Double beta decay: an interface between nuclear, particle and atomic physics

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Abstract. General properties of the nuclear matrix elements (NMEs) related to the various modes of neutrinoless double $\beta$ decays are examined and analyzed. The decays include the electron-emitting double beta-minus decays $\beta^-\beta^-$ and the various positron-emitting/electron capture decays. Special interest is devoted to the neutrinoless double electron capture decay with a resonance condition.

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1. Introduction

Numerous neutrino-oscillation experiments have provided a lot of information about the neutrino masses and mixings [1]. In particular, the mixing picture has been completed by the latest results on the so-called $\theta_{13}$ mixing angle. Only the squared neutrino mass differences can be accessed in these experiments, not the absolute mass scale. Complementary experiments are needed to learn about the absolute mass scale and mass hierarchy of the neutrinos. The neutrinoless double beta ($0\nu\beta\beta$) decay of atomic nuclei is a process that can provide us with this information, supplemented with the possibility to identify the neutrino as a Majorana particle, provided that the $0\nu\beta\beta$ really occurs in Nature. Possible detection of this decay mode would have several fundamental implications for particle physics.

Double beta decay experiments have thus far mainly concentrated on measuring the electron-emitting mode of $0\nu\beta\beta$ decays, hereafter denoted as $0\nu\beta^-\beta^-$ decays. These decays have favorable decay energies ($Q$ values) and are thus of great experimental interest at the present. Of secondary interest are the positron emitting/electron capture modes of double beta decays. There are three different types of such modes, namely the double positron emission ($0\nu\beta^+\beta^+$ decay), positron emission together with electron capture ($0\nu\beta^+\text{EC}$ decay) and the double electron capture ($0\nu\text{ECEC}$ decay). The last mode deserves particular attention since it cannot be an ordinary phase-space decay.
but needs either a resonance condition or higher-order mechanisms in order to spend the decay energy released in the transition.

All the above described modes of neutrinoless double beta decay can run through the Majorana mass of the neutrino. There are several other possibilities through which the decay can occur [1] but here we concentrate on the mass mode as inspired by the detection of the neutrino mass by the oscillation experiments. Decay rate of the mass mode is proportional to the square of the so-called effective neutrino mass, $\langle m_\nu \rangle$, being a linear combination of the mass eigenstates weighted by the two independent Majorana phases and the elements of the electron row of the neutrino mixing matrix.

Determination of the magnitude of $\langle m_\nu \rangle$ is the key issue in experiments on double beta decays. The effective mass can be extracted from the measured double-beta half-lives via the so-called nuclear matrix elements (NMEs) that intimately intertwine with the lepton aspects of the various modes of double beta decays [2, 3]. The NMEs contain the information on the nuclear wave functions of the initial and final states of the transition, in addition to the form of the effective operator(s) mediating the transition. To compute the NME we need to study details of nuclear structure by using suitable nuclear models, either microscopic or semi-microscopic [2]. These models are addressed in section 4 of this article.

2. Basic features of the neutrinoless double beta decays

Here we give the basic ingredients of the formalism of the neutrinoless double beta decays in order to enable a later discussion of the differences in the various formalisms used to describe these decays.

The $0\nu2\beta$-decay half-life can be written as [2, 4, 5]

$$\left(\frac{1}{t_{1/2}} (0^+_i \rightarrow 0^+_f)\right)_{\alpha}^{-1} = G_{\alpha}^{(0\nu)} \left( M_{\alpha}^{(0\nu)} \right)^2 |\langle m_\nu \rangle|^2,$$

(1)

where $\langle m_\nu \rangle$ is the effective neutrino mass [2]. The symbol $\alpha = \beta^-\beta^-, \beta^+\beta^+, \beta^+EC$ lists the various possible modes of neutrinoless double beta decays: double electron emission ($\beta^-\beta^-$), double positron emission ($\beta^+\beta^+$) and positron emission combined with electron capture ($\beta^+EC$) [2, 6]. The nuclear matrix element of (1) can be written as a linear combination of the Gamow–Teller, Fermi and tensor terms [7, 8], i.e.

$$M_{\alpha}^{(0\nu)}' = \left( \frac{g_A}{g_A^B} \right)^2 \left[ M_{GT}^{(0\nu)} - \left( \frac{g_V}{g_A} \right)^2 M_{F}^{(0\nu)} + M_{T}^{(0\nu)} \right],$$

(2)

where $g_A^B = 1.25$ is the bare-nucleon value of the weak-interaction axial-vector coupling constant. Values for the phase-space factors $G_{\alpha}^{(0\nu)}$ are given in [2, 4, 9, 10] for the value $g_A = 1.25$, as is required by the definition of the NME $M_{\alpha}^{(0\nu)}'$ in the above equations. Details of the associated NMEs are given e.g. in [2, 11].

The neutrinoless double electron capture $0\nuECEC$ cannot occur as such due to missing leptonic degrees of freedom in the final state. Instead, the resonant neutrinoless double electron capture (R$0\nuECEC$) can occur and it was studied in the works [12, 13]
from the lepton aspects points of view. There it was suggested that the fulfillment of a resonance condition in this decay could enhance the decay rates up to a factor of a million. The \( R_0 \nu ECEC \) decay proceeds between two atomic states as

\[
e^- + e^- + (A, Z) \rightarrow (A, Z - 2)^* \rightarrow (A, Z - 2) + \gamma + 2X,
\]

where the capture of two atomic electrons leaves the final nucleus in an excited state that decays by one or more gamma-rays (in case of an excited state) and the atomic vacancies are filled by outer electrons with emission of X-rays. The corresponding half-life for the \( 0^+ \) final states can be written as

\[
[T_{1/2}^{R_0\nu ECEC}]^{-1} = G_{\nu ECEC}^{ECEC} \left| \frac{1}{R_A} M'(0\nu) \right|^2 \frac{|(m_\nu)|^2 \Gamma}{(Q - E)^2 + \Gamma^2/4},
\]

where \( R_A = 1.2A^{1/3} \) fm is the nuclear radius and the NME is given in (2). The difference \( Q - E \) is the degeneracy of the initial and final states, \( Q \) being the difference between the masses of the initial and final atoms (decay \( Q \) value) and \( E \) is the total energy of the excited state in the final atom (consisting of the possible nuclear excitation energy, the excitation energy of the two holes in the electronic shells and the Coulomb repulsion between the holes). The quantity \( \Gamma \) is the decay width of the two holes in the atomic shells [12]. The atomic factor \( G_{\nu ECEC}^{ECEC} \) is given in [14, 15].

3. Ingredients of the pnQRPA calculations

The pnQRPA formalism is reviewed nicely in [2, 16, 17]. The pnQRPA was successfully used to explain the long two-neutrino double beta \((2\nu\beta\beta)\) decay half-lives in [18] by suppression of the associated NME relative to its simple single-particle estimate. The explanation called for the use of the strength parameter \( g_{pp} \) of the particle-particle part of the proton-neutron interaction in the \( 1^+ \) channel. This parameter governs the relative magnitudes of the particle-particle and particle-hole terms in the nuclear Hamiltonian. While the couplings of the particle-hole channel can be fixed by fitting the observed energy of the \( 1^+ \) GTGR, there is no direct way of fixing \( g_{pp} \). Since the original work a lot of studies of the effects of the \( g_{pp} \) have been done, e.g., in [17, 19, 20, 21, 22, 23].

The idea of fixing the value of the strength parameter \( g_{pp} \) by the data on half-lives of \( 2\nu\beta\beta \) decays (see the recent compilation [24]) was advocated in [25] and adopted in many subsequent works dealing with \( 0\nu\beta^-\beta^- \) decays. A shortcoming of the method is that it can be used only for those nuclei for which the \( 2\nu\beta\beta \) decay half-life is known experimentally. An alternative way to fix the value of \( g_{pp} \) would be to use the measured log \( ft \) value of the \( \beta^- \) decay of the lowest \( 1^+ \) state in the intermediate nucleus of the double beta decay. This method is the only alternative for those nuclei where the \( 2\nu\beta\beta \) decay half-life is not known [8, 26, 27, 28].

The short-range correlations between the two decaying nucleons in the \( 0\nu\beta^-\beta^- \) processes cause an effective repulsion between the two nucleons so as to prevent their overlap in the 1 fm region of their relative distance. This distance corresponds to the large average momentum exchange (\( \sim 200 \) MeV) occurring in the propagation
of the virtual Majorana neutrino between the two decay vertices. The use of the traditional Jastrow correlator [29] causes an unrealistically large suppression of the $0\nu\beta^-\beta^-$ NMEs as noticed in [30]. In this article it was proposed that the Jastrow short-range correlations should be replaced by the correlations effected by the unitary correlation operator method (UCOM) [31]. As pointed out in [30], the UCOM is a softer way to account for the short-range correlation effects in the double beta decays than the Jastrow method. Further refinements in the computation of the $0\nu\beta\beta$ decays were introduced in [7] in the form of finite-size dipole form factors of nucleons and higher-order nucleon currents, including the interference between the vector, axial-vector and induced pseudo-scalar contributions. All the latest calculations include these corrections in the $0\nu\beta\beta$ NMEs.

4. Comparison of the $0\nu\beta^-\beta^-$ NMEs calculated by different formalisms

Here we analyze the similarities and differences of the ground-state-to-ground-state $0\nu\beta^-\beta^-$ NMEs calculated in different theoretical formalisms. In Figs. 1 and 2 the NMEs calculated by the pnQRPA are compared with the corresponding NMEs of the interacting shell model (ISM) [32], the (proton-neutron) interacting boson model (IBA-2) [33, 34], the Gogny-based energy-density functional approach (EDF) [35] and the projected Hartree-Fock-Bogoliubov mean-field scheme (PHFB) [36]. The pnQRPA NMEs have been taken from [8, 37, 38, 39]. Here the unquenched value $g_A = 1.25$ for the axial-vector coupling constant has been adopted. In Fig. 1 the Jastrow short-range correlations are used and in Fig. 2 the UCOM short-range correlations are adopted. It should be noted that in the case of the decay of $^{48}$Ca an old formalism of Refs. [40, 41, 42] has been used and thus an update would be welcome. This is why a direct comparison of the pnQRPA results with the results of the other models is not straightforward in the case of $^{48}$Ca.

From Figs. 1 and 2 it is easy to deduce that the overall magnitudes of the NMEs for the pnQRPA and the IBA-2 are quite similar (magnitudes and spread) whereas the NMEs of the ISM are much smaller with very small spread. The NMEs of the EDF have similar magnitudes as those of the pnQRPA but a smaller spread. The NMEs (Jastrow and UCOM correlated) of the PHFB are by far the largest ones with clearly the largest spread. It seems that in bulk the NMEs calculated by using the pnQRPA, IBA-2 and EDF frameworks have quite similar magnitudes whereas the magnitudes of the ISM-calculated and the PHFB-calculated NMEs deviate notably from them, the ISM NMEs being quite small and the PHFB NMEs being quite large. The IBA-2 model is an advanced form of the generalized-seniority model and thus very closely related to the ISM in spirit. Also the valence spaces used in both models are restricted to one closed major shell. Hence, it is a big mystery why there is such a large difference between the magnitudes of the $0\nu\beta^-\beta^-$ NMEs produced by the two models.

All the different theoretical approaches (IBA-2, ISM, EDF and PHFB), except the pnQRPA, use the closure approximation in the calculations. This may introduce
Figure 1. Ground-state-to-ground-state NMEs of the discussed $0\nu\beta^-\beta^-$ decays for the four indicated calculations. All NMEs are calculated using the Jastrow short-range correlations. The mother nucleus is indicated on the $x$ axis. The value $g_A = 1.25$ is adopted.

Figure 2. The same as Fig. 1 but for different calculations and using the UCOM short-range correlations.
an error of some 10 percent in the calculations [43]. As noted above, the pnQRPA calculations avoid this complication by including all intermediate states in the $0\nu\beta^-\beta^-$ NMEs. The inclusion of all the spin-orbit partners in the single-particle basis is essential for the pnQRPA results to satisfy the Ikeda $3(N - Z)$ sum rule [16]. In [39] the different aspects of including single-particle states beyond the minimal one nuclear major shell were discussed and illustrated for the $0\nu\beta^-\beta^-$ ground-state-to-ground-state decays of $^{76}$Ge, $^{82}$Se, $^{128,130}$Te and $^{136}$Xe. A similar study was performed in [44, 45] for the $0\nu\beta^-\beta^-$ decays of $^{76}$Ge, $^{82}$Se and $^{136}$Xe to the first excited $0^+$ states in $^{76}$Se, $^{82}$Kr and $^{136}$Ba. In all these studies stressed was the importance of including all spin-orbit partners beyond the simple one valence major shell used in the shell-model calculations [46] of double-beta processes. Omission of these spin-orbit partners and the other single-particle states around the valence shell could cause a serious underestimation of the magnitudes of the $0\nu\beta^-\beta^-$ NMEs. This drawback not only affects the ISM calculations but also the IBA-2 calculations that are done using only one complete closed major shell. In relation to this defect it would be crucial for the ISM and IBA-2 calculations to analyze their computed rates for beta decays in medium-heavy and heavy nuclei. It should be further noted that in [39, 44, 45, 47] was performed a thorough study of the effects on the $0\nu\beta\beta$ NMEs by the use of different occupancies of the valence single-particle orbitals. Large effects could be found only for $^{76}$Ge.

Let us study next the importance of shell effects on the $0\nu\beta^-\beta^-$ NMEs. From Fig. 1 one immediately perceives the stunning similarity between the trends of the pnQRPA, IBA-2 and the ISM NMEs. Indeed the three models are one-to-one for the mass ranges $A \leq 82$ and $A \geq 124$. The striking similarity of the pnQRPA and the IBA-2 continues even beyond that, to the masses $96 \leq A \leq 116$. The only qualitative deviation is at $^{110}$Pd where a much weaker peaking of the NME is obtained in the IBA-2 model than in the pnQRPA. From Fig. 2 it is seen that the trends of the pnQRPA and the two mean-field based models (EDF and PHFB) are quite different. To study more closely these matters, we can take as a paradigm the generalized seniority (GS) scheme which is a reasonable approximation to a more complete shell-model calculation. The generalized seniority prescription advocated in [33] describes the $0\nu\beta^-\beta^-$ NMEs in the $N = 50 - 82$ major shell as smooth concave arches for different proton numbers $Z$. In this way one obtains the ratio

$$R = \frac{M^{(0\nu)}}{M_{\text{GS}}^{(0\nu)}}$$

which gives a measure how close the calculated NMEs of a nuclear model are to those of the simple generalized seniority scheme.

The ratios (5) are summarized in Table 1 for all the discussed nuclear models in the range $124 \leq A \leq 136$, i.e. between $^{124}$Sn and $^{136}$Xe. As can be seen the IBA-2, ISM and pnQRPA conform excellently to the GS scheme. It is even more striking to see that, in fact, the pnQRPA obeys by far the best the seniority scheme. On the other hand the EDF and PHFB are drastically off from the generalized-seniority trends which may point to missing shell effects in these two mean-field based schemes. In particular,
Table 1. Ratios (5) for the indicated nuclei in the five different model frameworks (first column).

| Model   | \( A = 124 \) | \( A = 128 \) | \( A = 130 \) | \( A = 136 \) |
|---------|----------------|----------------|----------------|----------------|
| IBA-2   | 0.912          | 1.00           | 1.00           | 1.13           |
| ISM     | 1.05           | 1.00           | 1.01           | 1.15           |
| pnQRPA  | 1.01           | 1.00           | 1.02           | 0.95           |
| EDF     | 1.36           | 1.00           | 1.39           | 1.56           |
| PHFB    | -              | 1.00           | 1.24           | -              |

The GS scheme predicts for the ratio

\[
R(Te) = \frac{M^{(0\nu)\beta^+}(^{128}\text{Te})}{M^{(0\nu)\beta^+}(^{130}\text{Te})}
\]

the value \( R_{GS}(\text{Te}) = 1.11 \). For the respective nuclear models this ratio is 1.11 (IBA-2), 1.10 (ISM), 1.10 (pnQRPA), 0.80 (EDF) and 0.90 (PHFB), thus indicating that the trend is not correct for the EDF and PHFB models.

5. Double positron-emission/electron-capture decays

The double positron-emission/electron-capture decays have generally smaller decay \( Q \) values than the double electron-emission decays [2]. On the positron-emission/electron-capture side the decay \( Q \) value depends on the mode.

![Figure 3](image_url)

*Figure 3.* Schematic representation of the \( 0\nu\beta^+\beta^+ \) decay (left panel), the \( 0\nu\beta^+\text{EC} \) decay (middle panel) and the \( R0\nu\text{ECEC} \) decay (right panel). In the last decay an atomic resonance state matches the decay energy. The horizontal dashed line represents the exchanged Majorana neutrino.

In Fig. 3 the two-positron emission \( (0\nu\beta^+\beta^+) \), the positron-emission plus electron capture \( (0\nu\beta^+\text{EC}) \) and the resonant neutrinoless double electron capture \( (R0\nu\text{ECEC}) \) modes of decay are displayed schematically. In these decays a Majorana neutrino is
exchanged as displayed by the horizontal dashed line in the figures. In all modes two protons are changed to two neutrons and one has to consider the short-range correlations between the decaying nucleons in the same way as done for the $0\nu\beta^-\beta^-$ decays \cite{30}. The $Q$ value is larger for the $0\nu\beta^+\text{EC}$ mode than for the $0\nu\beta^+\beta^+$ mode since there is one less positron in the final state and the rest-mass energy of the captured electron (minus the electron binding in the atomic orbital) can be exploited as decay energy. The neutrinoless ECEC cannot proceed as such since there are no leptons in the final state and hence the decay energy cannot be absorbed by them. Instead, the decay energy can be wasted by hitting a resonance in the final atom, as discussed in the section 2. This leads to the $R0\nu\text{ECEC}$ decay.

The orders of magnitude of the half-lives associated with the various positron-emitting transitions in nuclei have been assessed recently in \cite{14} for the decay of $^{106}\text{Cd}$ and in \cite{48} for the decay of $^{96}\text{Ru}$. Furthermore, in Table 2 is presented an overview of those resonant neutrinoless ECEC decays for which the associated decay $Q$ values have been measured by exploiting the Penning-trap techniques.

| Transition | $J^\pi$ | $Q - E$ [keV] | Atomic orbitals | $C^{\text{ECEC}}$ | Ref. |
|------------|--------|---------------|-----------------|-----------------|------|
| $^{74}\text{Se} \rightarrow ^{74}\text{Ge}$ | $2^+$ | 2.23 | L$_2$L$_3$ | $(0.2 - 100) \times 10^{43}$ | \cite{49} |
| $^{96}\text{Ru} \rightarrow ^{96}\text{Mo}$ | $2^+$ | 8.92(13) | L$_1$L$_3$ | | \cite{50} |
| $^{102}\text{Pd} \rightarrow ^{102}\text{Ru}$ | $0^+$ | $-3.90(13)$ | L$_1$L$_1$ | $(4.4 - 19) \times 10^{31}$ | \cite{51} |
| $^{106}\text{Cd} \rightarrow ^{106}\text{Pd}$ | $0^+$ | 8.39 | KK | $(2.1 - 5.7) \times 10^{30}$ | \cite{14} |
| $^{112}\text{Sn} \rightarrow ^{112}\text{Cd}$ | $(2,3)^-$ | $-0.33(41)$ | KL$_3$ | | \cite{51} |
| $^{136}\text{Ce} \rightarrow ^{136}\text{Ba}$ | $0^+$ | $-11.67$ | KK | $(3 - 23) \times 10^{32}$ | \cite{53} |
| $^{144}\text{Sm} \rightarrow ^{144}\text{Nd}$ | $2^+$ | 171.89(87) | KL$_3$ | | \cite{51} |
| $^{152}\text{Gd} \rightarrow ^{152}\text{Sm}$ | $0^+$ | 0.91(18) | KL$_1$ | $\sim 1 \times 10^{26}$ | \cite{54} |
| $^{156}\text{Dy} \rightarrow ^{156}\text{Gd}$ | $1^-$ | 0.75(10) | KL$_1$ | | \cite{55} |
| | $0^+$ | 0.54(24) | L$_1$L$_1$ | | \cite{55} |
| | $2^+$ | 0.04(10) | M$_1$M$_3$ | | \cite{55} |
| $^{162}\text{Er} \rightarrow ^{162}\text{Dy}$ | $2^+$ | 2.69(30) keV | KL$_3$ | | \cite{50} |
| $^{168}\text{Yb} \rightarrow ^{168}\text{Er}$ | $(2^-)$ | 1.52(25) keV | M$_1$M$_3$ | | \cite{50} |

In the table are also listed the theoretically estimated half-lives for the cases for which such exist. In the table a quantity $C^{\text{ECEC}}$ is given and it ties to the $R0\nu\text{ECEC}$ half-life through

$$T_{1/2}^{\text{R0}\nu\text{ECEC}} = \frac{C^{\text{ECEC}}}{\langle (m_\nu[\text{eV}])^2 \rangle} \text{years}, \tag{7}$$

where the effective neutrino mass should be given in units of eV.
6. Conclusions

In this paper I have presented the ranges of values of the nuclear matrix elements corresponding to the double $\beta^{-}$ decays of nuclei of masses $48 \leq A \leq 136$. All these nuclear matrix elements are analyzed with respect to the use of the closure approximation, size of the single-particle model space, short-range correlations and shell effects. One can conclude that thus far only the pnQRPA manages to avoid the use of the closure approximation in the NME calculations. Some of the recent models are mean-field based and seem to have trouble in reproducing shell effects. The IBA-2 and the ISM use only one closed major shell as their model space whereas the pnQRPA and the mean-field based models allow larger valence spaces. Although the IBA-2 maps to the seniority scheme and is thus closely related to the ISM, the magnitudes of the NMEs of the two models deviate notably from each other. These models also suffer of the lack of explicit inclusion of the spin-orbit partner orbitals in the calculations. Summarizing the above features one could argue that the pnQRPA is still the scheme that is most complete and best suited for reliable calculation of the values of the double-beta-decay nuclear matrix elements.

For the positron-emission/electron-capture decays there remains a whole lot of theoretical and experimental work to be done, especially in the case of the resonant neutrinoless ECEC decays.

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