Double beta decay of $^{100}\text{Mo}$: the deformed limit

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The double beta decay of $^{100}\text{Mo}$ to the ground state and excited states of $^{100}\text{Ru}$ is analysed in the context of the pseudo SU(3) scheme. The results of this deformed limit are compared with the vibrational one based on the QRPA formalism. Consistency between the deformed limit and the experimental information is found for various $\beta\beta$ transitions, although, in this approximation some energies and B(E2) intensities cannot reproduced.

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The two neutrino mode of the double beta decay ($\beta\beta_{2\nu}$) is an exotic but allowed second order process in the standard model. It has been detected in nine nuclei and has served as a tool to develop the most refined experimental

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detection methods for very low signals. It also represents a severe test on the nuclear structure description of those nuclei [1].

The \(^{100}\text{Mo}\) is an excellent subject of study. Its large Q-value, \(Q_{\beta\beta} = 3.034\text{MeV}\), favors its decay. Four groups have reported on the detection of the \(\beta\beta_{2\nu}\) of \(^{100}\text{Mo}\) to the ground state of \(^{100}\text{Ru}\) with half-lives of the order of \(10^{19}\text{yrs}\) [2,3,4,5]. Also the decay to the first excited \(0^{+}_1\) state has been reported [4,6].

This abundance of experimental information allowed a careful check of the nuclear models used to describe the two neutrino mode. The QRPA model, both in its conventional and number projected versions, was found to collapse when realistic particle-particle interactions are used [7,8]. Under the assumption that the excited 1130 keV \(0^{+}\) state in \(^{100}\text{Ru}\) is a member of a \(0^{+}, 2^{+}, 4^{+}\) two-phonon vibrational triplet the QRPA calculation exhibits an overestimation of the amplitude of the \(\beta\beta_{2\nu}\) decay to this excited state. However the decay to the ground state is reasonably well reproduced by using the same approximation. The single beta-decay transition between the initial and intermediate nuclei is also overestimated by the theory [7]. Assuming realistic nucleon-nucleon interactions similar results were found, i.e. the \(\beta\beta_{2\nu}\) decay amplitudes are overestimated. This result is particularly true for the decay to the first \(2^{+}\) state [10].

All the works dealing with the \(\beta\beta_{2\nu}\) decay of \(^{100}\text{Mo}\) found a strong dominance of one single particle transition: \((g_{7/2}(n))^2 \rightarrow (g_{9/2}(p))^2\). This lack of collectivity was mentioned as a possible cause of the failure of the QRPA to describe the \(\beta\beta_{2\nu}\) decay of this specific nucleus [8] while having success in others [7,11,12,13].

Other complementary explanation could be that deformation effects were destroying the one-phonon–two-phonon structure in \(^{100}\text{Ru}\), and substituting it with rotational bands built upon a deformed ground state or some vibrational
intrinsic excitations [10]. In the present paper we explore both possibilities using the pseudo SU(3) formalism.

The transition from spherical to deformed shapes in Mo isotopes was study microscopically several years ago, commenting on the deformed character of some first excited 0\(^+\) states [14]. In a similar way within the General Collective Model (GCM) [15] a study of the potential energy surfaces (PES) of the Ru isotopes [16] exhibited a transition from a harmonic oscillator (\(^{98}\)Ru) to a nucleus with triaxial dominance (\(^{108}\)Ru). All Ru isotopes between \(^{100}\)Ru and \(^{104}\)Ru behave very similar [16]. The PES has a global minimum at \(\beta = 0\), suggesting an harmonic oscillator for the low lying states. There is also a local minimum at \(\beta\) approximately 0.4 and \(\gamma = 24^\circ\), which suggests triaxial shapes for excited states. However the energy of the ground state lies above the potential barrier between the spherical and the triaxial minimum. As a consequence, the ground state, the first and second excited 2\(^+\) state are spread out between the global and triaxial minimum showing the behavior of an anharmonic oscillator, while the first excited 0\(^+\) and third excited 2\(^+\) state are peaked within the triaxial minimum. As a picture we obtain the spectrum of an anharmonic oscillator were the first excited 0\(^+\) state does not fit into it. Nevertheless the \(B(E2)\) transitions follow the characteristic of an anharmonic oscillator within a simple consideration, i.e., the transition from the first exited 0\(^+\) state to the first excited 2\(^+\) state is strong compared to the second excited 2\(^+\) state, which is weak. This did lead in the past to the assumption that \(^{100}\)Ru resembles more an anharmonic oscillator.

We will use the pseudo SU(3) model [17] to provide a microscopical description of the ground and excited low energy states in \(^{100}\)Ru, and the ground state of \(^{100}\)Mo including deformation. This exercise will supply a rotational limit in the description of these nuclei, to be compared with the spherical, vibrational limit obtained with the QRPA.
The double beta decay, when described in the pseudo SU(3) scheme, is strongly dependent on the occupation numbers for protons and neutrons in the normal and abnormal parity states $n^N_\pi, n^N_\nu, n^A_\pi, n^A_\nu$ [18]. In particular, the $\beta\beta_{2\nu}$ decays are allowed only if they fulfil the following relations:

$$n^A_\pi,f = n^A_\pi,i + 2, \quad n^A_\nu,f = n^A_\nu,i, \quad n^N_\pi,f = n^N_\pi,i, \quad n^N_\nu,f = n^N_\nu,i - 2$$

These numbers are determined by filling the Nilsson levels from below, as discussed in [18]. They are exhibited in Table 1 as the deformed occupation (def-o) case. Both $^{100}Mo$ and $^{100}Ru$ have deformations $\beta \approx 0.23$. This number must be taken carefully, given these nuclei do not exhibit a rotational spectra, but is a hint about their average deformations. We were forced to select a slightly higher deformation for neutrons than for protons. If not, the removed pair of neutrons in $^{100}Ru$ would come from the abnormal parity orbital, and in this case the expressions (1) would not be fulfilled suppressing the $\beta\beta_{2\nu}$ decay.

In the third and fourth row of Table 1 the occupations in the spherical occupation (sph-o) limit ($\beta \leq 0.09$) are given. This is a very interesting limiting case, in which all the proton holes belong to the abnormal $g_{9/2}$ orbit and all the neutron particles to the normal parity orbitals.

In the abnormal parity space only seniority zero configurations are taken into account. This is a very strong assumption, which in future works is expected to be improved, but is quite useful in order to simplify the calculations. Its effects in the present calculation are discussed below.

Under the assumption of a Hamiltonian consisting in a Nilsson mean field and a strong quadrupole-quadrupole interaction, the deformed wave functions of $^{100}Mo$ and $^{100}Ru$, with angular momentum $J$ and belonging to the ground state ($\sigma = g.s.$) or the excited ($\sigma = exc.$) band can be constructed according to [18]. The result is:
\[ |^{100}Mo(Ru), J^+ \sigma \rangle = \{2^{\otimes N}_\pi \}(\lambda_\pi, \mu_\pi); \{2^{\otimes N}_\nu \}(\lambda_\nu, \mu_\nu); 1(\lambda \mu)_\sigma K = 1J >_N \]
\[ (g_{9/2})^{n_\pi^2}; J_\pi^A = 0; (h_{11/2})^{n_\nu^2}; J_\nu^A = 0 >_A , \]
expectation value of the Hamiltonian between the $^{100}Ru$ wave functions only depends on the $(\lambda, \mu)$ and $J = L$ of the normal parity orbitals. Explicitly:

$$<^{100} Ru, (\lambda, \mu)K = 1, L = J M | H |^{100} Ru, (\lambda, \mu)K = 1, L = J M > =$$

$$N_s \hbar \omega - 2\chi C_2 - (\frac{3}{2}\chi + a)L(L + 1)$$

In the above expression $N_s$ represents the number of proton plus neutron phonons, which depends only on the normal parity occupations $n^N_\pi$ and $n^N_\nu$ and do not depend on the irrep or on the angular momentum $L$. The eigenvalues of the second order Casimir operator of SU(3) is $C_2 = (\lambda + \mu + 3)(\lambda + \mu) - \lambda\mu$. The irrep $(8, 6)$ has the maximum value of $C_2 = 190$ and yields the ground state band. The second $0^+$ and $2^+$ states were associated with the irrep $(10, 2)$, with $C_2 = 160$.

The two parameters of the Hamiltonian (3) are fitted by means of the excitation energies of the first $2^+$ and the first excited $0^+$ states. The results are $\chi = 18.83keV$, $a = 61.75keV$, which are reasonable numbers as an interpolation between those needed to reproduce the rotational spectra of $^{24}Mg$ \cite{19} and $^{238}U$ \cite{20}. In the comparison it must be taken into account that the Refs. \cite{19} and \cite{20} use symplectic extensions of SU(3) model and thus they need smaller coupling constants.

In Table 2 the experimental and theoretical low lying states in $^{100}Ru$ are presented, with the angular momentum, parity and energy stated in each level, as well as the corresponding irrep $(\lambda, \mu)$ of each band. As expected, the energies of the first $4^+$ and the second $2^+$ states are overestimated. This is a remainder that the present exercise is a rotational limit of a triaxial nucleus, whose low energy spectra evokes an anharmonic oscillator, as it was mentioned above.

The average quadrupolar moment $Q_0$ is related with a particular B(E2) value as follows:
\[ B(E2,0^+ \rightarrow 2^+) = \frac{5}{16\pi}|Q_0|^2 \] (6)

In the pseudo SU(3) scheme, this intrinsic quadrupolar moment is easily evaluated as \[22\]

\[ Q_0 = e_\pi^{eff} Q_\pi + e_\nu^{eff} Q_\nu \quad Q_\alpha = \frac{\eta_\alpha + 1}{\eta_\alpha} (2\lambda_\alpha + \mu_\alpha) \] (7)

where \(Q_0\) is given in units of \(e \ b_0^2\) with \(b_0^2 = \frac{\hbar}{M\omega} = 4.70 \text{fm}^2\). Using the wave functions of the ground state band [2] the intrinsic quadrupole moments are:

\[ Q_\pi = 5.33 \quad Q_\nu = 22.5 \] (8)

The experimental value is \(Q_0(\text{exp}) = 57.7 e \ b_0^2\). To reproduce this result unreasonable effective charges \(e_\pi^{eff} \approx 2.9 e\) and \(e_\nu^{eff} \approx 1.9 e\) would be needed. This failure of the pseudo SU(3) model in reproducing the quadrupole moment of \(^{100}\text{Ru}\) is related with the use of the seniority zero approximation for nucleons in abnormal parity orbitals. In the case of \(^{100}\text{Ru}\) case even in the def-o limit there are only two normal holes and the associated irrep \((0,4)\) gives a very little proton quadrupole moment. The greater part of the proton quadrupole moment must come from protons in the abnormal parity orbital \(g_{9/2}\), whose contribution is neglected in the seniority zero approximation. These limitations were discussed previously [21,22]. In this picture large effective charges are always needed in order to compensate this effect. For the case of \(^{100}\text{Ru}\) these effective charges are too large. Although we have presented here some limitations of the rotational model of \(^{100}\text{Ru}\), it is successful in describing the \(\beta\beta_{2\nu}\) decay of \(^{100}\text{Mo}\).

We turn now to the study of the two neutrino mode of the double beta decay \(\beta\beta_{2\nu}\) of \(^{100}\text{Mo}\) into the ground state, the first \(2^+\) and the first excited \(0^+\) states of \(^{100}\text{Ru}\). The mathematical expressions needed to evaluate the \(\beta\beta_{2\nu}\) to the ground state of \(^{100}\text{Ru}\) can be found in [18]. The same formulae works for the decay to the first excited \(0^+\) state, replacing the strong coupled
irrep $(8,6)$ by $(10,2)$. The decay to the first $2^+$ state requires a different expression, which can be found in [23]. The formulae for this decay resembles that of the decay to the $0^+$ states, but the energy denominator is elevated to the third power. Being in general this energy of the order of 10 $MeV$ this power implies a factor 100 of suppression for this matrix element [1,9,10].

In Table 3 the dimensionless $\beta\beta_{2\nu}$ matrix elements for the decay of $^{100}Mo$ to the ground state, the first $2^+$ and the first excited $0^+$ states of $^{100}Ru$ are presented. The first two rows include the results of the QRPA calculations obtained using a $\delta$-interaction [9] and an interaction derived from the Bonn one-boson-exchange potential using G-matrix techniques [10]. The third row shows the results for the pseudo SU(3) calculation using the def-o wave functions given in Eq. (2). The energy denominator used for the decay to the ground state, determined by fixing the energy of the Isobaric Analog State [18] is $E = E_0 - 2\hbar\omega k_r (\eta_\nu + \frac{1}{2}) + \Delta_C = 7.95 MeV$, where $E_0 = \frac{1}{2} Q_{\beta\beta} + m_e c^2$ and $\Delta_C$ is the Coulomb displacement energy. The matrix elements are given in units of the first or third power of the inverse electron mass [1], since the energy denominators have been divided by the electron rest mass. For the first $2^+$ state the energy denominator is equal to 7.68 MeV and for the first excited $0^+$ it is 7.39 MeV. The results for the sph-o pseudo SU(3) approach are given in the fourth row. As it was anticipated in the spherical occupation limit the decay to the excited $0^+$ state is absent.

The experimental matrix elements showed in Table 3 were extracted from the measured half-lives $T_{2\nu}^{1/2}$ using phase space integrals $G_{GT}$, which were obtained following the prescriptions given in [24] with $g_A/g_V = 1.0$. These data are reproduced in the last two rows of Table 3.

It is remarkable that the sph-o pseudo SU(3) limit reproduces quite well the experimental matrix element for the $\beta\beta_{2\nu}$ to the ground state and that the def-o pseudo SU(3) limit is able to do the same with the matrix element.
related with the $\beta\beta_{2\nu}$ decay to the first $0^+$ state. Both the ability to reproduce the numbers and the difficulty to fit both in the same model are pointing to the description or $^{100}$Ru as a triaxial nucleus.

The $\beta\beta_{2\nu}$ matrix element for the $0^+ \rightarrow 2^+$ decay is strongly cancelled in comparison with the QRPA one [10]. In the sph-o case, which successfully reproduce the $0^+ \rightarrow 0^+(g.s.)$ decay, the reduction has two contributions: i) the matrix element of the operator $\sigma_1 \cdot \sigma_2$ which connects the $0^+$ states is a factor ten greater than the matrix element of the operator $[\sigma_1 \otimes \sigma_2]^2$ which mediates the other decay; ii) the energy denominator in the pseudo SU(3) model is approximately three times greater than the energy denominator associated with the first intermediate state $1^+$, giving a $3^3 = 27$ additional reduction when compared with the QRPA result.

In order to estimate the effect of the quadrupole-quadrupole correlations over the $\beta\beta_{2\nu}$ matrix elements, we have performed also a simple estimation of these matrix elements under the pure seniority zero approximation. It is a model in which only the $g_{9/2}^\pi$ and $g_{7/2}^\nu$ orbitals are active, with the nucleons paired to angular momentum zero. There are 2 protons and 8 neutrons in $^{100}$Mo and 4 protons and 6 neutrons in $^{100}$Ru. These two (four) protons are described in the same way in this simple approach and in the sph-o pseudo SU(3) scheme but neutrons have strong mixing with their partners in the $N = 4$ oscillator shell in the pseudo SU(3) scheme which is absent in the other.

The seniority zero matrix elements [18] are exactly the same as the pure pairing ones [7,13], i.e.

$$ M_{2\nu}(0^+_i \rightarrow 0^+_j (g.s.)) = \sum_{pn} \frac{u_p v_n \bar{u}_p \bar{v}_n < p | \sigma | n >^2}{e_p + e_n - E_0} $$

$$ (9) $$

There exist only one $(p, n) = (g_{9/2}^\pi, g_{7/2}^\nu)$ configuration in this approach, limiting the sum to only one term. The pairing occupation numbers $v_n^2$ in
the initial (unbarred) and final (barred) nuclei are \( u_p^2 = 0.8, \bar{u}_p^2 = 0.4, v_n^2 = 1.0, \bar{v}_n^2 = 0.25 \). Using this numbers together with the energy denominator given above we have obtained the matrix element for the \( \beta \beta_{2\nu} \) in this seniority zero approach which is given in the fifth row of Table 3. The comparison with the pseudo SU(3) matrix elements exhibits a reduction by a factor two in the sph-o limit and by a factor three in the def-o one. This reduction is due to the quadrupole-quadrupole correlations, which strongly mix the \( g_{\frac{5}{2}} \) with their shell partners, and also mix these neutrons with the normal parity protons. Using an energy denominator consisting essentially of twice the pairing gap plus half the Q-value (\( \approx 3\text{MeV} \)) would increase the seniority zero matrix element making it worst when compared with the experimental value.

In the present paper we have studied the \( \beta \beta_{2\nu} \) of \( ^{100}\text{Mo} \) to \( ^{100}\text{Ru} \) in the context of the pseudo SU(3) model. It was also mentioned that in the geometrical model, while the \( ^{100}\text{Ru} \) ground state essentially feels an anharmonic oscillator potential, the first excited \( 0^+ \) state is concentrated in the deformed region. We have explored the possibility of a coexistence of shapes, trying to find out a possible explanation for the difficulties found in previous attempts to describe the \( \beta \beta_{2\nu} \) of \( ^{100}\text{Mo} \) to excited states of \( ^{100}\text{Ru} \) which described the first excited \( 0^+ \) state as a two phonon state.

We have used the pseudo SU(3) model as a deformed limit and compared it with the QRPA, which is taken as the spherical limit. Under this scheme, and with the additional approximation of a seniority zero wave function for the abnormal parity nucleons, we have generated a rotational spectrum for \( ^{100}\text{Ru} \) which does not resemble so much the experimental one. Also, we were not able to generate enough proton quadrupole moment since we have used the seniority zero approximation for abnormal parity nucleons. Besides this limitations, the description of the \( \beta \beta_{2\nu} \) was successful. We were able to reproduce the experimental nuclear matrix elements, without any parameter,
but using the *deformed occupation* pseudo SU(3) wave function for $\beta\beta_{2\nu}$ to the first excited $0^+$ state, and the *spherical occupation* pseudo SU(3) wave function for the $\beta\beta_{2\nu}$ to the ground state. Fitting both decays in the same model is not possible, at least within the present scenario.

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Table captions

**Table 1** Occupation numbers and \((\lambda's, \mu's)\) for the deformed occupation \((\text{def-o})\) and spherical occupation \((\text{sph-o})\) pseudo SU(3) wave function for \(^{100}\text{Mo}\) and \(^{100}\text{Ru}\).

**Table 2** Experimental and theoretically determined energies (in keV) for the ground state \((\text{g.s})\) and excited \((\text{exc.})\) band of \(^{100}\text{Ru}\).

**Table 3** The dimensionless \(\beta\beta_{2\nu}\) matrix elements for the decay of \(^{100}\text{Mo}\) to the ground state, the first \(2^+\) and the first excited \(0^+\) states of \(^{100}\text{Ru}\), evaluated with different models. The experimental matrix elements, measured half lives \(T_{2\nu}^{1/2}\) and phase space integrals \(G^{GT}\) are also listed.
Table 1

|   | $n^A_\pi$ | $n^A_\nu$ | $n^N_\pi$ | $n^N_\nu$ | $(\lambda_\pi, \mu_\pi)$ | $(\lambda_\nu, \mu_\nu)$ | $(\lambda, \mu)_{g.s.}$ | $(\lambda, \mu)_{e.x.c.}$ |
|---|---|---|---|---|---|---|---|---|
| Mo | 4 | 2 | 10 | 6 | (0, 4) | (12, 0) | (12, 4) |   |
| def−o |   |   |   |   |   |   |   |   |
| Ru | 6 | 2 | 10 | 4 | (0, 4) | (8, 2) | (8, 6) | (10, 2) |
| Mo | 2 | 0 | 12 | 8 | (0, 0) | (10, 4) | (10, 4) |   |
| sph−o |   |   |   |   |   |   |   |   |
| Ru | 4 | 0 | 12 | 6 | (0, 0) | (12, 0) | (12, 0) |   |

Table 2

| $J^+$ | $irrep$ | $g.s. \text{ band}$ | $exc. \text{ band}$ |
|---|---|---|---|
| $th.$ | $exp.$ | $th.$ | $exp.$ |
| 0$^+$ | (8, 6) | (10, 2) |   |
| 2$^+$ | 0 | 1130 | 1130 |
| 4$^+$ | 540 | 1362 | 1670 |
| 4$^+$ | 1800 | 1227 |   |
| Process                  | $Q_{RP A}$ [9] | $Q_{RP A}$ [10] | $\text{pseudoSU}(3)(\text{def} - o)$ | $\text{pseudoSU}(3)(\text{sph} - o)$ | $\text{seniority} 0$ | $\text{experiment}$ |
|--------------------------|----------------|----------------|------------------------------------|------------------------------------|---------------------|--------------------|
| $0^+ \rightarrow 0^+(g.s.)$ | $-0.256$       | $0.197$        | $-0.108$                            | $0.152$                            | $-0.323$            | $\pm 0.150$       |
| $0^+ \rightarrow 0^+(\text{exc.})$ | $-0.256$       | $-0.271$       | $0.098$                             | $7.3 \times 10^{-5}$               | $< 0.106$           |                    |
| $0^+ \rightarrow 2^+$     |                |                | $1.53 \times 10^{-4}$              |                                    |                     |                    |

**Additional Data**

| $T_{2
u}^{1/2}$ [$10^{19} \text{yr}$] | 1.15           | 178            | > 11.5                             |                      |
| $G_{\text{GT}}$ [$10^{-20} \text{yr}^{-1}$] | 387           | 6.61           | 76.6                               |                      |