

Quasiparticle random phase approximation analysis of the double beta decay of ^{100}Mo to the ground state and excited states of ^{100}Ru

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The beta decay rate of the 1^+ ground state of ^{100}Tc to the ground and excited states of ^{100}Mo and ^{100}Ru has been calculated using a combination of the charge-conserving and charge-nonconserving modes of the quasiparticle random phase approximation theory. These results, as well as the calculated $E2$ decay properties of ^{100}Mo and ^{100}Ru , are compared with data. In addition, the two-neutrino double beta decay rates of ^{100}Mo to the ground state and excited states of ^{100}Ru are evaluated and analyzed using available experimental data. For completeness, the neutrinoless double beta decay rate of ^{100}Mo is calculated and used to extract the value of the effective neutrino mass and the parameters of a general weak-interaction Hamiltonian.

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I. INTRODUCTION

In recent years there has been a great number of ingenious measurements of both the two-neutrino double beta decay ($2\nu\beta\beta$) as well as the neutrinoless ($0\nu\beta\beta$) mode [1, 2]. Along with the accumulation of experimental information there has been a steadily increasing number of calculations on both modes of double beta decay (for a recent review see [2]). Until very recently, the measurements and the calculations have been performed for the ground-state to ground-state transitions and only a very limited number of measurements [1] and theoretical work [3–5] has been devoted to double beta decay transitions to excited states of the decay daughter. In particular, there exists recent measurements for the $2\nu\beta\beta$ and $0\nu\beta\beta$ decay of ^{100}Mo to the ground state [6, 7] and excited states [8] of ^{100}Ru .

In Ref. [3] the first steps were taken to see if the measured $2\nu\beta\beta$ decay half-lives for the ground-state and excited-state transitions could be described consistently with the electron capture (EC) and β^- transitions from the first 1^+ state of the intermediate nucleus ^{100}Tc to the ground state of ^{100}Mo and ^{100}Ru , respectively. The authors of [3] used a schematic delta force for their nucleon-nucleon interaction in their quasiparticle random phase approximation (QRPA) calculations and assumed the excited 0^+ final state of ^{100}Ru to be a collective vibrational state built of two QRPA phonons. The conclusion of [3] was that all the above-mentioned physical observables could not be described simultaneously (with the same interaction-strength parameters) within the QRPA framework using schematic nucleon-nucleon interactions.

In the present work we aim at extending the work of [3] to a QRPA calculation of both the beta decay of ^{100}Tc as well as the $2\nu\beta\beta$ and $0\nu\beta\beta$ decay properties of ^{100}Mo assuming realistic nucleon-nucleon interactions derived from the Bonn one-boson-exchange potential [9] using the G -matrix techniques. Our calculation includes

both the lowest 2^+ excitation (2_1^+) as well as the 0^+ and 2^+ two-phonon excitations ($0_{2\text{ph}}^+$, $2_{2\text{ph}}^+$) in ^{100}Ru . The 2_1^+ excitation is described using the framework of [4, 10] and the two-phonon excitations are treated according to [5]. In addition, to explore the justification of assuming spherical collective excitations, we calculate the electric quadrupole transition strength $B(E2; 2_1^+ \rightarrow 0_{\text{g.s.}}^+)$ for both ^{100}Mo and ^{100}Ru within the QRPA framework and compare it with experiment.

Our theoretical formalism is reviewed in Sec. II. The determination of the single-particle space and parameters of the theory as well as the results are presented and discussed in Sec. III. The summary and final conclusions are presented in Sec. IV.

II. THEORETICAL FRAMEWORK

The ground state and the excited states of an even-even nucleus are treated using the QRPA theory including two-quasineutron and two-quasiproton excitations in the QRPA matrix [11] (hereafter denoted by pp - nn QRPA). The diagonalization of the QRPA matrix leads to the excited states $|I_k^{\pi'} M\rangle$ of the even-even nucleus, where M labels the magnetic substates and k numbers the states for a particular angular momentum I and parity π' in the order of ascending energy. These states are QRPA phonons defined by

$$|I_k^{\pi'} M\rangle = Q^\dagger(I_k^{\pi'} M)|\text{QRPA}\rangle, \quad (1)$$

where $|\text{QRPA}\rangle$ is the correlated QRPA ground state and the operator Q^\dagger is the QRPA phonon-creation operator [10–14]. In an analogous way, the states $|J_m^\pi M\rangle$ of the odd-odd nucleus are defined as pn QRPA phonons [14, 15] of the type

$$|J_m^\pi M\rangle = \Gamma^\dagger(J_m^\pi M)|\text{QRPA}\rangle, \quad (2)$$

where J is the angular momentum, π the parity, m the state index, and M as before. The pn QRPA operator Γ^\dagger is defined in [14, 15].

In the past the pn QRPA formalism has been successfully used to explain the quenching observed in the β^+ /EC decay [13] and the $2\nu\beta\beta$ decay [15, 16]. There the quenching can be explained theoretically by the inclusion of the particle-particle interaction channel of the nucleon-nucleon force in the nuclear many-body calculation. Furthermore, our recent analysis [17] of the neutron-rich palladium isotopes has shown that also the β^- type transitions may show a rather strong dependence on the strength of the particle-particle channel of the nucleon-nucleon interaction. The same conclusion has been reached by Griffiths and Vogel in [3].

The single beta decay and the $2\nu\beta\beta$ decay rates can be used to fix the parameters of the model (e.g., the schematic or realistic nucleon-nucleon interaction used in the calculation) thus leaving the $0\nu\beta\beta$ decay rate as a parameter-independent prediction [18, 19] and enabling one to obtain information on the Majorana mass of the neutrino and the contribution of the right-handed currents to the weak interactions.

For single beta decay transitions the comparative half-life, ft , is defined for the pure Gamow-Teller β^+ /EC and β^- transitions in [20–22]. For the various $2\nu\beta\beta$ decay modes the half-life is given in [4] and for the $0\nu\beta\beta$ decay mode the corresponding expression is given in [18]. The relevant nuclear matrix elements have been computed for beta decay transitions to the ground state of the final double-even nucleus in [10]. Concerning transitions to excited states the relevant matrix elements are more complicated and are given in Ref. [10] for a one-phonon pp - nn QRPA excitation and in Ref. [5] for a two-phonon pp - nn QRPA excitation.

The method of calculating electric transitions of multipolarity I (EI) from the even-even excited state $|I_k^\pi M\rangle$, k labeling the states, to the correlated ground state [QRPA] is described in [23]. The adequacy of the single-particle basis can be probed by the energy-weighted sum rule (EWSR) [23] based on unperturbed two-quasiparticle states

$$\begin{aligned} S(EI) &= \frac{1}{2} \langle \text{BCS} | [T_I^{(E)}, [\hat{H}, T_I^{(E)}]] | \text{BCS} \rangle \\ &= \sum_{ab} E_{ab}^{(2\text{qp})} B(EI; 0_{\text{BCS}}^+ \rightarrow |ab; I\rangle), \end{aligned} \quad (3)$$

where \hat{H} is the nuclear Hamiltonian and 0_{BCS}^+ denotes the BCS ground state. The two-quasiparticle states are of the form

$$|ab; IM\rangle = A^\dagger(ab, IM)|\text{BCS}\rangle, \quad (4)$$

where A^\dagger is the quasiparticle pair creation operator [13] and $E_{ab}^{(2\text{qp})}$ is the two-quasiparticle energy. On the other hand, assuming momentum-independent interactions, the sum rule can be approximated by [24]

$$S(EI) \approx 3.44Ze^2I(I+1)(1.44)^I A^{2(I-1)/3}. \quad (5)$$

The above equations are used to test how well a cho-

sen harmonic-oscillator single-particle basis (for protons and neutrons separately) exhausts the EWSR. We apply this method to the electric quadrupole operator $T_2^{(E)}$ in the case of $0^+ \rightarrow 2^+$ transitions in Sec. IV. The EWSR can furthermore be used to test the correctness of the QRPA calculation since it is model independent. In the present work we have used both the $B(E2)$ and the EWSR to check the consistency of the QRPA wave functions used for the description of one- and two-phonon states involved in the $2\nu\beta\beta$ transitions.

III. RESULTS AND DISCUSSION

A. Outline of the nuclear-structure calculation and the scaling of the nucleon-nucleon interaction

In this section we review the main steps of the numerical calculation of the various beta decay observables and the determination of the renormalization parameters of the nucleon-nucleon G -matrix interaction [13]. Adjusting the force parameters to the available low-energy nuclear-structure data leaves both the $2\nu\beta\beta$ as well as $0\nu\beta\beta$ decay rates as parameter-free predictions in contrast to earlier calculations [15, 16, 19]. We also discuss the electric quadrupole decay to the lowest 2^+ state in ^{100}Mo and ^{100}Ru to enable a wider comparison of the predictions of the QRPA scenario and the experimental data.

We have performed all the calculations using two different basis-state sets: a basis of two (three) oscillator major shells, namely $3\hbar\omega$, $4\hbar\omega$ ($3\hbar\omega$, $4\hbar\omega$, $5\hbar\omega$), including for the smaller basis the intruder orbital $0h_{11/2}$ coming from the first excluded higher oscillator shell $5\hbar\omega$. This yields altogether 10 (15) single-particle states in the smaller (bigger) basis. The nucleus ^{40}Ca acts as core for both of these sets and the smaller (bigger) basis extends to the $N=Z=82$ ($N=Z=126$) shell closure. For both sets the single-particle energies were chosen to be the same, namely based on the Coulomb-corrected Woods-Saxon energies [23] with modifications near the Fermi energy of ^{100}Mo and ^{100}Ru . The modifications were made to the relative spacing of the neutron orbitals $1d_{5/2}$, $2s_{1/2}$, $2d_{3/2}$, $1g_{7/2}$ and the proton orbitals $2p_{1/2}$ and $0g_{9/2}$ according to the reaction data as described in [3]. Some additional adjustments of the other proton orbitals were made to see the effect upon the reduced electric quadrupole transition probability $B(E2; 2_1^+ \rightarrow 0_{g.s.}^+)$ in ^{100}Mo and ^{100}Ru .

The monopole matrix elements of the G matrix [9] have been used to calculate the BCS ground state of ^{100}Mo and ^{100}Ru . These monopole matrix elements are scaled by the proton (neutron) pairing strength parameter $g_{\text{pair}}^{(p)}$ ($g_{\text{pair}}^{(n)}$) which is adjusted as described in [13]. The adopted single-particle basis has a small but noticeable effect upon these values as shown in Table I.

An interesting feature of the calculations is that the relevant beta decay observables are not affected by the variations in the pairing-strength parameters; only for decays involving high-lying 1^+ states of ^{100}Tc there are significant changes. This means that also the $2\nu\beta\beta$ -decay

TABLE I. The values of the overall scaling parameters of the different channels of the nucleon-nucleon G -matrix interaction for ^{100}Mo and ^{100}Ru . The small (large) basis contains 10 (15) single-particle orbitals as discussed in the text.

Quantity	(Mo) small	(Mo) large	(Ru) small	(Ru) large
$g_{\text{pair}}^{(p)}$	1.20	1.10	1.20	1.12
$g_{\text{pair}}^{(n)}$	1.00	0.97	1.00	0.93
G_{ph}	1.11	0.84	0.93	0.74
G_{pp}	1.00	1.00	1.00	1.00
g_{ph}	1.20	1.20	1.20	1.20
g_{pp}	1.12	0.79	1.12	0.79

observables are not much affected by the choice of the pairing-strength parameters due to the suppression produced by the energy denominators [4]. A feature, which does not become explicit in the presented final results, is that changes in the pairing-strength parameters induce some qualitative changes in the β^- decay strength of the first 1^+ state of ^{100}Tc to 2^+ states above the two-phonon states in ^{100}Ru . Unfortunately, due to lack of experimental information, this behavior in the β^- strength function cannot be analyzed further.

The overall strength of the proton-proton and neutron-neutron interaction (the $T=1$ channel) is determined by the scales G_{ph} (the overall scale for the particle-hole matrix elements) and G_{pp} (the overall scale for the particle-particle matrix elements). The parameter G_{ph} was adjusted such that the first calculated 2^+ state in ^{100}Mo , and separately in ^{100}Ru , agrees with the experimental energy. The resulting parameter values are indicated in Table I. The particle-particle strength parameter G_{pp} has no significant effect upon neither the energy nor the γ decay properties of the 2_1^+ state so that the simple choice of $G_{\text{pp}} = 1$ (unrenormalized particle-particle G -matrix interaction) was made both for ^{100}Mo and ^{100}Ru .

The renormalization of the proton-neutron interaction (a mixture of $T=0$ and $T=1$ channels) is accomplished [13] by the scale parameter of the particle-hole interaction, g_{ph} , and the scale parameter of the particle-particle interaction, g_{pp} , in the pn QRPA calculation. The value of g_{ph} is fixed by comparing the calculated and semiempirical [25] energy of the Gamow-Teller giant resonance in the odd-odd nucleus ^{100}Tc . The resulting value is $g_{\text{ph}} = 1.2$ for both basis sets as shown in Table I. The value of the parameter g_{pp} has been determined by calculating the β^- decay rate $B(\text{GT}; ^{100}\text{Tc}(1_1^+) \rightarrow ^{100}\text{Ru}(0_{\text{g.s.}}^+))$ and comparing it with the corresponding experimental [26] value $\log ft = 4.60$.

B. Results for the beta decay rates and electric quadrupole transitions

In Table II we summarize our calculated results for the $E2$ matrix elements and for those beta decay observables for which experimental data is available. As seen from Table II the changes in the reduced electric transition probabilities $B(E2; 2_1^+ \rightarrow \text{g.s.})$ are small when going from

TABLE II. The $B(E2)$ values for the $2_1^+ \rightarrow \text{g.s.}$ transition in ^{100}Mo (Mo) and ^{100}Ru (Ru). All the $\log ft$ values refer to β^+ ($\log ft_+$) or β^- ($\log ft_-$) transitions from the first 1^+ state of ^{100}Tc . The final state is indicated in the parenthesis. The column “small” (“large”) symbolizes the calculation using 10 (15) single-particle states.

Quantity	Small	Large	Expt.
$B(E2)^a$ (Mo) [W.u.]	20.0	24.6	34^b
$B(E2)^a$ (Ru) [W.u.]	16.2	19.9	53.1^b
$\log ft_+(0_{\text{g.s.}}^+)$	3.64	3.48	$4.45_{-0.30}^{+0.18}$ ^c
$\log ft_-(0_{\text{g.s.}}^+)$	4.6	4.6	$4.60(1)^b$
$\log ft_-(2_1^+)$	4.5	4.5	$6.5(4)^b$
$\log ft_-(2_{2\text{ph}}^+)$	6.0	6.1	$7.1(3)^b$
$\log ft_-(0_{2\text{ph}}^+)$	5.1	5.2	$5.0(1)^b$

^aBare charges: $e_{\text{eff}}^{(p)} = 1.0$, $e_{\text{eff}}^{(n)} = 0.0$.

^bFrom Ref. [26].

^cFrom Ref. [27].

the small to the large model space. The $B(E2)$ of Mo is better reproduced as the one of Ru, the theory giving a far too small $B(E2)$ for Ru. This is the case even in the large basis where the core-polarization effects should already be small. The cause of this difference between the experimental and theoretical $B(E2)$ values in ^{100}Ru may go beyond the spherical QRPA, and thus suggests that deformation may play a role for the nuclei under study. Concerning the EWSR the smaller basis fulfills only about 30% of the unperturbed EWSR, whereas the larger one a good 80%, both for protons and neutrons.

The possibility of deformation effects is also supported by the too large calculated decay rate $B(\text{GT}; ^{100}\text{Tc}(1_1^+) \rightarrow ^{100}\text{Ru}(2_1^+))$ for which the corresponding $\log ft_-(2_1^+)$ is listed in Table II. In our calculations this property persisted for every reasonable spherical single-particle set which we chose for the basis. This clear pattern is, however, distorted by comparing the calculated two-phonon results [$\log ft_-(0_{2\text{ph}}^+)$, $\log ft_-(2_{2\text{ph}}^+)$ in Table II] with the corresponding experimental ones. In this case the theoretical results reproduce relatively well the experimental data, especially in the case of the transition to the 0^+ two-phonon state. This is, as such, rather surprising since the two-phonon states are built of two 2_1^+ phonons, and one would expect similar level of agreement or disagreement with experiment if the experimental 0^+ and 2^+ states belonged to a true two-phonon triplet.

In addition to difficulties in predicting the $B(E2)$ values and the $\log ft_-(2_1^+)$ value, the QRPA fails in predicting the experimental [27] rate of the electron-capture (EC) transition $B(\text{GT}; ^{100}\text{Tc}(1_1^+) \rightarrow ^{100}\text{Mo}(0_{\text{g.s.}}^+))$, as seen in Table II for the quantity denoted by $\log ft_+(0_{\text{g.s.}}^+)$. This feature may either be a sign of deformation effects or an indication of an abnormal sequence of single-particle levels. The experimental $\log ft_+(0_{\text{g.s.}}^+)$ can be reproduced by shifting upwards the orbitals $\nu 1d_{3/2}$ and $\nu 0g_{7/2}$. The upward shifting, however, leads to unrealistically strong cancellation effects in the $2\nu\beta\beta$ decay amplitude, contrasting the findings of [27, 28].

Our observations confirm the conclusions of [3] where a schematic δ force was used for the nucleon-nucleon interaction. Thus it seems that at least some of the relevant observables in the Mo-Tc-Ru system cannot be reproduced simultaneously with a consistent set of interaction-strength parameters.

C. Results for the $2\nu\beta\beta$ and $0\nu\beta\beta$ decay modes

In Table III we depict our results for the $2\nu\beta\beta$ decay to the ground state ($0_{g.s.}^+$), to the first 2^+ state (2_1^+), and to the 0^+ and 2^+ two-phonon states (0_{2ph}^+ , 2_{2ph}^+) of the final nucleus ^{100}Ru . The variation of the observables, when going from the smaller (10 single-particle states) to the larger (15 single-particle states) basis is negligible for the two-phonon transitions, whereas for the ground-state transition the extension of the basis has a considerable effect. The main reason for this is the strong cancellation among the various intermediate 1^+ contributions in the smaller basis [compare the columns " $M_{GT}^{(2\nu)}(1_1^+)$ " and " $M_{GT}^{(2\nu)}$ " for the smaller and larger basis]. The larger basis leads to smaller total cancellation and the value of the double Gamow-Teller matrix element is largely exhausted by the first intermediate 1^+ state, as also discovered in [3, 28].

In addition to the cancellation effect in the ground-state transition, there is a coherent summing effect in the transition to the two-phonon 0^+ state. In this case the coherent contribution of the 1^+ states above the ^{100}Tc ground state is made possible by the small power of the energy denominator ($s = 1$) appearing in M_{GT} [4], in contrast with the 2^+ transitions ($s = 3$).

Comparison of the calculated and experimental half-lives in Table III reveals that the predicted $2\nu\beta\beta$ half-life of the transition to the ground state is shorter than the corresponding experimental one. This may be due to the fact that the theory fails in the description of the transition $^{100}\text{Mo}(0_{g.s.}^+) \rightarrow ^{100}\text{Tc}(1_1^+)$ as discussed before. This effect is still more important for the $2\nu\beta\beta$ transition to the 2_1^+ state in ^{100}Ru since in this case the contribution of the other intermediate states is completely negligible. In addition, the transition $^{100}\text{Tc}(1_1^+) \rightarrow ^{100}\text{Ru}(2_1^+)$ is poorly described by the QRPA.

Because the other intermediate 1^+ states seem to have

a vanishing contribution, the predicted half-life can be corrected by factors which take into account the difference between the experimental and theoretical beta decay observables. After such a correction the $0^+ \rightarrow 2_1^+$ half-life acquires the value $t_{1/2}^{(2\nu)}(0^+ \rightarrow 2_1^+) \approx 5 \times 10^{23}$ yr, well above the reported experimental limit of Table III. For the $0^+ \rightarrow 0_{2ph}^+$ transition such correction is not as straightforward to perform due to non-negligible contributions from higher intermediate 1^+ states. In this case only the "left branch" $^{100}\text{Mo}(0_{g.s.}^+) \rightarrow ^{100}\text{Tc}(1_1^+)$ contributes to the correction since the "right branch" $^{100}\text{Tc}(1_1^+) \rightarrow ^{100}\text{Ru}(0_{2ph}^+)$ is correctly predicted by the QRPA, as seen in Table II. Performing this very crude correction would yield a half-life value of $t_{1/2}^{(2\nu)}(0^+ \rightarrow 0_{2ph}^+) \approx 2 \times 10^{20}$ yr. The above half-life value is calculated assuming that the two-phonon states are degenerate at energy $E_{2ph} = 1080$ keV. The correction in the phase space due to the deviation from the corresponding experimental value $E_{exp}(0_{2ph}^+) = 1130$ keV is small and does not alter the above half-life estimate significantly.

The results of the neutrinoless mode are presented in Tables IV–VI. In Table IV we summarize the values of the various nuclear matrix elements entering the half-life [29] in units of $M_{GT}^{(s)}$, the double Gamow-Teller matrix element corresponding to s -wave electrons. The symbols for the matrix elements are those of Ref. [18]. As for the other calculated $0\nu\beta\beta$ emitters [18, 19] the s -wave recoil term $M_R^{(s)}$ plays a significant role in rendering a relatively large value for the coefficient $C_{\eta\eta}^{(0)}$ of the half-life expression [18, 29], as seen from Table V. This, in turn, yields the value of the effective coupling parameter $\langle\eta\rangle$ of a right-handed leptonic current with a left-handed hadronic current rather small (see Table VI).

The upper limits of the quantities displayed in Table VI are obtained from the half-life in standard manner [29]. The recent experimental half-life limit [7] sets the upper limit of the effective neutrino mass, $|\langle m_\nu \rangle| \leq 2.67$ eV, rather low for the ^{100}Mo decay. In a previous analysis [29] the most stringent mass limit has been set by the ^{128}Te ($|\langle m_\nu \rangle| \leq 2.00$ eV) and ^{76}Ge ($|\langle m_\nu \rangle| \leq 2.32$ eV) decays.

The present analysis reveals that the p -wave contribution to the half-life coefficients $C^{(0)}$ is not large and

TABLE III. Calculated $2\nu\beta\beta$ matrix elements $M_{GT}^{(2\nu)}(1^+)$ (only the first intermediate 1^+ state contributes) and $M_{GT}^{(2\nu)}$ (all the intermediate 1^+ states contribute) and the half-life, $t_{1/2}^{(2\nu)}$, for the decay of ^{100}Mo to the ground state ($J_f = 0_{g.s.}^+$), the first 2^+ state ($J_f = 2_1^+$), and to the 0^+ and 2^+ two-phonon states ($J_f = 0_{2ph}^+$, 2_{2ph}^+) of the final nucleus ^{100}Ru in the single-particle basis containing 10 (small) and 15 (large) single-particle states. The matrix elements are given in powers of the inverse electron rest mass as in [4, 5].

J_f	$M_{GT}^{(2\nu)}(1_1^+)$	Small		Large		Expt. (10^{18} yr)
		$M_{GT}^{(2\nu)}$	$t_{1/2}^{(2\nu)}$ (10^{18} yr)	$M_{GT}^{(2\nu)}(1_1^+)$	$t_{1/2}^{(2\nu)}$ (10^{18} yr)	
$0_{g.s.}^+$	0.246	0.121	7.66	0.312	0.197	$11.5_{-2.0}^{+3.0}$ ^a
2_1^+	-0.027	-0.028	754	-0.034	-0.033	> 150 ^b
0_{2ph}^+	-0.183	-0.265	69.9	-0.202	-0.271	> 80 ^b
2_{2ph}^+	-0.0076	-0.0076	214000	-0.0081	-0.0082	> 65 ^b

^aFrom Ref. [6].

^bFrom Ref. [8].

TABLE IV. Ratios $\chi = M/M_{\text{GT}}^{(s)}$ for the various nuclear matrix elements M defined in [18] for the $0\nu\beta\beta$ decay of ^{100}Mo . The quantity $M_{\text{GT}}^{(s)}$ is the s -wave double Gamow-Teller matrix element. The symbols in the table define the labeling of the ratio χ as $(s)F \leftrightarrow \chi_F^{(s)}$. The calculation is carried out using 10 (“small”) and 15 (“large”) single-particle states.

χ	Small	Large
$(s)F$	-0.503	-0.497
$(s)\omega F$	-0.469	-0.448
$(s)\omega\text{GT}$	0.994	0.958
$(s)R$	1.56	1.42
$(p)qF+$	-0.165	-0.181
$(p)q\text{GT}$	0.941	0.752
$(p)qT$	0.083	0.041
$(p)qP+$	0.325	0.307
$(s)-$	-1.41	-1.36
$(s)+$	0.576	0.556
$(p)-$	-0.410	-0.345
$(p)+$	0.504	0.519
$(s)m$	-1.56	-1.54
$(p)m$	-2.03×10^{-4}	-2.80×10^{-4}
$\Delta(p)m$	9.93×10^{-5}	4.50×10^{-5}
$\Delta(p)-$	-4.90×10^{-4}	-4.19×10^{-4}
$\Delta(p)+$	-2.72×10^{-4}	-1.80×10^{-4}
P	0.197	0.187
ΔP	2.01×10^{-4}	1.37×10^{-4}
$ M_{\text{GT}}^{(s)} $ (fm $^{-1}$)	0.402	0.545

certainly does not change the qualitative pattern emerging from the s -wave contribution. This was also noticed in the previous studies [18, 19]. Another important feature of the $0\nu\beta\beta$ matrix elements is that they are, to a large extent, independent of the contribution coming from the intermediate 1^+ states [18]. The ^{100}Mo decay supports this observation, the most contribution being in the double Gamow-Teller matrix element $M_{\text{GT}}^{(s)}$, where the 1^+ contribution is at most 30% for all reasonable values ($0 \leq g_{\text{pp}} \leq 1.0$) of the scaling strength of the particle-particle channel of the G -matrix interaction. The other intermediate multipoles J^π are only very weakly affected by g_{pp} so that it is reasonable to use the same value of g_{pp} for all multipoles of the G -matrix interaction.

TABLE V. The coefficients $C_x^{(0)}$ of the $0\nu\beta\beta$ decay half-life expression [18] for the ^{100}Mo decay in units of inverse years (yr $^{-1}$) calculated using 10 (“small”) and 15 (“large”) single-particle states.

$C_x^{(0)}$ ^a	Small	Large
mm	5.53×10^{-13}	1.00×10^{-12}
$m\lambda$	-3.27×10^{-13}	-5.85×10^{-13}
$m\eta$	8.94×10^{-11}	1.48×10^{-10}
$\lambda\lambda$	1.31×10^{-12}	2.30×10^{-12}
$\eta\eta$	2.17×10^{-8}	3.28×10^{-8}
$\lambda\eta$	-8.10×10^{-13}	-1.35×10^{-12}

^aAll $C_x^{(0)}$ in units of inverse years.

TABLE VI. The upper limit on the effective neutrino mass $\langle m_\nu \rangle$ and the effective coupling constants $\langle \lambda \rangle$ and $\langle \eta \rangle$ of the right-handed weak currents for the $0\nu\beta\beta$ decay of ^{100}Mo as extracted from the experimental half-life limit $t_{1/2}^{(0\nu)}(\text{exp}) \geq 4.4 \times 10^{22}$ yr [7]. The columns “small” and “large” denote calculation using 10 and 15 single-particle states, respectively.

Quantity	Small	Large
$ \langle m_\nu \rangle $ (eV)	3.59	2.67
$ \langle \lambda \rangle $	4.17×10^{-6}	3.14×10^{-6}
$ \langle \eta \rangle $	3.55×10^{-8}	2.88×10^{-8}

IV. SUMMARY AND CONCLUSIONS

We have calculated the electric quadrupole decay rate of the first excited 2^+ state in ^{100}Mo and ^{100}Ru , as well as a number of beta and double beta ($2\nu\beta\beta$ and $0\nu\beta\beta$) decay observables in the ^{100}Mo - ^{100}Tc - ^{100}Ru isobaric chain and compared them with the available experimental data. The calculations have been performed exploiting the usual charge-conserving QRPA and the charge-nonconserving proton-neutron QRPA (pn QRPA) framework using a smaller (10 single-particle states) and a bigger (15 single-particle states) single-particle set to test the effects of the size of the model space. The energies of the single-particle orbitals in the vicinity of the Fermi energy have been extracted from experiment, whereas the energy of the other orbitals has been taken from a Coulomb-corrected Woods-Saxon potential. By using the experimental level spacing near the Fermi energy we want to end up with as realistic a description of the final observables as possible. The nucleon-nucleon interaction is obtained from the Bonn one-boson-exchange potential through the G -matrix method.

Our analysis has shown that it is impossible in the QRPA framework to reproduce simultaneously all the experimental data on the beta decay of ^{100}Tc to the ground and excited one- and two-phonon states of ^{100}Mo and ^{100}Ru . This leads to difficulties also in the description of the $2\nu\beta\beta$ decay rates of ^{100}Mo to the ground state as well as to the one-phonon and two-phonon excited states of the final nucleus ^{100}Ru . Thus our findings give support to the conclusions of Griffiths and Vogel [3] who use a schematic δ force, rather than a realistic G -matrix force, as their nucleon-nucleon interaction. Furthermore, we have found that the first intermediate 1^+ state exhausts a lion share of the $2\nu\beta\beta$ amplitude of ^{100}Mo for the transitions to the excited states of ^{100}Ru . In the case of the $2\nu\beta\beta$ transition to the ground state of ^{100}Ru , the contribution coming from the excited 1^+ states of ^{100}Tc are of the order of one third to one half of the 1_1^+ contribution. This result can be accommodated within the error bar set up by [27] for the experimental $2\nu\beta\beta$ half-life. Thus our analysis shows that the model is not in contradiction with data concerning the effect of the intermediate 1^+ states.

In addition to the above discrepancies, we find that, in spite of the rather large model space used, the reduced electric quadrupole transition probability $B(E2; 2_1^+ \rightarrow$

$0_{g.s.}^+$) is not well reproduced for ^{100}Ru . One possible reason for this could be deformation effects which would destroy the one-phonon-two-phonons structure in ^{100}Ru and substitute it with rotational bands built upon a deformed ground state or some vibrational intrinsic excitations (β or γ vibrations). The same could happen also to ^{100}Mo and/or ^{100}Tc nuclei. Recent analysis of the possible deformation and coexistence in ^{100}Mo and ^{100}Tc nuclei has been performed in [30, 31].

Despite the difficulties in predictions based upon the 1^+ excitations in the intermediate nucleus ^{100}Tc we have calculated the $0\nu\beta\beta$ decay rate of ^{100}Mo and compared it with the experimental lower limit of the decay half-life to extract upper limits for the values of some basic observables appearing in the grand-unification theories based upon various different gauge groups. A fact which may justify such a calculation in this case is that the decay properties of the 1^+ states in ^{100}Tc do not affect significantly the $0\nu\beta\beta$ decay transition rate since the vir-

tual $0\nu\beta\beta$ transitions go through intermediate states of all angular momenta and both parities. Thus the other intermediate multipolarities are effective in masking the 1^+ contribution. However, this still leaves the question open if the QRPA description of the other multipoles suffers from the same symptoms as the description of the decay properties of the first 1^+ state. Only the use of a theory containing the deformation degree of freedom could yield information about the possible contribution of deformation to the quantities calculated here by using the spherical QRPA theory.

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