

Neutrinoless double beta decay of  $^{76}\text{Ge}$ ,  $^{82}\text{Se}$ ,  $^{100}\text{Mo}$ , and  $^{136}\text{Xe}$  to excited  $0^+$  statesF. Šimković,<sup>1,3</sup> M. Nowak,<sup>2</sup> W. A. Kamiński,<sup>2</sup> A. A. Raduta,<sup>1,4</sup> and Amand Faessler<sup>1</sup><sup>1</sup>*Institute of Theoretical Physics, University of Tuebingen, D-72076 Tuebingen, Germany*<sup>2</sup>*Department of Theoretical Physics, Maria Curie-Skłodowska University, PL-20 031 Lublin, Poland*<sup>3</sup>*Department of Nuclear Physics, Comenius University, Mlynská dolina F1, SK-842 15 Bratislava, Slovakia*<sup>4</sup>*Institute of Physics and Nuclear Engineering, P.O. Box MG6, Bucharest, Romania**and Department of Theoretical Physics and Mathematics, P.O. Box MG11, Bucharest University, Romania*

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The neutrinoless double-beta-decay ( $0\nu\beta\beta$  decay) transition to the first excited  $0^+$  collective final state is examined for  $A=76, 82, 100$ , and  $136$  nuclei by assuming light and heavy Majorana neutrino exchange mechanisms as well as the trilinear  $R$ -parity violating contributions. Realistic calculations of nuclear matrix elements have been performed within the renormalized quasiparticle random phase approximation. Transitions to the first excited two-quadrupole phonon  $0^+$  state are described within a boson expansion formalism and alternatively by using the operator recoupling method. We present the sensitivity parameters to different lepton number violating signals, which can be used in planning the  $0\nu\beta\beta$ -decay experiments. The half-life of  $0\nu\beta\beta$  decay to the first excited state  $0_1^+$  is by a factor of 10–100 larger than that of the transition to the ground state,  $0_{\text{g.s.}}^+$ .

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## I. INTRODUCTION

Neutrinoless double beta decay ( $0\nu\beta\beta$  decay), which violates the total lepton number by two units, is the most sensitive low-energy probe for physics beyond the standard model (SM) [1–5]. The observation of the  $0\nu\beta\beta$  decay would provide unambiguous evidence that at least one of the neutrinos is a Majorana particle with nonzero mass [6]. This conclusion is valid without specifying which from the plethora of possible  $0\nu\beta\beta$ -decay mechanisms triggered by the exchange of neutrinos, neutralinos, gluinos, leptoquarks, etc., is the leading one. The current experimental upper limits on the  $0\nu\beta\beta$ -decay half-life impose stringent constraints, e.g., on the parameters of grand unification theory (GUT) and supersymmetric (SUSY) extensions of the SM.

There is a continuous, both experimental and theoretical, activity in the field of  $0\nu\beta\beta$  decay. An interesting issue is what are the implications of the neutrino oscillation phenomenology to  $0\nu\beta\beta$  decay. We note that the results of the solar [7], atmospheric [8], and terrestrial [9] neutrino experiments provide convincing evidence of neutrino oscillations, which require nonvanishing masses for neutrinos as well as neutrino mixing [10]. The neutrino oscillations are sensitive to the differences of the masses squared and cannot distinguish between Dirac and Majorana neutrinos. Nevertheless, if assumptions about the character (Dirac or Majorana neutrinos), the phases, and the neutrino mixing pattern are considered, one can derive estimates for the effective Majorana electron neutrino mass  $\langle m_\nu \rangle$  responsible for  $0\nu\beta\beta$  decay. The current viable analysis implies the effective neutrino mass  $\langle m_\nu \rangle$  to be within the range  $10^{-3} \text{ eV} \leq \langle m_\nu \rangle \leq 1 \text{ eV}$  [11,12]. The present generation of  $0\nu\beta\beta$ -decay experiments [13–15] achieve sensitivities of  $T_{1/2}^{0\nu} \sim 10^{24} - 10^{25} \text{ yr}$  for different isotopes [13–15]. It corresponds to  $\langle m_\nu \rangle \approx 0.5 - 1.0 \text{ eV}$  [16,17]; i.e., these  $0\nu\beta\beta$ -decay experiments allow one already to discriminate among various neutrino mixing schemes.

Neutrino oscillations imply that perhaps we are close to the observation of  $0\nu\beta\beta$  decay. This would be a major achievement. Maybe it is enough to increase the sensitivity to  $\langle m_\nu \rangle$  by about an order of magnitude; i.e., the  $0\nu\beta\beta$ -decay experiments should be sensitive to half-lives of  $10^{27} - 10^{28} \text{ yr}$  for the ground to ground transitions. We hope that these data will stimulate new experimental activities. Ambitious plans are underway to push the upper constraints on lepton number violating parameters farther down. By using several tons of enriched  $^{76}\text{Ge}$ , the GENIUS experiment is expected to probe  $\langle m_\nu \rangle$  up to  $10^{-2} \text{ eV}$  [18]. The CUORE experiment intends to search for rare events with the help of a cryogenic  $\text{TeO}_2$  detector with high-energy resolution [19]. The ongoing NEMO 3 experiment, now under construction in the Fréjus underground laboratory, will measure up to 10 kg of different double-beta-decay isotopes [20]. Both CUORE and NEMO 3 have a chance to reach a sensitivity to the effective neutrino mass  $\langle m_\nu \rangle$  on the order of 0.1 eV [17].

It is worth examining also other possibilities to increase the sensitivity of  $0\nu\beta\beta$ -decay experiments. Until now, attention was concentrated mostly on the  $0\nu\beta\beta$ -decay transition to the ground state of the final nucleus. However, there might be a chance that the transitions to the excited  $0^+$  and/or  $2^+$  final states are more favorable experimentally, at least for a particular mechanism for  $0\nu\beta\beta$  decay [15,21]. Generally speaking, transitions to the excited states are suppressed due to the reduced  $Q_{\beta\beta}$  value. However, this restriction can be compensated by a possible lower background due to a coincidence of the  $\beta$  particles with the  $\gamma$  or  $\gamma$ 's from the excited final state. The possible advantage depends on the ratio of the corresponding nuclear matrix elements to the excited and ground states. If their values are comparable, the  $0\nu\beta\beta$ -decay experiment measuring transitions to ground and excited final states could be of a similar sensitivity.

Recently, this issue received increasing attention from many experts in the field. The  $0\nu\beta\beta$  decay of  $^{76}\text{Ge}$  and

$^{100}\text{Mo}$  to the first excited  $2_1^+$  final state has been investigated in Ref. [22] by assuming massive Majorana neutrinos and right-handed weak currents. It was found that the zero neutrino-double-beta decay transition probabilities for the  $0^+ \rightarrow 2^+$  decay are strongly suppressed due to higher partial waves of the emitted electrons needed in the  $0^+ \rightarrow 0_{\text{g.s.}}^+$  transition. But in the case of  $0\nu\beta\beta$  decay to the lowest and first excited  $0^+$  states the two emitted electrons are preferentially in an  $s_{1/2}$  wave. Therefore, this decay channel is more favored. Recently, the first realistic calculation for  $0^+ \rightarrow 0_1^+$  decay has been performed for  $A=76$  and  $82$  nuclei within a higher quasiparticle random phase approximation (QRPA) [23]. The  $0\nu\beta\beta$ -decay mechanisms mediated by light Majorana neutrinos within the left-right symmetric model have been discussed. The conclusion was that the transition to excited collective  $0^+$  final states is reduced compared with the decay to the ground state. It would be worthwhile to test this result also within other nuclear approaches.

The aim of this work is to examine the  $0\nu\beta\beta$  decay of  $^{76}\text{Ge}$ ,  $^{82}\text{Se}$ ,  $^{100}\text{Mo}$ , and  $^{136}\text{Xe}$  to the first excited  $0_1^+$  state. We shall discuss the mechanisms induced by light and heavy Majorana neutrino exchange as well as those with trilinear  $R$ -parity violation. The nuclear matrix elements will be evaluated within the renormalized QRPA (RQRPA) [24,25], which takes into account the Pauli exclusion principle. We shall also consider the contributions to  $0\nu\beta\beta$  decay coming from the momentum-dependent induced nucleon currents, which has been found to be significant for ground state to ground state transitions [16]. We note that these contributions were ignored in a similar study [23]. The collective two-quadrupole phonon state  $0_1^+$  will be described by two different approaches proposed in Refs. [26] and [27–29], respectively. Finally the sensitivity parameters for a given isotope, associated with different lepton number violating signals and nuclear transitions, will be calculated. Also a discussion about possible projects of future experimental searches for  $0\nu\beta\beta$  decay to excited final states  $0^+$  will be presented.

The paper is organized as follows. In Sec. II, basic formulas relevant to the  $0\nu\beta\beta$ -decay mechanisms are presented. In Sec. III two approaches meant to calculate the transitions to ground and excited states are described. In Sec. IV we calculate the  $0\nu\beta\beta$ -decay matrix elements for  $A=76, 82, 100$ , and  $136$  nuclei via the RQRPA. We also determine the sensitivity of transitions to the collective excited state  $0_1^+$  and to lepton number violation associated with the Majorana neutrino mass and  $R$ -parity breaking. The perspectives of measuring  $0^+ \rightarrow 0_1^+$  decays are analyzed. The summary and final conclusions are presented in Sec. IV.

## II. $0\nu\beta\beta$ -DECAY HALF-LIFE

The theory of light and heavy Majorana neutrino mass modes of  $0\nu\beta\beta$  decay has been reviewed, e.g., in Refs. [1,2,4,16]. The trilinear  $R$ -parity violating mode of  $0\nu\beta\beta$  decay has been presented in Refs. [30–33]. Without going into details of the derivations, we summarize the basic ingredients of these modes of  $0\nu\beta\beta$  decay.

### A. Majorana neutrino mass mechanism

The half-life of  $0\nu\beta\beta$  decay associated with the light and heavy Majorana neutrino mass mechanism is given as

$$[T_{1/2}^{0\nu}]^{-1} = G_{01} \left| \frac{\langle m_\nu \rangle}{m_e} M_{\langle m_\nu \rangle}^{\text{light}} + \eta_N M_{\eta_N}^{\text{heavy}} \right|^2. \quad (2.1)$$

Here,  $G_{01}$  is the integrated kinematical factor [1,34]. The lepton number nonconserving parameters, i.e., the effective electron Majorana neutrino mass  $\langle m_\nu \rangle$  and  $\eta_N$ , are given as follows:

$$\langle m_\nu \rangle = \sum_1^3 (U_{ek}^L)^2 \xi_k m_k, \quad \eta_N = \sum_1^3 (U_{ek}^L)^2 \Xi_k \frac{m_p}{M_k}, \quad (2.2)$$

with  $m_p$  ( $m_e$ ) being the proton (electron) mass.  $U^L$  is the unitary mixing matrix connecting left-handed neutrino weak eigenstates  $\nu_{lL}$  to mass eigenstates of light  $\chi_k$  and heavy  $N_k$  Majorana neutrinos with masses  $m_k$  ( $m_k \ll 1$  MeV) and  $M_k$  ( $M_k \gg 1$  GeV), respectively. We have

$$\nu_{lL} = \sum_{k=\text{light}} U_{lk}^L \chi_{kL} + \sum_{k=\text{heavy}} U_{lk}^L N_{kL} \quad (l=e, \mu, \tau). \quad (2.3)$$

$\nu_k, N_k$  satisfy the Majorana condition  $\nu_k \xi_k = C \bar{\nu}_k^T$ ,  $N_k \Xi_k = C \bar{N}_k^T$ , where  $C$  denotes the charge conjugation while  $\xi, \Xi$  are phase factors; the eigenmasses are assumed positive.

The nuclear matrix elements associated with the exchange of light ( $M_{\langle m_\nu \rangle}^{\text{light}}$ ) and heavy neutrinos ( $M_{\eta_N}^{\text{heavy}}$ ), including contributions from induced nucleon currents, can be written as a sum of Fermi, Gamow-Teller, and tensor components [16]:

$$\mathcal{M}_K = -\frac{M_F^K}{g_A^2} + M_{GT}^K + M_T^K \quad (K = \langle m_\nu \rangle, \eta_N). \quad (2.4)$$

Here,  $g_A = 1.25$ . Using the second quantization formalism,  $\mathcal{M}_K$  can be expressed in terms of relative coordinates as follows:

$$\begin{aligned} \mathcal{M}_K = & \sum_{J^\pi} \sum_{\substack{pnp'n' \\ m_i m_f J}} (-)^{j_n + j_{p'} + J + \mathcal{J}} (2J+1) \left\{ \begin{matrix} j_p & j_n & J \\ j_{n'} & j_{p'} & \mathcal{J} \end{matrix} \right\} \\ & \times \langle p(1), p'(2); \mathcal{J} | f(r_{12}) \tau_1^+ \tau_2^+ \mathcal{O}_K(12) f(r_{12}) | \\ & \times n(1), n'(2); \mathcal{J} \rangle \\ & \times \langle 0_f^+ | [c_p^\dagger, \tilde{c}_{n'}]_J | J^\pi m_f \rangle \langle J^\pi m_f | J^\pi m_i \rangle \\ & \times \langle J^\pi m_i | [c_p^\dagger, \tilde{c}_n]_J | 0_i^+ \rangle. \end{aligned} \quad (2.5)$$

Here,  $f(r_{12})$  is the short-range correlation function [4] and  $\mathcal{O}_K(12)$  ( $K = \langle m_\nu \rangle, \eta_N$ ) represents the coordinate- and spin-dependent part of the two-body  $0\nu\beta\beta$ -decay transition operator

$$\mathcal{O}_{\mathcal{K}}(12) = -\frac{H_F^{\mathcal{K}}(r_{12})}{g_A^2} + H_{GT}^{\mathcal{K}}(r_{12})\sigma_{12} + H_T^{\mathcal{K}}(r_{12})\mathbf{S}_{12}. \quad (2.6)$$

Also, the following notation has been used:

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = |\mathbf{r}_{12}|, \quad \hat{\mathbf{r}}_{12} = \frac{\mathbf{r}_{12}}{r_{12}},$$

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{\mathbf{r}}_{12})(\vec{\sigma}_2 \cdot \hat{\mathbf{r}}_{12}) - \sigma_{12}, \quad \sigma_{12} = \vec{\sigma}_1 \cdot \vec{\sigma}_2, \quad (2.7)$$

where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are coordinates of the beta decaying nucleons. The radial part of the light and heavy neutrino exchange potentials  $H_I^{(m_\nu)}(r_{12})$  and  $H_I^{\eta N}(r_{12})$  ( $I=F, GT, T$ ) can be written as

$$H_I^{(m_\nu)}(r_{12}) = \frac{2}{\pi g_A^2} \frac{R}{r_{12}} \int_0^\infty \frac{\sin(qr_{12})}{q + E^m(J) - (E^i + E^f)/2} h_I(q^2) dq,$$

$$H_I^{\eta N}(r_{12}) = \frac{1}{m_p m_e} \frac{2}{\pi g_A^2} \frac{R}{r_{12}} \int_0^\infty \sin(qr_{12}) h_I(q^2) q dq, \quad (2.8)$$

with

$$h_F(q^2) = g_V^2(q^2) g_A^2,$$

$$h_{GT}(q^2) = g_A^2(q^2) + \frac{1}{3} \frac{g_P^2(q^2) q^4}{4m_p^2} - \frac{2}{3} \frac{g_A(q^2) g_P(q^2) q^2}{2m_p}$$

$$+ \frac{2}{3} \frac{g_M^2(\vec{q}^2) \vec{q}^2}{4m_p^2},$$

$$h_T(q^2) = \frac{2}{3} \frac{g_A(q^2) g_P(q^2) q^2}{2m_p} - \frac{1}{3} \frac{g_P^2(q^2) q^4}{4m_p^2} + \frac{1}{3} \frac{g_M^2(\vec{q}^2) \vec{q}^2}{4m_p^2}. \quad (2.9)$$

Here,  $R = r_0 A^{1/3}$  is the mean nuclear radius [16] with  $r_0 = 1.1$  fm.  $E^i$ ,  $E^f$ , and  $E^m(J)$  are the energies of the initial, final, and intermediate nuclear states with angular momentum  $J$ , respectively. The momentum dependence of the vector, weak magnetism, axial vector, and pseudoscalar form factors [ $g_V(q^2)$ ,  $g_M(q^2)$ ,  $g_A(q^2)$ , and  $g_P(q^2)$ ] can be found in Ref. [16].

We note that the overlap factor  $\langle J^\pi m_f | J^\pi m_i \rangle$  and the one-body transition densities  $\langle J^\pi m_i | [c_p^\dagger \tilde{c}_n]_J | 0_i^+ \rangle$  and  $\langle 0_f^+ | [c_p^\dagger \tilde{c}_n]_J | J^\pi m_f \rangle$  entering Eq. (2.5) must be computed in a nuclear model.

### B. Trilinear $R$ -parity violating mechanisms

The minimal supersymmetric standard model (MSSM), which is the simplest extension of the SM, preserves  $R$  parity, i.e., also the total lepton number. We recall that  $R$  parity is a discrete multiplicative symmetry defined as  $R_p = (-1)^{3B+L+2S}$ , where  $S$ ,  $B$ , and  $L$  are the spin, the baryon,

and the lepton quantum number. Thus  $R_p = +1$  for SM particles and  $R_p = -1$  for superpartners.

Generally, one can add trilinear  $R$ -parity violating terms to the superpotential of the MSSM:

$$W_{R_p} = \lambda_{ijk} L_i L_j E_k^c + \lambda'_{ijk} L_i Q_j D_k^c + \mu_j L_j H_2 + \lambda''_{ijk} U_i^c D_j^c D_k^c, \quad (2.10)$$

where  $i, j, k$  denote generation indices. Here  $L$  and  $Q$  stand for the lepton and quark doublet left-handed superfields while  $E^c$ ,  $U^c$ , and  $D^c$  for the charge conjugated lepton, up, and down quark singlet superfields, respectively. The terms proportional to  $\lambda$  and  $\lambda'$  violate the lepton number while those proportional to  $\lambda''$  violate the baryon number.

The  $0\nu\beta\beta$  decay can be induced by different trilinear  $R$ -parity violating mechanisms, partially determined by different products of the parameters  $\lambda$  and  $\lambda'$  [12,33,35]. Here, we consider those mechanisms which lead to the most stringent constraint on the  $\lambda'_{111}$  parameter. They are triggered by an exchange of gluinos and neutralinos. The corresponding Feynman diagrams can be found, e.g., in Refs. [17,33]. If the masses of the SUSY particles are assumed to be of about the same value, there is a dominance of the gluino-exchange mechanism [33]. This conclusion is expected to be valid also for the  $0\nu\beta\beta$ -decay transitions to excited  $0^+$  states.

The  $0\nu\beta\beta$ -decay half-life, associated with exchange of gluinos, is [4,33]

$$[T_{1/2}(0^+ \rightarrow 0^+)]^{-1} = G_{01} |(\eta_{\tilde{g}} + 4\eta'_{\tilde{g}}) \mathcal{M}_{\lambda'_{111}}|^2. \quad (2.11)$$

The effective  $R_p$  violating parameters  $\eta_{\tilde{g}}$  and  $\eta'_{\tilde{g}}$  can be expressed by means of the fundamental parameters of the MSSM as follows:

$$\eta_{\tilde{g}} = \frac{\pi\alpha_s}{6} \frac{\lambda'_{111}}{G_F^2 m_{\tilde{d}_R}^4} \frac{m_P}{m_{\tilde{g}}} \left[ 1 + \left( \frac{m_{\tilde{d}_R}}{m_{\tilde{u}_L}} \right)^4 \right],$$

$$\eta'_{\tilde{g}} = \frac{\pi\alpha_s}{12} \frac{\lambda'_{111}}{G_F^2 m_{\tilde{d}_R}^4} \frac{m_P}{m_{\tilde{g}}} \left( \frac{m_{\tilde{d}_R}}{m_{\tilde{u}_L}} \right)^2. \quad (2.12)$$

Here,  $\alpha_s = g_s^2/(4\pi)$  is the  $SU(3)_c$  gauge coupling constant.  $m_{\tilde{u}_L}$ ,  $m_{\tilde{d}_R}$ , and  $m_{\tilde{g}}$  are masses of the  $u$  squark,  $d$  squark, and gluino.

At the level of hadronization, the dominant mechanism is the pion realization of the underlying  $\Delta L = 2$  quark-level  $0\nu\beta\beta$  transition  $dd \rightarrow uu + 2e^-$  [33]. The nuclear matrix element  $\mathcal{M}_{\lambda'_{111}}$  can be written as a sum of contributions originating from one- and two-pion-exchange modes. Thus, we have [33]

$$\mathcal{M}_{\lambda'_{111}} = \mathcal{M}^{1\pi} + \mathcal{M}^{2\pi} = \left( \frac{m_A}{m_p} \right)^2 \frac{m_p}{m_e} \left( \frac{4}{3} \alpha^{1\pi} (M_{GT}^{1\pi} + M_T^{1\pi}) \right. \\ \left. + \alpha^{2\pi} (M_{GT}^{2\pi} + M_T^{2\pi}) \right), \quad (2.13)$$

where

$$M_{GT}^{k\pi} = \langle 0_f^+ | \sum_{i \neq j} \tau_i^+ \tau_j^+ \vec{\sigma}_i \cdot \vec{\sigma}_j F_{GT}^{(k)}(m_\pi r_{ij}) \frac{R}{r_{ij}} | 0_i^+ \rangle,$$

with  $k=1,2$ ,

$$M_T^{k\pi} = \langle 0_f^+ | \sum_{i \neq j} \tau_i^+ \tau_j^+ [3(\vec{\sigma}_i \cdot \hat{\mathbf{r}}_{ij})(\vec{\sigma}_j \cdot \hat{\mathbf{r}}_{ij}) - \vec{\sigma}_i \cdot \vec{\sigma}_j] F_T^{(k)}(m_\pi r_{ij}) \frac{R}{r_{ij}} | 0_i^+ \rangle, \quad (2.14)$$

with

$$F_{GT}^{(1)}(x) = e^{-x}, \quad F_T^{(1)}(x) = (3 + 3x + x^2) \frac{e^{-x}}{x^2}, \quad (2.15)$$

$$F_{GT}^{(2)}(x) = (x-2)e^{-x}, \quad F_T^{(2)}(x) = (x+1)e^{-x}. \quad (2.16)$$

Here,  $m_A (= 850 \text{ MeV})$  and  $m_\pi$  are the mass scale of the nucleon form factor and the mass of the pion, respectively. Values of the structure coefficients  $\alpha^{k\pi}$  ( $k=1,2$ ) are [33]  $\alpha^{1\pi} = -4.4 \times 10^{-2}$  and  $\alpha^{2\pi} = 2 \times 10^{-1}$ .

Having in mind forthcoming calculations within the RQRPA, it is useful to rewrite  $\mathcal{M}_{\lambda'_{111}}$  in the form given by Eqs. (2.5) and (2.6) ( $\mathcal{K} = \lambda'_{111}$ ). One finds that the Fermi part of the pion-exchange potential is equal to zero [ $H_F^{\lambda'_{111}}(r_{12}) = 0$ ] and the Gamow-Teller and tensor parts are given by

$$H_{GT}^{\lambda'_{111}}(r_{12}) = \left( \frac{m_A}{m_p} \right)^2 \frac{m_p}{m_e} \left( \frac{4}{3} \alpha^{1\pi} F_{GT}^{1\pi}(m_\pi r_{12}) + \alpha^{2\pi} F_{GT}^{2\pi}(m_\pi r_{12}) \right),$$

$$H_T^{\lambda'_{111}}(r_{12}) = \left( \frac{m_A}{m_p} \right)^2 \frac{m_p}{m_e} \left( \frac{4}{3} \alpha^{1\pi} F_T^{1\pi}(m_\pi r_{12}) + \alpha^{2\pi} F_T^{2\pi}(m_\pi r_{12}) \right). \quad (2.17)$$

### III. ONE-BODY TRANSITION DENSITIES

The nuclear matrix element  $\mathcal{M}_{\mathcal{K}}$  ( $\mathcal{K} = \langle m_\nu \rangle, \eta_N \lambda'_{111}$ ), in Eq. (2.5), is associated with the  $0\nu\beta\beta$  decay to the ground state,  $0_{g.s.}^+$ , or to any of the excited  $0^+$  states in the final nucleus. Its evaluation requires the description of the initial ( $|0_i^+\rangle$ ), final ( $|0_f^+\rangle$ ), and intermediate states (all in different nuclei) with angular momentum and parity  $J^\pi$  ( $|J^\pi m_{i,f}\rangle$ ), within a given nuclear model. Then, the one-body transition density, entering the expression for  $\mathcal{M}_{\mathcal{K}}$ , can be calculated and consequently the chosen matrix element is readily obtained.

The standard QRPA (based on the quasiboson approximation) and the RQRPA have been intensively used to calculate nuclear matrix elements for the double beta decay [4,16,23–25,32–34]. The RQRPA includes anharmonicities (the ground state is less correlated than in the standard QRPA)

and there is no collapse of its first solution within the physical range of the particle-particle interaction strength. Within schematic models, it has been shown that by including the Pauli exclusion principle (PEP) in the QRPA, good agreement with the exact solution of the many-body problem can be achieved even beyond the critical point of the standard QRPA [36]. The RQRPA takes into account the PEP in an approximate way. Nevertheless, it is enough to avoid the main drawback of the standard QRPA and to reduce the sensitivity of the calculated observables to the details of the nuclear model. The RQRPA has been used in our previous studies of the double beta decay [4,16,29,32,33,37]. Here we apply this approach to calculate the  $0\nu\beta\beta$  decay to first excited states  $0^+$ .

The final nuclei for  $A=76, 82, 100$ , and  $136$  double beta decaying systems are  $^{76}\text{Se}$ ,  $^{82}\text{Kr}$ ,  $^{100}\text{Ru}$ , and  $^{136}\text{Ba}$ , respectively. The first excited  $0_1^+$  state of these nuclei is believed to be a member of the vibrational triplet  $0^+, 2^+, 4^+$ . This state can be described as follows:

$$|0_1^+\rangle = \frac{1}{\sqrt{2}} \{ \Gamma_2^{1\dagger} \otimes \Gamma_2^{1\dagger} |0\rangle_{g.s.} \}, \quad (3.1)$$

where  $\Gamma_2^{1\dagger}$  is the creation quadrupole phonon operator. The experimental energies of  $0_1^+$  [ $E(0_1^+)$ ] and  $2_1^+$  [ $E(2_1^+)$ ] states relative to the ground state energies are

$$\begin{aligned} [E(0_1^+), E(2_1^+)] &= [1.122, 0.559] \text{ MeV} && \text{for } A=76 \\ &= [1.488, 0.777] \text{ MeV} && \text{for } A=82 \\ &= [1.130, 0.540] \text{ MeV} && \text{for } A=100 \\ &= [1.579, 0.818] \text{ MeV} && \text{for } A=136. \end{aligned} \quad (3.2)$$

One notices that the energy of the  $0_1^+$  excited state is about twice the energy of the  $2_1^+$  excited state.

The nuclear states of interest are described as charge changing ( $pn$ -RQRPA) and charge conserving ( $ppnn$ -RQRPA) modes of the RQRPA approach.

In the framework of the  $pn$ -RQRPA, the  $m$ th excited state of the intermediate odd-odd nucleus, with the angular momentum  $J$  and projection  $M$ , is created by applying the phonon operator  $Q_{JM}^{m\dagger}$  on the vacuum state  $|0_{RPA}^+\rangle$ :

$$|m, JM^\pi\rangle = Q_{JM}^{m\dagger} |0_{RPA}^+\rangle \quad \text{with} \quad Q_{JM}^m |0_{RPA}^+\rangle = 0. \quad (3.3)$$

Here  $|0_{RPA}^+\rangle$  is the ground state of the initial or the final nucleus and the phonon operator  $Q_{JM}^{m\dagger}$  is defined by the ansatz

$$Q_{JM}^{m\dagger} = \sum_{pn} [X_{(pn, J^\pi)}^m A^\dagger(pn, JM) + Y_{(pn, J^\pi)}^m \tilde{A}(pn, JM)]. \quad (3.4)$$

$X_{(pn, J^\pi)}^m$ ,  $Y_{(pn, J^\pi)}^m$  denote free variational amplitudes, which are calculated by solving the RQRPA equations.



The first excited  $2^+$  state of the daughter nucleus is assumed to have one-quadrupole-phonon character. Within the  $ppnn$ -RQRPA (allowing for two-proton and two-neutron quasiparticle excitations only) this state is defined by

$$|2_1^+\rangle = \Gamma_{2M^+}^\dagger |0_{RPA}^+\rangle \quad \text{with} \quad \Gamma_{2M^+}^\dagger |0_{RPA}^+\rangle = 0, \quad (3.5)$$

where

$$\begin{aligned} \Gamma_{2M^+}^\dagger = & \sum_{p \leq p'} [R_{(p,p',2^+)}^1 A^\dagger(p,p',2M) \\ & + S_{(p,p',2^+)}^1 \tilde{A}(p,p',2M)] \\ & + \sum_{n \leq n'} [R_{(n,n',2^+)}^1 A^\dagger(n,n',2M) \\ & + S_{(n,n',2^+)}^1 \tilde{A}(n,n',2M)]. \end{aligned} \quad (3.6)$$

$A^\dagger(\tau\tau',JM)$  and  $A(\tau\tau',JM)$  ( $\tau=p,n$  and  $\tau'=p',n'$ ) are the two quasiparticle creation and annihilation operators coupled to the good angular momentum  $J$  with projection  $M$ , respectively, defined by

$$\begin{aligned} A^\dagger(\tau\tau',JM) = & \frac{[1 + (-1)^J \delta_{\tau\tau'}]}{(1 + \delta_{\tau\tau'})^{3/2}} \sum_{m_\tau, m'_\tau} C_{j_\tau m_\tau j_\tau m'_\tau}^{JM} a_{m_\tau}^\dagger a_{m'_\tau}^\dagger, \\ A(\tau\tau',JM) = & [A^\dagger(\tau\tau',JM)]^\dagger. \end{aligned} \quad (3.7)$$

The vacua defined by Eqs. (3.5) and (3.3) are in principle different from each other. However, the differences induce corrections to the matrix elements considered, of higher order, and therefore they are neglected. The quasiparticle creation and annihilation operators ( $a_{m_\tau}^\dagger$  and  $a_{m_\tau}$ ,  $\tau=p,n$ ) have been defined through the Bogoliubov-Valatin transformation

$$\begin{pmatrix} a_{m_\tau}^\dagger \\ \tilde{a}_{m_\tau} \end{pmatrix} = \begin{pmatrix} u_\tau & v_\tau \\ -v_\tau & u_\tau \end{pmatrix} \begin{pmatrix} c_{m_\tau}^\dagger \\ \tilde{c}_{m_\tau} \end{pmatrix}, \quad (3.8)$$

where  $c_{m_\tau}^\dagger$  ( $c_{m_\tau}$ ) denotes the particle creation (annihilation) operator acting on a single-particle level with quantum numbers  $(n_\tau, l_\tau, j_\tau)$ . The parameters  $u, v$  are occupation amplitudes and the tilde symbol indicates the time-reversal operation, e.g.,  $\tilde{a}_{m_\tau} = (-1)^{j_\tau - m_\tau} a_{\tau - m_\tau}$ .

Let us now denote by  $\mathcal{D}_{pn}$  and  $\mathcal{D}_{\tau\tau'}$  ( $\tau=p,n$ ) the following expectation values:

$$\begin{aligned} \langle 0_{RPA}^+ | [A(pn, JM), A^\dagger(p'n', JM)] | 0_{RPA}^+ \rangle &= \delta_{pp'} \delta_{nn'} \mathcal{D}_{pn}, \\ \langle 0_{RPA}^+ | [A(\tau\tau', JM), A^\dagger(\sigma\sigma', JM)] | 0_{RPA}^+ \rangle \\ &= (\delta_{\tau\sigma} \delta_{\tau'\sigma'} - (-1)^{j_\tau + j_{\tau'} - J} \delta_{\tau\sigma'} \delta_{\tau'\sigma}) \mathcal{D}_{\tau\tau'}. \end{aligned} \quad (3.9)$$

Here, the exact expressions of the commutators are taken into account. The calculation of  $\mathcal{D}$  factors is discussed in Refs. [25,38].

Solving the  $pn$ -RQRPA ( $ppnn$ -RQRPA) equations, one gets the renormalized amplitudes  $\bar{X}, \bar{Y}$  ( $\bar{R}, \bar{S}$ ) with the usual normalization  $\bar{X}\bar{X} - \bar{Y}\bar{Y} = 1$  ( $\bar{R}\bar{R} - \bar{S}\bar{S} = 1$ ). They are related to  $X$  ( $R$ ) and  $Y$  ( $S$ ) amplitudes, characterizing the standard QRPA phonon operator by

$$\begin{aligned} \bar{X}_{(pn, J^\pi)}^m &= \sqrt{\mathcal{D}_{pn}} X_{(pn, J^\pi)}^m, & \bar{Y}_{(pn, J^\pi)}^m &= \sqrt{\mathcal{D}_{pn}} Y_{(pn, J^\pi)}^m, \\ \bar{R}_{(\tau\tau', J^\pi)}^m &= \sqrt{\mathcal{D}_{\tau\tau'}} R_{(\tau\tau', J^\pi)}^m, & \bar{S}_{(\tau\tau', J^\pi)}^m &= \sqrt{\mathcal{D}_{\tau\tau'}} S_{(\tau\tau', J^\pi)}^m. \end{aligned} \quad (3.10)$$

In the quasiparticle representation, the beta transition density operator can be written as

$$\begin{aligned} [c_p^\dagger \tilde{c}_n]_{JM} = & u_p v_n A^\dagger(pn, JM) + u_n v_p \tilde{A}(pn, JM) \\ & + u_p u_n B^\dagger(pn, JM) - v_p v_n \tilde{B}(pn, JM). \end{aligned} \quad (3.11)$$

If we restrict our consideration to the ground state to ground state  $0\nu\beta\beta$  decay, we end up with the following expressions for one-body densities [16,25]:

$$\begin{aligned} \langle J^\pi m_i | [c_p^\dagger \tilde{c}_n]_{JM} | 0_i^+ \rangle = & \sqrt{2J+1} (u_p^{(i)} v_n^{(i)} \bar{X}_{(pn, J^\pi)}^{m_i} \\ & + v_p^{(i)} u_n^{(i)} \bar{Y}_{(pn, J^\pi)}^{m_i}) \sqrt{\mathcal{D}_{pn}^{(i)}}, \end{aligned} \quad (3.12)$$

$$\begin{aligned} \langle 0_f^+ | [\widetilde{c_p^\dagger \tilde{c}_n}]_{JM} | J^\pi m_f \rangle = & \sqrt{2J+1} (v_p^{(f)} u_n^{(f)} \bar{X}_{(pn, J^\pi)}^{m_f} \\ & + u_p^{(f)} v_n^{(f)} \bar{Y}_{(pn, J^\pi)}^{m_f}) \sqrt{\mathcal{D}_{pn}^{(f)}}. \end{aligned} \quad (3.13)$$

Here, the index  $i$  ( $f$ ) indicates that the quasiparticles and the excited states of the nucleus are defined with respect to the initial (final) nuclear ground state  $|0_i^+\rangle$  ( $|0_f^+\rangle$ ). The overlap matrix elements entering Eq. (2.5) are explicitly given in Ref. [39].

The beta transition density from the intermediate states  $|J^\pi m\rangle$  to the first excited  $0^+$  state of the daughter nucleus, which is considered to be of two-quadrupole phonon character for the nuclei with  $A = 76, 82, 100$ , and  $136$ , can be written as

$$\begin{aligned} \langle 0_1^+ | [\widetilde{c_p^\dagger \tilde{c}_n}]_{JM} | J^\pi m \rangle \\ = \langle 0_{RPA}^+ | \frac{1}{\sqrt{2}} \{ \Gamma_2 \otimes \Gamma_2 \}^0 \{ [c_p^\dagger \tilde{c}_n]_{JM} \otimes Q_{J^\pi}^{m\dagger} \}^0 | 0_{RPA}^+ \rangle \sqrt{2J+1}. \end{aligned} \quad (3.14)$$

There are two basic approaches to calculate this expression. We shall discuss them in the next sections.

### A. Recoupling approach

The first calculation of the two-neutrino double-beta-decay ( $2\nu\beta\beta$ -decay) transition to an excited  $0^+$  final state was presented in Ref. [26]. The formalism proposed was

developed in the Tamm-Dancoff approximation (TDA). It was claimed that the contributions coming from the background graphs are negligible. The dominant contribution is obtained by calculating, through a recoupling procedure, the

scalar product of two pairs of proton-neutron quasiparticle creation operators, originating from the beta transition  $[c_p^\dagger \widetilde{c}_n]_{JM}$  and the phonon  $Q_{JM}^{m\dagger}$  operators:

$$\{A^\dagger(pn, J) \otimes A^\dagger(p'n', J)\}^0 = - \sum_{J'} (-1)^{j_n + j_{p'} + J + J'} \frac{(\delta_{pp'}(-)^{J'+1} + 1)}{(1 + \delta_{pp'})^{1/2}} \frac{(\delta_{nn'}(-)^{J'+1} + 1)}{(1 + \delta_{nn'})^{1/2}} (2J' + 1)^{1/2} \begin{Bmatrix} j_n & j_p & J \\ j_{p'} & j_{n'} & J' \end{Bmatrix} \times \{A^\dagger(pp', J') \otimes A^\dagger(nn', J')\}^0. \quad (3.15)$$

Henceforth we shall denote this approach as the recoupling method (RCM).

By using Eq. (3.14), the beta transition matrix element takes the form

$$\langle 0_1^+ | [c_p^\dagger \widetilde{c}_n]_{JM} | J^\pi M, m_f \rangle = \sqrt{10} \sum_{p'n'} (1 + \delta_{pp'})^{1/2} (1 + \delta_{nn'})^{1/2} \left( \frac{\mathcal{D}_{pp'}^{(f)} \mathcal{D}_{nn'}^{(f)}}{\mathcal{D}_{pn}^{(f)}} \right)^{1/2} \begin{Bmatrix} j_n & j_p & J \\ j_{p'} & j_{n'} & 2 \end{Bmatrix} \times (u_p^{(f)} v_n^{(f)} \bar{X}_{(p'n', J^\pi)}^{m_f} \bar{R}_{(pp', 2^+)}^{m_f} \bar{R}_{(nn', 2^+)}^{m_f} - v_p^{(f)} u_n^{(f)} \bar{Y}_{(p'n', J^\pi)}^{m_f} \bar{S}_{(pp', 2^+)}^{m_f} \bar{S}_{(nn', 2^+)}^{m_f}). \quad (3.16)$$

Obviously, in the above expression, the full expression of the RPA phonon operator was used. In comparing this transition density to  $0_1^+$  with that one leading to the ground state, we find two important differences. First, the dominant contribution in Eq. (3.16) is a product of three forward-going amplitudes. This fact implies that the transition amplitude is not expected to be very sensitive to the nuclear ground state correlations. Second, the leading term in Eq. (3.16) is multiplied by the factor  $u_p^{(f)} v_n^{(f)}$  (i.e., “ $\beta^-$ ” like) while the leading term of the beta ground state transition in Eq. (3.13) contains the factor  $v_p^{(f)} u_n^{(f)}$  (i.e., “ $\beta^+$ ” like).

The drawback of this approach is that the transition density, in Eq. (3.16), contains significant unphysical contributions. To clarify this point we transform the second part of the right-hand side (RHS) of Eq. (3.14), which up to a multiplicative constant should represent the excited state  $0_1^+$  in the  $(A, Z+2)$  nucleus. From the transition operator written in quasiparticle representation we keep, for illustration, the operator  $A^\dagger(pn, J)$ , which is further expressed in terms of the  $pn$ -QRPA bosons. The final result is

$$\{A^\dagger(pn, J) \otimes Q_{J^\pi}^{m\dagger}\}^0 | 0_{RPA_f}^+ \rangle = \sum_{m'} \left[ X_{(pn, J^\pi)}^{m'} \{Q_{J^\pi}^{m'\dagger} \otimes Q_{J^\pi}^{m\dagger}\}^0 | 0_{RPA_f}^+ \rangle + \frac{1}{\sqrt{2J+1}} Y_{(pn, J^\pi)}^m | 0_{RPA_f}^+ \rangle \right]. \quad (3.17)$$

The second term in the above equation is obtained by using the commutator algebra for  $Q_{J^\pi}^{m\dagger}$  and its Hermitian conjugate operator, and then Eq. (3.3). From Eq. (3.17) it follows that within the RCM procedure we have produced a linear combination of a state associated with the  $(A, Z)$  nucleus and the ground state characterizing the  $(A, Z+2)$  nucleus. We note

that the desired  $0_1^+$  excited state of the  $(A, Z+2)$  nucleus is missing. The RCM does not allow one to eliminate the admixture of these states, which due to the recoupling procedure are related to the  $0_1^+$  excited state. Moreover, it is worth noting that the component in the  $(A, Z+2)$  nucleus is proportional to the  $Y$  amplitude, as prescribed by the method presented in the next subsection, and not to the forward-going amplitude of the proton-neutron dipole phonon as suggested by the RCM approach. Thus, the validity of this recoupling procedure is questionable in the framework of the QRPA.

The RCM has been modified by introducing a multiple commutator method (MCM) and applied to calculate different lepton number conserving modes of the double beta decay [40]. This version of the RCM has been also used for describing the  $0\nu\beta\beta$  decay to excited collective  $0^+$  states [23].

## B. Boson expansion approach

A pioneering approach to study the double beta decay to excited states of the final nucleus was proposed in Refs. [27,28]. It is the so-called boson expansion method (BEM). Applications of the BEM approach to study the single beta and  $2\nu\beta\beta$  decay to the first excited quadrupole state ( $2_1^+$ ) and the two-quadrupole-phonon states ( $0_{2-ph, 2_{2-ph}}^+$ ) of even-even isotopes were presented in Refs. [27,28]. Recently, the renormalized version of the BEM was applied to the transition  $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$  [29]. The new version has the virtue of exploiting the complementary features of the BEM and RQRPA methods. As a matter of fact this improved version of the BEM is adopted in the present paper.

Within the BEM approach, the operators involved on the RHS of Eq. (3.11) are written as polynomials of the RPA bosons [27,28], so that the mutual commutation relations are consistently preserved by the boson mapping. We shall fol-

low this procedure with some simplifications, which do not influence the final form of the one-body transition density.

By exploiting the fact that  $Q_{J^\pi}^m |0_{RPA_f}^+\rangle = 0$ , we introduce a commutator in the expression for the one-body transition operator to the  $0_1^+$  state. In addition, we evaluate this commutator by satisfying exact commutation relations. Thus we obtain

$$\begin{aligned} \langle 0_1^+ | [c_p^\dagger \tilde{c}_n]_{JM} | J^\pi M, m_f \rangle & \\ &= (-1)^{J-M} \langle 0_1^+ | [[c_p^\dagger \tilde{c}_n]_{J-M}, Q_{J^\pi}^{\dagger m}] | 0_{RPA_f}^+ \rangle \\ &= (v_p^{(f)} u_n^{(f)} X_{(pn, J^\pi)}^{m_f} + u_p^{(f)} v_n^{(f)} Y_{(pn, J^\pi)}^{m_f}) \\ &\quad \times \sum_{\tau=p, n} \frac{\langle 0_1^+ | B^\dagger(\tau\tau, 00) | 0_{RPA_f}^+ \rangle}{\sqrt{(2j_\tau + 1)}}. \end{aligned} \quad (3.18)$$

We omitted the terms  $A^\dagger(\tau\tau, 00)$  and  $A(\tau\tau, 00)$ , since in the boson expansion formalism they consist of terms comprising products of odd numbers of phonon operators  $Q_{JM^\pi}^{m^\dagger}$ ,  $Q_{JM^\pi}^m$ ,  $\Gamma_{2M^+}^{1^\dagger}$ , and  $\Gamma_{2M^+}^1$ , and consequently do not contribute to the above matrix element.

We proceed by performing the boson expansion of the operator  $B^\dagger(\tau\tau, 00)$  with the result

$$\begin{aligned} B^\dagger(\tau\tau, 00) &= \mathcal{B}_{11}^{20}(\tau\tau) \{ \Gamma_{2^+}^{1^\dagger} \otimes \Gamma_{2^+}^{1^\dagger} \}^0 + \mathcal{B}_{11}^{02}(\tau\tau) \{ \Gamma_{2^+}^1 \otimes \Gamma_{2^+}^1 \}^0 \\ &\quad + \mathcal{B}_{11}^{11}(\tau\tau) \{ \Gamma_{2^+}^{1^\dagger} \otimes \Gamma_{2^+}^1 \}^0. \end{aligned} \quad (3.19)$$

The upper indices, accompanying the expansion coefficients, indicate the number of the creation and annihilation phonon operators involved in the given terms while the lower indices suggest that the phonon operators correspond to the first root of the  $ppnn$ -QRPA equations. We note that relevant to the problem studied here is the coefficient  $\mathcal{B}_{11}^{20}(\tau\tau)$ , which can be determined by the following procedure. Commuting Eq. (3.19) twice with  $\Gamma_{2^+}^{1^\dagger}$  and then taking the expectation value of the result in the boson vacuum, one obtains

$$\begin{aligned} \mathcal{B}_{11}^{20}(\tau\tau) &= \frac{1}{2} \sum_M C_{2M, 2-M}^{00} \langle 0 | [ \Gamma_{2M}^1, [ \Gamma_{2-M}^{1^\dagger}, B^\dagger(\tau\tau, 00) ] ] | 0 \rangle \\ &= - \sqrt{\frac{5}{2j_\tau + 1}} \left( \sum_{\tau'(\tau' < \tau)} \bar{R}_{(\tau\tau', 2^+)}^1 \bar{S}_{(\tau\tau', 2^+)}^1 \right. \\ &\quad \left. + \sum_{\tau'(\tau' < \tau)} \bar{R}_{(\tau'\tau, 2^+)}^1 \bar{S}_{(\tau'\tau, 2^+)}^1 \right). \end{aligned} \quad (3.20)$$

In the above equations, all commutators are exactly evaluated except for the last one for which the renormalized quasiboson approximation is used [27–29].

Now, by a straightforward calculation, one arrives at the final expression for the one-body transition density leading to the final excited  $0_1^+$  two phonon state:

$$\begin{aligned} \langle 0_1^+ | [c_p^\dagger \tilde{c}_n]_{JM} | J^\pi M, m_f \rangle &= (v_p^{(f)} u_n^{(f)} \bar{X}_{(pn, J^\pi)}^{m_f} \\ &\quad + u_p^{(f)} v_n^{(f)} \bar{Y}_{(pn, J^\pi)}^{m_f}) \\ &\quad \times (\mathcal{D}_{pn})^{-1/2} \xi(p, p', n, n'), \end{aligned} \quad (3.21)$$

where

$$\begin{aligned} \xi(p, p', n, n') &= \sqrt{10} \left[ \frac{1}{2j_n + 1} \left( \sum_{n'(n < n')} \bar{R}_{(nn', 2^+)}^1 \bar{S}_{(nn', 2^+)}^1 \right. \right. \\ &\quad \left. \left. + \bar{R}_{(n'n, 2^+)}^1 \bar{S}_{(n'n, 2^+)}^1 \right) \frac{1}{2j_p + 1} \right. \\ &\quad \times \left( \sum_{p'(p < p')} \bar{R}_{(pp', 2^+)}^1 \bar{S}_{(pp', 2^+)}^1 \right. \\ &\quad \left. \left. + \bar{R}_{(p'p, 2^+)}^1 \bar{S}_{(p'p, 2^+)}^1 \right) \right]. \end{aligned} \quad (3.22)$$

It is worthwhile to notice that if we replace the factor  $\xi(p, p', n, n')$  with unity and consider small ground state correlations, i.e.,  $\mathcal{D}_{pn} \simeq 1$ , we obtain the ground state transition density from Eq. (3.13). We note that the transition density to the ground state is proportional to  $(\mathcal{D}_{pn})^{1/2}$ —i.e., it is suppressed by anharmonic effects—while the transition density to the excited  $0_1^+$  state is proportional to  $1/(\mathcal{D}_{pn})^{1/2}$ —i.e., it is enhanced by large ground state correlations.

We remark that the BEM expression given in Eq. (3.21) differs considerably from the the RCM expression given in Eq. (3.16). We see that the BEM transition density in Eq. (3.21) consists of products of forward- and backward-going variational amplitudes of the  $ppnn$ -RQRPA. It means that the final result exhibits sensitivity to the particle-particle interaction of the nuclear Hamiltonian. In addition, the BEM transition amplitude is a “ $\beta^+$ ”-like amplitude since the leading term is proportional to  $u_n^f v_p^f$ . This implies a possible strong dependence on the ground state correlations. The fact that the RCM and the MCM approaches differ considerably from the BEM procedure, when the final state is of multiple phonon character, was noticed already in Ref. [28]. The BEM avoids the operators recoupling and therefore the problem concerning the unphysical RCM contributions does not appear.

#### IV. NUMERICAL RESULTS AND DISCUSSIONS

The formalism described in the previous sections was applied to the transitions  $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$ ,  $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$ ,  $^{100}\text{Mo} \rightarrow ^{100}\text{Ru}$ , and  $^{136}\text{Xe} \rightarrow ^{136}\text{Ba}$ . The  $pn$ -RQRPA and the  $ppnn$ -RQRPA calculations have been performed for the same sets of basis states as in Ref. [16], which are identical for protons and neutrons. The single-particle energies were obtained by using a Coulomb-corrected Woods-Saxon potential. The realistic interaction employed is the Brueckner  $G$  matrix of the Bonn one-boson-exchange potential. The trun-

TABLE I. Nuclear matrix elements of light and heavy Majorana neutrino-exchange modes for  $0\nu\beta\beta$  decay in  $A=76, 82, 100,$  and  $136$  nuclei. Both transitions to the ground state ( $0_{\text{g.s.}}^+$ ) and the first  $0_1^+$  excited states (which is assumed to be a two-phonon state) of the final nucleus are considered. The calculations have been performed within renormalized QRPA with the help of the recoupling (RCM) and the boson expansion (BEM) approaches for the evaluation of the one-body transition density (f.s. means “final state”).

A	f.s.	Method	Light neutrino exchange mechanism				Heavy neutrino exchange mechanism			
			$M_F^{(m\nu)}$	$M_{GT}^{(m\nu)}$	$M_T^{(m\nu)}$	$\mathcal{M}_{(m\nu)}$	$M_F^{\eta N}$	$M_{GT}^{\eta N}$	$M_T^{\eta N}$	$\mathcal{M}_{\eta N}$
76	$0_{\text{g.s.}}^+$		-1.26	2.18	-0.190	2.80	-37.4	28.7	-20.1	32.6
	$0_1^+$	RCM	-0.570	0.933	-0.022	1.28	-4.00	1.42	-0.39	3.59
	$0_1^+$	BEM	-0.371	0.796	-0.039	0.994	-12.0	9.62	-1.06	16.3
82	$0_{\text{g.s.}}^+$		-1.15	2.07	-0.172	2.64	-34.4	25.4	-17.4	30.0
	$0_1^+$	RCM	-0.617	0.971	-0.024	1.34	-4.11	1.40	-0.014	4.02
	$0_1^+$	BEM	-0.342	0.762	-0.033	0.947	-11.2	8.61	-0.498	15.2
100	$0_{\text{g.s.}}^+$		-1.28	2.62	-0.230	3.21	-44.3	34.2	-32.9	29.7
	$0_1^+$	RCM	-0.305	1.059	0.016	1.27	-2.98	1.21	0.483	3.60
	$0_1^+$	BEM	-0.397	1.52	-0.008	1.76	-14.1	11.1	-3.90	16.2
136	$0_{\text{g.s.}}^+$		-0.504	0.496	-0.161	0.66	-21.7	16.8	-16.6	14.1
	$0_1^+$	RCM	-1.66	3.40	-0.038	4.42	-11.4	4.37	0.445	12.1
	$0_1^+$	BEM	-0.205	0.347	-0.038	0.441	-8.69	6.98	-1.99	10.5

cation of the single-particle space requires a renormalization of two-body matrix elements. The scaling of the pairing strength in the BCS calculation was adjusted to fit the empirical pairing gaps according to Ref. [41]. In the RQRPA calculations, the particle-particle and particle-hole channels of the  $G$ -matrix interaction are renormalized by multiplying them by the parameters  $g_{pp}$  and  $g_{ph}$ , which, in principle, should be close to unity. Our adopted value for  $g_{ph}$  was  $g_{ph}=0.8$ , as in our previous calculations [4,16]. We shall present the relevant nuclear matrix elements for  $g_{pp}=1$ . Nevertheless, their sensitivity to  $g_{pp}$  within the interval 0.80–1.20, which can be regarded as physical, will be discussed. We note that in our calculations the  $pn$ -RQRPA and  $ppnn$ -RQRPA channels are coupled through the equation for the renormalization factors  $D$  [25]. Our numerical analysis

shows that the quadrupole QRPA energies of the daughter nucleus are independent of  $g_{pp}$ .

The results of our calculations are summarized in Tables I, II, and IV and in Fig. 1. In Table I the dimensionless nuclear matrix elements of light and heavy neutrino-exchange modes of the  $0\nu\beta\beta$  decay of  $^{76}\text{Ge}$ ,  $^{82}\text{Se}$ ,  $^{100}\text{Mo}$ , and  $^{136}\text{Xe}$  are presented for both transitions to the ground and excited states. The displayed  $0\nu\beta\beta$ -decay matrix elements to the first excited states  $0_1^+$  were obtained within the RCM and BEM approaches. The particular contributions to the full matrix elements coming from Fermi, Gamow-Teller, and tensor terms in Eq. (2.4) are shown as well. The modifications coming from induced nucleon currents are included in the Gamow-Teller and tensor components [16]. We find that the tensor contribution plays an important role when the

TABLE II. The  $0\nu\beta\beta$ -decay nuclear matrix elements associated with the trilinear  $R$ -parity violating mode for  $A=76, 82, 100,$  and  $136$ . The same notation is used as in Table I.

A	f.s.	method	$\mathcal{R}_p$ SUSY mechanism						
			$M_{GT}^{1\pi}$	$M_T^{1\pi}$	$\mathcal{M}^{1\pi}$	$M_{GT}^{2\pi}$	$M_T^{2\pi}$	$\mathcal{M}^{2\pi}$	$\mathcal{M}_{\lambda', 111}$
76	$0_{\text{g.s.}}^+$		1.30	-1.02	-24.3	-1.34	-0.652	-601	-625.
	$0_1^+$	RCM	0.254	-0.009	-21.7	-0.139	-0.014	-46.3	-68.0
	$0_1^+$	BEM	0.482	-0.027	-40.2	-0.475	-0.050	-158	-198
82	$0_{\text{g.s.}}^+$		1.234	-0.873	-31.9	-1.258	-0.572	-551	-583
	$0_1^+$	RCM	0.253	0.011	-23.4	-0.135	-0.000	-40.8	-64.2
	$0_1^+$	BEM	0.462	0.001	-40.9	-0.449	-0.030	-144	-185
100	$0_{\text{g.s.}}^+$		1.433	-1.726	-25.9	-1.525	-1.048	-775	-750
	$0_1^+$	RCM	0.204	0.018	-19.6	-0.102	0.017	-25.6	-45.2
	$0_1^+$	BEM	0.532	-0.208	-28.6	-0.509	-0.129	-192	-221
136	$0_{\text{g.s.}}^+$		0.606	-0.840	20.7	-0.742	-0.543	-387	-367
	$0_1^+$	RCM	0.783	0.033	-72.1	-0.383	0.021	-109	-181
	$0_1^+$	BEM	0.284	-0.084	-17.7	-0.318	-0.076	-119	-136



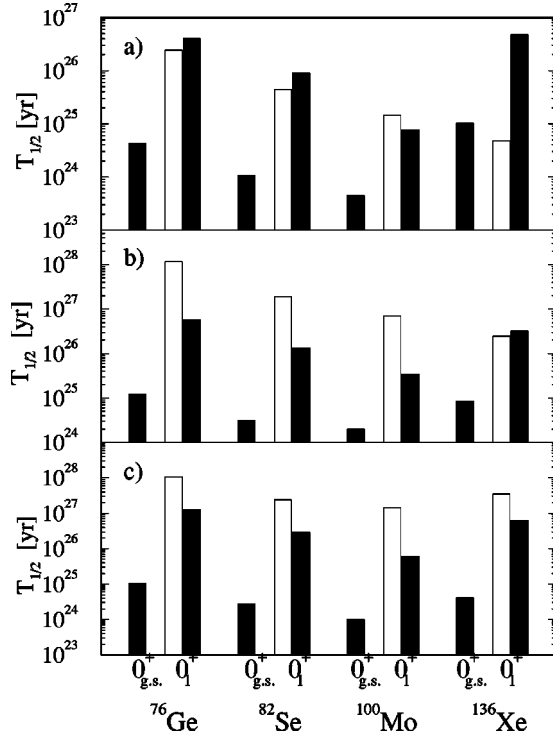


FIG. 1. Calculated half-lives of the  $0\nu\beta\beta$  decay of  $^{76}\text{Ge}$ ,  $^{76}\text{Se}$ ,  $^{100}\text{Mo}$ , and  $^{136}\text{Xe}$  for transitions to the ground  $0_{g.s.}^+$  and  $0_1^+$  excited states of the final nuclei assuming  $\langle m_{\nu} \rangle_{ee} = 1$  eV (a),  $\eta_N = 10^{-7}$  (b), and  $\lambda'_{111} = 10^{-4}$  (c). The black bars correspond to results describing ground state to ground state transitions as well as the results obtained for the transitions to the  $0_1^+$  excited state within the boson expansion method (BEM). The open bars denote results obtained for transitions to the  $0_1^+$  state via the recoupling method (RCM).

mechanism is mediated by heavy neutrinos and tends to cancel the contributions by Fermi and Gamow-Teller transition amplitudes. By glancing at Table I we find that the nuclear matrix elements involving the first excited  $0_1^+$  state are suppressed in comparison with those associated with transitions to the ground state. In the case of BEM calculations of  $M_{(m_{\nu})}^{light}$ , the suppression factor is about 2.8, 2.8, 1.8, and 1.5 for  $A = 76, 82, 100,$  and  $136$ , respectively. The RCM values are close to the BEM ones for  $A = 76, 82,$  and  $100$  nuclei. One notices an anomaly in the case of the  $A = 136$  system, where the RCM transition to the excited state is by a factor of 6.7 stronger than that to the ground state. It could be connected with the fact that  $^{136}\text{Xe}$  is a closed shell nucleus for neutrons ( $N = 82$ ) and therefore the unphysical contributions to this transition in the RCM approach might be larger. We note that it is not possible to compare directly nuclear matrix elements  $M_{(m_{\nu})}^{light}$  in Table I with those calculated in Ref. [23] for  $A = 76$  and  $82$ , since Ref. [23] does not include contributions from the induced currents. Nevertheless, we note that the ratio of the nuclear matrix elements of the transition to ground and excited states is equal to about 3 in Ref. [23]. This value is in good agreement with results of this article, despite the fact that the two formalisms differ from each other in many aspects.

From Table I it follows that the  $0\nu\beta\beta$  decay, mediated by heavy neutrinos to excited final states for  $A = 76, 82,$  and  $100$ , are weaker than those associated with ground state to ground state transitions, by about a factor of 1.3–2.0 (8–9) in the BEM (RCM). Here, the difference between the BEM and RCM predictions is more significant than for the light Majorana neutrino-exchange mechanism. We note also that for the  $A = 136$  system, the RCM value of  $M_{\eta_N}^{heavy}$  is comparable with the BEM one; i.e., within the RCM, the behavior of this nucleus is different from that of the remaining nuclei.

In Table II, the nuclear matrix elements associated with the trilinear  $R$ -parity violating mode of  $0\nu\beta\beta$  decay are displayed. Both the one-pion- and two-pion-exchange Gamow-Teller and tensor contributions to  $M_{\lambda'_{111}}$  are shown. In Refs. [32,33], it was shown that there is a dominance of the two-pion-exchange mode for the  $0\nu\beta\beta$ -decay transitions connecting the initial and final ground states, due to a larger structure coefficient  $\alpha^{2\pi}$  and because of a strong mutual cancellation of the one-pion-exchange Gamow-Teller and tensor contributions. We see that the second reason does not hold in the case of transitions to  $0_1^+$  excited states. We have found that the one-pion mode plays a more important role for this transition, giving a significant contribution to  $M_{\lambda'_{111}}$ . By comparing the values of nuclear matrix elements for ground and excited state transitions, we see that the second one is reduced by a factor of 2.7–3.4 within the BEM. The RCM values are considerably smaller for  $A = 76, 82,$  and  $100$  systems. A different situation is again found for the  $0\nu\beta\beta$  decay of  $^{136}\text{Xe}$  where the RCM value is close to the BEM result.

One purpose of our study is also the sensitivity of results for  $M_{(m_{\nu})}^{light}$ ,  $M_{\eta_N}^{heavy}$ , and  $M_{\lambda'_{111}}$  to the details of the nuclear model. We have examined the  $0\nu\beta\beta$  transition matrix elements as a function of the renormalization factor for the strength of the particle-particle interaction,  $g_{pp}$ , considered in the physical interval (see Table III). We see that the BEM values for the transition to excited  $0_1^+$  states exhibit a very similar dependence on  $g_{pp}$  as those for the transitions to the ground state. On the other hand, the RCM values are insensitive to changes of  $g_{pp}$ . Thus, our expectations from the previous section, hinging on the forms of the BEM and RCM one-body transition densities, have been confirmed. We note that a similar behavior has been found also for other nuclear systems.

As was already mentioned in the Introduction there is additional suppression of the  $0\nu\beta\beta$  decay to excited  $0^+$  final states coming from the smaller kinematical factor  $G_{01}$  [see Eq. (2.1)]. The values of  $G_{01}$  are given in Table IV. One finds that the ratio  $G_{01}(0_{g.s.}^+)/G_{01}(0_1^+)$  is about 12, 11, 5.2, and 21 for  $A = 76, 82, 100,$  and  $136$  systems, respectively. The corresponding half-lives to the excited  $0^+$  final state are larger by this factor.

For a given nuclear isotope the characteristics of  $0\nu\beta\beta$  decay refer to both the nuclear matrix element and the kinematical factor. For a chosen isotope, it is worthwhile to introduce sensitivity parameters with respect to different lepton number violating parameters. Large numerical values of these parameters may define those transitions and isotopes

TABLE III. The calculated nuclear matrix elements of the  $0\nu\beta\beta$  decay of  ${}^{76}\text{Ge}$  associated with exchange of light and heavy neutrinos and gluinos for different values of  $g_{pp}$  within its expected physical range in the RQRPA.

$g_{pp}$	$0_{\text{g.s.}}^+$	$M_{\langle m_\nu \rangle}^{\text{light}}$		$M_{\eta_N}^{\text{heavy}}$			$M_{\lambda'_{111}}$								
		$0_1^+$	BEM	$0_1^+$	RCM	$0_{\text{g.s.}}^+$	$0_1^+$	BEM	$0_1^+$	RCM	$0_{\text{g.s.}}^+$	$0_1^+$	BEM	$0_1^+$	RCM
0.8	3.8	1.34	1.30	39	19	3.7	-686	-225	-71						
1.0	2.8	0.99	1.28	33	16	3.6	-625	-198	-68						
1.2	1.6	0.58	1.20	27	13	3.3	-564	-163	-63						

which are the most promising candidates for a lepton number violating signal in the  $0\nu\beta\beta$  decay. These parameters are defined as follows [16,17]:

$$\begin{aligned}\zeta_{\langle m_\nu \rangle}(Y) &= 10^7 |\mathcal{M}_{\langle m_\nu \rangle}| \sqrt{G_{01}} \text{ year}, \\ \zeta_{\eta_N}(Y) &= 10^6 |\mathcal{M}_{\eta_N}| \sqrt{G_{01}} \text{ year}, \\ \zeta_{\lambda'_{111}}(Y) &= 10^5 |\mathcal{M}_{\lambda'_{111}}| \sqrt{G_{01}} \text{ year}.\end{aligned}\quad (4.1)$$

TABLE IV. The sensitivity factors  $\zeta_{\langle m_\nu \rangle}$ ,  $\zeta_{\eta_N}$ , and  $\zeta_{\lambda'_{111}}$  [see Eqs. (4.1)] and calculated  $0\nu\beta\beta$ -decay half-lives  $T_{1/2}$  for transitions to both ground and excited  $0_1^+$  states of the final nucleus ( $A=76, 82, 100$ , and 136) by assuming  $\langle m_\nu \rangle = 1$  eV,  $\eta_N = 10^{-7}$ , and  $\lambda'_{111} = 10^{-4}$ .  $G_{01}$  is the kinematical factor.

	${}^{76}\text{Ge}$	${}^{82}\text{Se}$	${}^{100}\text{Mo}$	${}^{136}\text{Xe}$
$0_{\text{g.s.}}^+ \rightarrow 0_{\text{g.s.}}^+$ $0\nu\beta\beta$ -decay transition				
$E_i - E_f$ [MeV]	3.067	4.027	4.055	3.503
$G_{01}$ [ $\text{yr}^{-1}$ ]	$7.98 \times 10^{-15}$	$3.52 \times 10^{-14}$	$5.73 \times 10^{-14}$	$5.92 \times 10^{-14}$
$\zeta_{\langle m_\nu \rangle}$	2.49	4.95	7.69	1.60
$\zeta_{\eta_N}$	2.90	5.64	7.10	3.43
$\zeta_{\lambda'_{111}}$	5.57	10.9	17.9	8.92
$T_{1/2}$ ( $\langle m_\nu \rangle = 1$ eV) [yr]	$4.21 \times 10^{24}$	$1.07 \times 10^{24}$	$4.42 \times 10^{23}$	$1.02 \times 10^{25}$
$T_{1/2}$ ( $\eta_N = 10^{-7}$ ) [yr]	$1.19 \times 10^{25}$	$3.14 \times 10^{24}$	$1.98 \times 10^{24}$	$8.50 \times 10^{24}$
$T_{1/2}$ ( $\lambda'_{111} = 10^{-4}$ ) [yr]	$1.04 \times 10^{25}$	$2.73 \times 10^{24}$	$1.01 \times 10^{24}$	$4.07 \times 10^{24}$
$0_{\text{g.s.}}^+ \rightarrow 0_1^+$ $0\nu\beta\beta$ -decay transition				
$E_i - E_f$ [MeV]	1.945	2.539	2.925	1.924
$G_{01}$ [ $\text{yr}^{-1}$ ]	$6.58 \times 10^{-16}$	$3.25 \times 10^{-15}$	$1.11 \times 10^{-14}$	$2.81 \times 10^{-15}$
RCM calculation				
$\zeta_{\langle m_\nu \rangle}$	0.328	0.764	1.34	2.34
$\zeta_{\eta_N}$	0.092	0.229	0.379	0.641
$\zeta_{\lambda'_{111}}$	0.174	0.366	0.476	0.959
$T_{1/2}$ ( $\langle m_\nu \rangle = 1$ eV) [yr]	$2.42 \times 10^{26}$	$4.47 \times 10^{25}$	$1.46 \times 10^{25}$	$4.76 \times 10^{24}$
$T_{1/2}$ ( $\eta_N = 10^{-7}$ ) [yr]	$1.18 \times 10^{28}$	$1.90 \times 10^{27}$	$6.95 \times 10^{26}$	$2.43 \times 10^{26}$
$T_{1/2}$ ( $\lambda'_{111} = 10^{-4}$ ) [yr]	$1.06 \times 10^{28}$	$2.42 \times 10^{27}$	$1.43 \times 10^{27}$	$3.52 \times 10^{26}$
BEM calculation				
$\zeta_{\langle m_\nu \rangle}$	0.255	0.540	1.85	0.234
$\zeta_{\eta_N}$	0.418	0.866	1.71	0.557
$\zeta_{\lambda'_{111}}$	0.508	1.055	2.33	0.721
$T_{1/2}$ ( $\langle m_\nu \rangle = 1$ eV) [yr]	$4.02 \times 10^{26}$	$8.96 \times 10^{25}$	$7.59 \times 10^{24}$	$4.77 \times 10^{26}$
$T_{1/2}$ ( $\eta_N = 10^{-7}$ ) [yr]	$5.72 \times 10^{26}$	$1.33 \times 10^{26}$	$3.43 \times 10^{25}$	$3.23 \times 10^{26}$
$T_{1/2}$ ( $\lambda'_{111} = 10^{-4}$ ) [yr]	$1.26 \times 10^{27}$	$2.91 \times 10^{26}$	$5.97 \times 10^{25}$	$6.23 \times 10^{26}$

that in order to get a limit on  $\langle m_\nu \rangle$  of 1 eV, by measuring the transition to the excited  $0_1^+$  final state, the experimentalists should reach the level of about  $10^{28}$  yr for the half-life. By comparing the theoretical values of  $T_{1/2}^{0\nu}$  for decay to the ground state with the predictions for the transition to the excited state  $0_1^+$ , both yielded by BEM, we note that the second ones are larger by about one to two orders of magnitude. This situation is shown also in Fig. 1. The question, for experimentalists, is whether the coincidence between the de-excitation  $\gamma$  and the emitted electrons allows one to reduce the background in the  $0\nu\beta\beta$ -decay experiment to a sufficient extent so that the constraints on lepton number violating parameters deduced from the transition to the  $0^+$  excited state can compete with those associated with transitions to the ground state. It might be that in the case of the  $0\nu\beta\beta$  decay of  $^{100}\text{Mo}$  to the excited  $0_1^+$  state triggered by light or heavy Majorana neutrino-exchange mechanisms, the suppression of the half-life by a factor of 17 relative to the transition to ground state is compensated by diminishing the background events.

The expected improved experimental upper limits on the  $0\nu\beta\beta$ -decay half-life  $T_{1/2}^{0\nu\text{-expt}}$ , imply more stringent limits on lepton number violating parameters  $\langle m_\nu \rangle$ ,  $\eta_N$ , and  $\lambda'_{111}$ . By using the sensitivity parameters  $\zeta$ 's given in Table IV, they can be deduced in a straightforward way as follows:

$$\begin{aligned} \frac{\langle m_\nu \rangle}{m_e} &\leq \frac{10^{-5}}{\zeta_{\langle m_\nu \rangle}} \sqrt{\frac{10^{24} \text{ yr}}{T_{1/2}^{0\nu\text{-expt}}}}, & \eta_N &\leq \frac{10^{-6}}{\zeta_{\eta_N}} \sqrt{\frac{10^{24} \text{ yr}}{T_{1/2}^{0\nu\text{-expt}}}}, \\ (\lambda'_{111})^2 &\leq \kappa^2 \left( \frac{m_q^-}{100 \text{ GeV}} \right)^4 \left( \frac{m_g^-}{100 \text{ GeV}} \right) \frac{10^{-7}}{\zeta_{\lambda'_{111}}} \sqrt{\frac{10^{24} \text{ yr}}{T_{1/2}^{0\nu\text{-expt}}}}, \end{aligned} \quad (4.2)$$

with  $\kappa = 1.8$  [4]. One finds that in order to push down the upper constraint on  $\langle m_\nu \rangle$  below 0.1 eV in the  $0\nu\beta\beta$ -decay experiment to the excited  $0_1^+$  final state, one has to measure the half-life of  $4.02 \times 10^{28}$ ,  $8.96 \times 10^{27}$ ,  $7.59 \times 10^{26}$ , and  $4.77 \times 10^{28}$  yr for  $A = 76, 82, 100$ , and  $136$  isotopes, respectively. The best present limits on this type of decay are on the level of  $10^{21}$ – $10^{22}$  yr (see review in [21]). But we would like to mention that some progress in measuring transitions to excited states is expected in the future. For example, experiment MAJORANA with 500 kg of  $^{76}\text{Ge}$  plan to have a sensitivity of  $10^{28}$  yr [15].

## V. SUMMARY AND CONCLUSIONS

The  $0\nu\beta\beta$  decay is a sensitive tool to study lepton number violating mechanisms, which are associated with the Majorana neutrino mass and  $R$ -parity violating supersymmetry. Neutrino oscillations indicate that we may be close to the observation of this exotic rare process. This stimulates both experimental and theoretical studies, which can be helpful to limit the effective Majorana neutrino mass  $\langle m_\nu \rangle$  below the

0.1 eV level. It is an open question whether the future  $0\nu\beta\beta$ -decay experiments measuring transitions to the excited final states can be of comparable sensitivity to different lepton number violating parameters as the ground to ground transitions. Experimental studies of transitions to an excited  $0_1^+$  final state allow us to reduce the background by gamma-electron coincidences. Drawbacks are lower  $Q$  values and possibly suppressed nuclear matrix elements. The theoretical studies of the corresponding nuclear transitions are of great interest.

We evaluated  $0\nu\beta\beta$ -decay nuclear matrix elements for transitions to first excited  $0_1^+$  final states for  $A = 76, 82, 100$ , and  $136$  nuclei. The calculations have been performed within two known approaches, the boson expansion method (BEM) and recoupling two pairs of quasiparticle operators (RCM). The results of these two types of calculations differ from each other considerably especially in the case of the exchange of heavy particles for  $A = 76, 82$ , and  $100$  systems. We indicated the drawbacks of the second approach. We also found anomalous behaviors of the RCM results for  $A = 136$  nuclei. The resulting matrix elements are summarized in Table I and Table II. The suppression of the decay matrix elements to  $0_1^+$  in comparison with the decay to  $0_{g.s.}^+$  depends on the isotope and  $0\nu\beta\beta$ -decay mechanism. An average suppression factor of about 2–3 is predicted by the BEM. Contrary to the RCM results, the BEM ones significantly depend on the strength of the two-body interaction.

Further, we have calculated the sensitivity parameters to different signals of lepton number violation associated with transitions to excited final states. We compared them with the ground to ground transitions. We have found the largest sensitivity to these parameters in the  $A = 100$  nuclear system. By comparing with the decay to  $0_{g.s.}^+$  we find a suppression by a factor of about 4.1 for Majorana neutrino-exchange mechanisms. It means that the corresponding theoretical half-life is larger than that associated with the transition to  $0_{g.s.}^+$  by a factor of 17. In order to reach the sensitivity to a neutrino mass  $\langle m_\nu \rangle \approx 0.1$  eV in the  $0\nu\beta\beta$  decay to an excited  $0^+$  state, it is necessary to measure half-lives of at least  $8 \times 10^{26}$  yr (as predicted by the BEM). Perhaps, this limit might be expected to be reached by the  $0\nu\beta\beta$ -decay  $^{100}\text{Mo}$  experiment in the near future.

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