Double-beta decay of ^{100}Mo: The deformed limit

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The double-beta decay of ^{100}Mo to the ground state and excited states of ^{100}Ru is analyzed in the context of the pseudo-SU(3) scheme. This deformed limit is compared with the vibrational one based on the quasiparticle random-phase approximation. 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 be 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 it represents a severe test on the nuclear-structure description of those nuclei [1].

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

This abundance of experimental information allowed a careful check of the nuclear models used to describe the two neutrino mode. The quasiparticle random-phase approximation (QRPA) model, both in its conventional and number projected versions, was found to collapse when realistic particle-particle interactions are used [6,7]. Under the assumption that the excited 1130-keV 0^+ state in ^{100}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 [8]. This result is particularly true for the decay to the first 2^+ state [9]. However the decay to the ground state is reasonably well reproduced by using the same approximation.

All the works dealing with the $\beta\beta_{2\nu}$ decay of ^{100}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 [7] while having success in others [1,6].

Another complementary explanation could be that deformation effects were destroying the one-phonon–two-phonon structure in ^{100}Ru, and substituting it with rotational bands built upon a deformed ground state or some vibrational intrinsic excitations [9]. In this paper we explore both possibilities using the pseudo-SU(3) formalism.

Within the general collective model (GCM) a study of the potential energy surfaces (PES) of the Ru isotopes [10] 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 [10]. The PES has a global minimum at $\beta = 0$, suggesting a harmonic oscillator for the low-lying states. There is also a local minimum at β approximately 0.4 and $\gamma = 24°$, 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^+ states 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 where the first excited 0^+ state does not fit into it.

We will use the pseudo-SU(3) model 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 $n_\pi^N, n_\nu^N, n_\pi^A, n_\nu^A$ [11]. In particular, the $\beta\beta_{2\nu}$ decays are allowed only if they fulfill the following relations: $n_{\pi,f}^A = n_{\pi,i}^A + 2$, $n_{\nu,f}^A = n_{\nu,i}^A$ $n_{\pi,f}^N = n_{\pi,i}^N$, $n_{\nu,f}^N = n_{\nu,i}^N - 2$. These numbers are determined by filling the Nilsson levels from below, as discussed in [11]. They are exhibited in Table I as the *deformed occupation* (def-o) case. Both ^{100}Mo and ^{100}Ru have deformations $\beta \approx 0.23$. 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

TABLE I. Occupation numbers and (λ's,μ's) for the *deformed occupation* (def-o) and *spherical occupation* (sph-o) pseudo-SU(3) wave function for ^{100}Mo and ^{100}Ru.

		n_π^A	n_ν^A	n_π^N	n_ν^N	(λ_π,μ_π)	(λ_ν,μ_ν)	$(\lambda,\mu)_{\text{g.s.}}$	$(\lambda,\mu)_{\text{exc}}$
def-o	Mo	4	2	10	6	(0,4)	(12,0)	(12,4)	
	Ru	6	2	10	4	(0,4)	(8,2)	(8,6)	(10,2)
sph-o	Mo	2	0	12	8	(0,0)	(10,4)	(10,4)	
	Ru	4	0	12	6	(0,0)	(12,0)	(12,0)	

the abnormal parity orbital, and in this case the above expressions would not be fulfilled suppressing the $\beta\beta 2_\nu$ decay.

In the third and fourth rows of Table I 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 but is useful in order to simplify the calculations.

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 (σ = g.s.) or the excited (σ = exc) band can be constructed according to [11]. The result is

$$|^{100}\text{Mo (Ru)}, J^+\sigma\rangle = |\{2^{\frac{n_\pi^N}{2}}\}(\lambda_\pi,\mu_\pi);\ \{2^{\frac{n_\nu^N}{2}}\}(\lambda_\nu,\mu_\nu);\ 1(\lambda\mu)_\sigma K=1J\rangle_N \\ |(g_{9/2})^{n_\pi^A},\ J_\pi^A=0;\ (h_{11/2})^{n_\nu^A},\ J_\nu^A=0\rangle_A. \tag{1}$$

Each (λ's,μ's) are also depicted in Table I. In this approach, instead of assuming the first excited 0^+ and the second 2^+ states as parts of a two phonon triplet, together with the first 4^+ states, it is assumed that the first $0^+, 2^+, 4^+$ states of ^{100}Ru are the low energy sector of a rotational band based in the normal $(\lambda,\mu)_{\text{g.s.}} = (8,6)$ strong coupled pseudo-SU(3) configuration and that the second $0^+, 2^+$ excited states belong to a second rotational band described by the $(\lambda,\mu)_{\text{exc}} = (10,2)$ pseudo-SU(3) configuration. Note that in the sph-o case the proton normal parity orbitals ($\tilde{N}=3$) are filled, giving rise to the irrep $(0,0)$. It implies that there exists only one strong coupled stated $(0,0)_\pi \times (12,0)_\nu = (12,0)$, and in our restrictive Hilbert space there is not a 0^+ excited state.

In order to analyze the spectra and transitions amplitudes of ^{100}Ru we have selected a simplified version of the pseudo-SU(3) Hamiltonian [11], i.e.,

$$H = \sum_\alpha H_\alpha - \tfrac{1}{2}\chi \mathbf{Q}^a\cdot\mathbf{Q}^a + aL^2\ ,\quad \alpha=\pi,\nu, \tag{2}$$

where the algebraic quadrupole operator $\mathbf{Q}^a = \sum_s \{q_{\pi s} + q_{\nu s}\}$ acts only within a shell and H_α is the spherical Nilsson Hamiltonian.

The abnormal parity sector of the wave function contributes with a constant to the eigenvalues of this Hamiltonian, because the seniority zero approximation inhibits any dependence with the total angular momentum. Thus, the expectation value of the Hamiltonian between the ^{100}Ru wave functions only depends on the (λ,μ) and $J=L$ of the normal parity orbitals. Explicitly:

$$\langle^{100}\text{Ru}, (\lambda,\mu)K=1, L=J\ M|H|^{100}\text{Ru}, (\lambda,\mu)K=1, L=J\ M\rangle = N_s\hbar\omega - 2\chi C_2 - (\tfrac{3}{2}\chi + a)L(L+1). \tag{3}$$

In the above expression N_s represents the number of proton plus neutron phonons, which depends only on the normal parity occupations n_π^N and n_ν^N 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 $\chi = 18.83$ keV, $a = 61.75$ keV, which are reasonable numbers as an interpolation between those needed to reproduce the rotational spectra of ^{24}Mg [12] and ^{238}U [13].

In Table II 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 (λ,μ) of each band. As expected, the energies of the first 4^+ and the second 2^+ states are overestimated. This is a reminder 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.

In the pseudo-SU(3) scheme, the intrinsic quadrupolar

TABLE II. Experimental and theoretically determined energies (in keV) for the ground state (g.s.) end excited (exc) band of ^{100}Ru.

	g.s. band		exc band	
J^+	Theor.	Expt.	Theor.	Expt.
irrep	(8,6)		(10,2)	
0^+	0	0	1130	1130
2^+	540	540	1362	1670
4^+	1800	1227		

moment Q_0 is easily evaluated as [14]

$$Q_0 = e_\pi^{\rm eff} Q_\pi + e_\nu^{\rm eff} Q_\nu \ , \quad Q_\alpha = \frac{\eta_\alpha + 1}{\eta_\alpha}(2\lambda_\alpha + \mu_\alpha) \ , \quad (4)$$

where Q_0 is given in units of $e\ b_0^2$ with $b_0^2 = \frac{\hbar}{M\omega} = 4.70$ fm^2. Using the wave functions of the ground-state band (1) the intrinsic quadrupole moments are $Q_\pi = 5.33$, $Q_\nu = 22.5$, while the experimental value is $Q_0(\exp) = 57.7e\ b_0^2$. To reproduce this result unreasonable effective charges $e_\pi^{\rm eff} \approx 2.9e$ and $e_\nu^{\rm eff} \approx 1.9e$ would be needed. This failure of the pseudo-SU(3) model in reproducing the quadrupole moment of ^{100}Ru is related with the use of the seniority zero approximation for nucleons in abnormal parity orbitals. In the case of ^{100}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. In this picture large effective charges are always needed in order to compensate this effect [14]. For the case of ^{100}Ru these effective charges are too large.

We turn now to the study of the two neutrino mode of the double-beta decay $\beta\beta_{2\nu}$ of ^{100}Mo into the ground state, the first 2^+ and the first excited 0^+ states of ^{100}Ru. The mathematical expressions needed to evaluate the $\beta\beta_{2\nu}$ to the ground state of ^{100}Ru can be found in [11]. The same formulas work 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 [15]. The formulas for this decay resemble 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 [1,8,9].

In Table III 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 δ interaction [8] and an interaction derived from the Bonn one-boson-exchange potential using G-matrix techniques [9]. The third row shows the results for the pseudo-SU(3) calculation using the def-o wave functions given in Eq. (1). The energy denominator used for the decay to the ground state, determined by fixing the energy of the isobaric analog state [11] is $E = E_0 - 2\hbar\omega k_\pi(\eta_\nu + \frac{1}{2}) + \Delta_C = 7.95$ MeV, where $E_0 = \frac{1}{2}Q_{\beta\beta} + m_e c^2$ and Δ_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 shown in Table III 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 [16] with $g_A/g_V = 1.0$. These data are reproduced in the last two rows of Table III.

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 $0^+ \to 2^+$ decay is strongly canceled in comparison with the QRPA one [9]. In the sph-o case, which successfully reproduces the $0^+ \to 0^+$(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 10 greater than the matrix element of the operator $[\sigma_1 \otimes \sigma_2]^2$ which mediates the

TABLE III. 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, evaluated with different models. The experimental matrix elements, measured half-lifes $T_{2\nu}^{1/2}$ and phase-space integrals G_{GT} are also listed.

	$0^+ \to 0^+$(g.s.)	$0^+ \to 0^+$(exc)	$0^+ \to 2^+$
QRPA [8]	-0.256	-0.256	
QRPA [9]	0.197	-0.271	-0.033
Pseudo-SU(3) (def-o)	-0.108	0.098	1.53×10^{-4}
Pseudo-SU(3) (sph-o)	0.152		7.3×10^{-5}
Seniority 0	-0.323		
Experiment	±0.150	±0.092	<0.106
$T_{2\nu}^{1/2}$ [10^{19} yr]	1.15 [2,3]	178 [5]	>11.5 [17]
G_{GT} [10^{-20} yr^{-1}]	387	6.61	76.6

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 $g^{\pi}_{9/2}$ and $g^{\nu}_{7/2}$ 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 [11] are exactly the same as the pure pairing ones [6], i.e.,

$$M_{2\nu}[0^+_i \to 0^+_f(\text{g.s.})] = \sum_{pn} \frac{u_p v_n \bar{u}_n \bar{v}_p \langle p||\sigma||n\rangle^2}{e_p + e_n - E_0} \ . \quad (5)$$

There exists only one $(p,n) = (g^{\pi}_{9/2}, g^{\nu}_{7/2})$ configuration in this approach, limiting the sum to only one term. The pairing occupation numbers v^2_α in the initial (unbarred) and final (barred) nuclei are $u^2_p = 0.8$, $\bar{v}^2_p = 0.4$, $v^2_n = 1.0$, $\bar{u}^2_n = 0.25$. Using these 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 III. The comparison with the pseudo-SU(3) matrix elements exhibits a reduction by a factor 2 in the sph-o limit and by a factor 3 in the def-o one. This reduction is due to the quadrupole-quadrupole correlations, which strongly mix the $g^{\nu}_{7/2}$ 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 (≈ 3 MeV) would increase the seniority zero matrix element making it worse when compared with the experimental value.

In this paper we have studied the $\beta\beta_{2\nu}$ of ^{100}Mo to ^{100}Ru in the context of the pseudo-SU(3) model. 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}Mo to excited states of ^{100}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}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 limitation, 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.

Two important experimental facts were not considered in this contribution. They are (i) the ground state of the intermediate nucleus, ^{100}Tc, exhausts the two neutrino double-beta matrix elements and (ii) it has not been possible to describe theoretically the electron capture of ^{100}Tc into the ground state of ^{100}Mo [8,9]. To incorporate this information to the pseudo-SU(3) analysis of the double-beta decay requires a major step forward: the description of the intermediate odd-odd nuclei. We plan to investigate it using a recently developed computer code [18].

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