J)[8]	(J)[9]	(U)[9]	(J)[17]
1.25	4.029	5.355	3.92 – 4.51	4.68	5.73	2.300
1.00	3.249	4.195	3.46 – 3.83	3.33	3.92	-

Table 6. Interestingly, our present results for the Jastrow correlator, $M^{(0\nu)} = 2.779$, are closer to the shell-model result than the previous values quoted in [7]. The reduction of the magnitude of the pnQRPA calculated NME, which yields a value close to the shell-model result, is significant. The reason for the reduction of the magnitude of the $0\nu\beta\beta$ NME can be summarized by looking at the multipole decomposition of the NME. For the Fermi matrix element the reduction stems from the 0^+ intermediate states. For the Gamow–Teller matrix element $M_{\rm GT}^{(0\nu)}$ the significant changes concentrate on the 1^+ and 2^- contributions. The wave function of the 2_1^- state plays a key role when seeking the reason for the reduction of the magnitude of the Gamow–Teller matrix element. The quality of the lowest 2^- state in the intermediate nucleus ^{76}As can be tested by

Table 7. Beta-minus decay $\log ft$ values for transitions from the $2^-_{\rm g.s.}$ of ^{76}As to the ground state and one- and two-phonon states in ^{76}Se.

	$0^+_{\rm g.s.}$	2^+_1	0^+_2	2^+_2	4^+_1
Exp.	9.7	8.1	10.3	8.2	11.1
Present calc.	9.7	7.4	9.0	8.4	10.7
[7]	9.0	7.7	9.2	8.7	10.9

computing the β^- decay $\log ft$ values for transitions from this state to the ground state and one- and two-phonon states in ^{76}Se. The results obtained are compared with the data and the calculations of [7] in Table 7. As can be seen there is a drastic improvement in the $\log ft$ value of the ground-state-to-ground-state transition. This transition tests exclusively the 2_1^- wave function whereas the rest of the transitions depend also on the final-state wave function, built from the 2_1^+ collective phonon in the ^{76}Se nucleus. It is worth pointing out that in the present calculation the quasiparticle spectrum is more compressed than in the calculation of Ref. [7]. This increases the collectivity of the 2_1^+ state in ^{76}Se and thus results in smaller effective charges when trying to reproduce the data on the E2 transition probability from this state. The single β^- decay is a non-trivial way to check the reduction in the $0\nu\beta\beta$ NME: The β^- NME is reduced by 58% from the old value [7]. This is in nice agreement with the 56% reduction of the $0\nu\beta\beta$ NME. The main component of the wave function driving both transitions is the proton $0f_{5/2}$ orbital coupled to the neutron $0g_{9/2}$ orbital. In the present calculation the wave function of the 2_1^- state is more fragmented and thus reduces the pnQRPA amplitude responsible for the transitions. On the other hand, the occupation of the neutron $0g_{9/2}$ orbital has increased which also reduces the decay amplitudes since they are proportional to the emptiness of $\nu 0g_{9/2}$. Similar considerations, though in a more complicated way, apply to the intermediate 1^+ contribution. Our calculations [12] show that the main contributions to the $0\nu\beta\beta$ NME come from inside the pfg subspace. The corrected occupations in the BCS calculation most likely reproduce better the shell-model occupations and thus the pnQRPA result comes closer to the shell-model result of [17]. The small contributions from outside the pfg subspace partly explain the deviations from the shell model result. Our presently computed variations $M^{(0\nu)} = 2.279 - 2.779$ (Jastrow) and $M^{(0\nu)} = 3.231 - 4.112$ (UCOM) in the $0\nu\beta\beta$ NME can be converted to the following half-life limits

$$t_{1/2}^{(0\nu)} = (5.36 - 8.04) \times 10^{24}\,\mathrm{yr}/(\langle m_\nu \rangle[\mathrm{eV}])^2 \text{ (Jastrow)} , \quad (3)$$

$$t_{1/2}^{(0\nu)} = (2.45 - 4.00) \times 10^{24}\,\mathrm{yr}/(\langle m_\nu \rangle[\mathrm{eV}])^2 \text{ (UCOM)} . \quad (4)$$

To conclude, we have performed a pnQRPA-based calculation of the nuclear matrix elements involved in the neutrinoless double beta decay of ^{76}Ge. The recently available data on the neutron pairing correlations in ^{76}Ge and ^{76}Se have been used to modify the basic Woods–Saxon mean field to reproduce the neutron occupations of the pfg subspace in a BCS calculation. The subsequently calculated $0\nu\beta\beta$ nuclear matrix elements are smaller in magnitude than the ones obtained in a standard calculation using the Woods–Saxon single-particle energies. This stems from the reduction in the contributions of the 0^+, 1^+ and 2^- intermediate states, with a special emphasis on the first 2^- state [12].

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