0νββ nuclear matrix elements and the occupancy of individual orbits

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The measured occupancies of valence orbits in ^{76}Ge and ^{76}Se are used as a guideline for modification of the effective mean field energies that results in better description of these quantities. With them, in combination with the self-consistent renormalized quasiparticle random phase approximation (SRQRPA) method that ensures conservation of the mean particle number in the correlated ground state, we show that the resulting 0νββ nuclear matrix element for the ^{76}Ge → ^{76}Se transition is reduced by ∼25% compared to the previous QRPA value, and therefore the difference between the present approach and the interacting shell model predictions becomes correspondingly smaller. Analogous modification of the mean field energies for the $A = 82$ system also results in a reduction of 0νββ matrix element for the ^{82}Se → ^{82}Kr transition, making it also closer to the shell model prediction.

I. INTRODUCTION

The fundamental importance of the search for 0νββ decay is widely accepted (see, e.g., the *APS Study of Physics of Neutrinos* [1]). Observing the decay would tell us that the total lepton number is not a conserved quantity, and that, consequently, neutrinos are massive Majorana fermions. Experimental searches for the 0νββ decay, of ever increasing sensitivity, are being pursued worldwide (for a recent review of the field, see [2]). However, interpreting existing results as a measurement of the neutrino effective mass, and planning new experiments, depends crucially on the knowledge of the corresponding nuclear matrix elements that govern the decay rate. Accurate determination of the nuclear matrix elements, and a realistic estimate of their uncertainty, is therefore an integral part of the study.

The nuclear matrix elements for 0νββ decay must be evaluated using tools of nuclear structure theory. Unfortunately, there are no observables that could be directly linked to the magnitude of 0νββ nuclear matrix elements and that could be used to determine them in an essentially model independent way. In the past, knowledge of the 2νββ-decay rate and of the ordinary β decay ft values were used to constrain the nuclear model parameters, in particular when the quasiparticle random phase approximation (QRPA) was employed [3,4]. Clearly, when other relevant data become available, and the nuclear model is constrained to reproduce them, confidence in the deduced 0νββ nuclear matrix elements would increase. Recently a set of such data, the occupation numbers of neutron valence orbits in the initial ^{76}Ge and final ^{76}Se nuclei, were determined in a series of measurements of cross sections for neutron adding and removing transfer reactions [5]. A similar series of measurements involving proton transfer reactions also became recently available [6].

Here we examine in detail how sensitive the matrix elements are to these quantities, and how much the previously determined nuclear matrix elements change when the input of the nuclear model is modified so that occupancies of individual orbits are correctly reproduced. As in the previous calculations [3], we use the QRPA method and its generalizations.

The occupation numbers for orbits with angular momentum j (and any other quantum numbers) in the initial nucleus, measured experimentally, are simply

$$n_j^{\exp} = \langle 0_{\mathrm{init}}^+ | \Sigma_m c_{j,m}^+ c_{j,m} | 0_{\mathrm{init}}^+ \rangle, \tag{1}$$

and the same quantity is determined for the ground state $|0_{\mathrm{fin}}^+\rangle$ of the final nucleus. Here $c_{j,m}^+$ is the creation operator for a proton in the orbit j_p or a neutron in the orbit j_n and $c_{j,m}$ is the corresponding annihilation operator. The states $|0_{\mathrm{init}}^+\rangle$ and $|0_{\mathrm{fin}}^+\rangle$ are the true ground states with all correlations in them.

Theoretically, for pure pairing BCS wave functions, the occupation numbers

$$n_j^{\mathrm{BCS}} = \langle 0_{\mathrm{BCS}}^+ | \Sigma_m c_{j,m}^+ c_{j,m} | 0_{\mathrm{BCS}}^+ \rangle = v_j^2 \times (2j+1), \tag{2}$$

depend only on the amplitudes v_{j_p} or v_{j_n} that are obtained by solving the gap equations. The amplitudes v are constrained by the requirement that the expectation value of the total neutron and proton numbers are conserved, i.e.,

$$N(\mathrm{or}\ Z) = \Sigma_{n(p)} n_{n(p)}^{\mathrm{BCS}} \equiv \Sigma_{n(p)} v_{n(p)}^2 \times (2j_{n(p)}+1). \tag{3}$$

Here, and in the following, we use n and p to label all quantum numbers of the corresponding neutron or proton orbits.

However, in the correlated QRPA ground state the occupation numbers are no longer the pure BCS quantities. Instead, they depend, in addition, on the solutions of the QRPA equations of motion for all multipoles J, and can be evaluated using

$$n_{n(p)}^{\mathrm{QRPA}} = \langle 0_{\mathrm{QRPA}}^+ | \Sigma_m c_{n(p),m}^+ c_{n(p),m} | 0_{\mathrm{QRPA}}^+ \rangle$$
$$\simeq (2j_{n(p)}+1) \times \left[v_{n(p)}^2 + \left(u_{n(p)}^2 - v_{n(p)}^2 \right) \xi_{n(p)} \right], \tag{4}$$

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where

$$\xi_{n(p)} = (2j_{n(p)} + 1)^{-1/2} \langle 0^+_{\text{QRPA}} | [a^+_{n(p)} a_{n(p)}]_{00} | 0^+_{\text{QRPA}} \rangle \quad (5)$$

is the expectation value of the number of quasiparticles in the orbit $n(p)$. (Here $a^+_{j_{n(p)},m}$, $a_{j_{n(p)},m}$ are the creation and annihilation operators for the quasiparticle with quantum numbers $n(p),m$.)

The quasiparticle occupation numbers $\xi_{n(p)}$ can be obtained iteratively using the equations of motion of the renormalized quasiparticle random phase approximation (RQRPA) and of the self-consistent RQRPA(SRQRPA) through the renormalization factors $\mathcal{D}_{pn}$:

$$\begin{aligned}
\mathcal{D}_{pn} &= 1 - \xi_p - \xi_n \\
&= 1 - \frac{1}{2j_p + 1} \Sigma_{n'} \mathcal{D}_{pn'} \left(\Sigma_{J,k}(2J+1) |\overline{Y}^{J,k}_{pn'}|^2 \right) \\
&\quad - \frac{1}{2j_n + 1} \Sigma_{p'} \mathcal{D}_{p'n} \left(\Sigma_{J,k}(2J+1) |\overline{Y}^{J,k}_{p'n}|^2 \right), \quad (6)
\end{aligned}$$

where $\overline{Y}^{J,m}_{pn} = \mathcal{D}^{1/2}_{pn} Y^{J,m}_{pn}$.

Note that the occupation numbers $n^{\text{QRPA}}_{n(p)}$ are no longer constrained by the same requirement, Eq. (3), that the particle number is conserved on average, as the BCS occupation numbers are.

The past applications of QRPA to the evaluation of the $0\nu\beta\beta$ nuclear matrix elements used standard parametrizations of the nuclear mean field, usually in the form of the Coulomb corrected Woods-Saxon potential fitted globally to a variety of nuclear properties (typically used parameters are those quoted in [7] or in [8]). In few papers [9] attempts were made to modify the single particle energy input in order to better describe the energy levels of the $\beta\beta$-decay candidate nuclei. It turns out that, at least in the $A = 76$ case, the quantities $n^{\text{BCS}}_{n(p)}$ based on the Woods-Saxon potential single particle energies, do not agree well with the experimental results of [5]. In particular, the occupancy of the neutron $g_{9/2}$ orbit appears to be underestimated.

Shortly after the data of Ref. [5] became available, a new publication [10] appeared, where the neutron single particle energies (only the valence orbits $g_{9/2}$, $f_{5/2}$, $p_{1/2}$, and $p_{3/2}$) were modified so that the neutron number occupancies of ^{76}Ge and ^{76}Se, for which the quantities $n^{\text{BCS}}_{n(p)}$ were used, were better reproduced. The proton mean field energies were also modified so that the one-quasiparticle energies in the odd-Z nuclei ^{77}As and ^{77}Br were also better described. The authors of Ref. [10] conclude that this modifications result in sizable reduction of the $0\nu\beta\beta$ nuclear matrix element for the ^{76}Ge $\to$ ^{76}Se transition.

In the present work we carefully analyze the rôle of the constraints represented by the knowledge of the orbit occupancies $n^{\text{exp}}_{n(p)}$. Clearly, these quantities reflect presence of correlations beyond pairing correlations described by $n^{\text{BCS}}_{n(p)}$. As a closest substitute for these correlations we use here $n^{\text{QRPA}}_{n(p)}$. Moreover, to describe such correlations, we use the SRQRPA that, as the simple BCS, and unlike the QRPA or RQRPA, conserves the neutron and proton particle numbers on average. (We describe the method in more detail in the next section).

Let us stress that the comparison between the measured and calculated occupancies in the experimental Refs. [5,6], as well as in the theoretical paper [10], was based on equating the experimental values $n^{\text{exp}}_{n(p)}$ with the BCS values $n^{\text{BCS}}_{n(p)}$. As pointed out above this is not really a justified comparison as far as the QRPA and its generalizations are concerned.

The paper is organized as follows. In the next section we briefly describe the SRQRPA method, and illustrate the effect of QRPA correlations on the occupation numbers. In Sec. III we discuss the modifications of the mean field energies for the $A = 76$ system that results in better description of the occupation numbers of valence orbits. We also show that using the modified mean field energies improves the description of the contribution of low-lying states to the $2\nu\beta\beta$ matrix element. In Sec. IV we present our result for the ^{76}Ge $\to$ ^{76}Se $0\nu\beta\beta$ nuclear matrix element and show that the mean field adjustment needed in order to better describe the orbit occupancies leads to reduction of the difference between the QRPA and nuclear shell model results [11]. Analogous modifications are applied in Sec. V to the $A = 82$ system with two more protons and four more neutrons then in $A = 76$. It also results in a noticeable reduction of $M^{0\nu}$ for the ^{82}Se $0\nu\beta\beta$ decay. We describe the contribution of individual orbits to the $0\nu\beta\beta$ matrix element in Sec. VI and conclude in Sec. VII.

II. SELF-CONSISTENT QUASIPARTICLE RANDOM PHASE METHOD

The standard QRPA method consists of two steps. First, the like-particle pairing interaction is taken into account by employing the quasiparticle representation. In the second step the linearized equations of motion are solved in order to describe small amplitude vibrational-like modes around that minimum. In the renormalized version of QRPA the violation of the Pauli exclusion principle is partially corrected.

The drawback of QRPA and RQRPA is the fact that, unlike in BCS, and as mentioned already earlier, the particle number is not conserved automatically, even on average, i.e.,

$$\Sigma_{j_n} n^{\text{QRPA}}_{j_n} \neq N \quad (7)$$

and the same is true for the proton states. Naturally, in the limit of negligibly small amplitudes, when the quasiparticle occupation numbers ξ_p and ξ_n in Eq. (6) are small, the inequality in Eq. (7) is correspondingly small as well. However, for realistic Hamiltonians the differences between the left-hand and right-hand sides of Eq. (7) in QRPA is of the order of unity (an extra or missing neutron or proton).

The self-consistent renormalized QRPA method (SRQRPA) removes this drawback by treating the BCS and QRPA vacua simultaneously. For the neutron-proton systems, of interest in the present context, the method was proposed and tested on the exactly solvable simplified models in Ref. [12]. It is a generalization of the procedure proposed earlier in [13].

Here we briefly describe the basic features of SRQRPA. In QRPA, RQRPA, and SRQRPA the phonon operators are defined as

$$Q^{\dagger(k)}_{J,M} = \Sigma_{pn} \left[X^k_{(pn)J} A^\dagger_{(pn)J,M} - Y^k_{(pn)J} \tilde{A}_{(pn)J,M} \right], \quad (8)$$

where $X^k_{(pn)J}$ and $Y^k_{(pn)J}$ are the usual variational amplitudes, and $A^\dagger_{(pn)J,M}$ is the angular momentum coupled two-quasiparticle creation operator. The X and Y amplitudes, as well as the corresponding energy eigenvalues ω_k are determined by solving the QRPA eigenvalue equations for each J^π

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}. \qquad (9)$$

The matrices $\mathcal{A}$ and $\mathcal{B}$ above are determined by the hamiltonian rewritten in terms of the coupled quasiparticle operators:

$$\mathcal{A}^J_{pn,p'n'}$$
$$= \langle 0^+_{\mathrm{QRPA}}|[\bar{A}_{(pn)J,M}, [\hat{H}, \bar{A}^\dagger_{(p'n')J,M}]]|0^+_{\mathrm{QRPA}}\rangle$$
$$\mathcal{B}^J_{pn,p'n'}$$
$$= \langle 0^+_{\mathrm{QRPA}}|[\bar{A}^\dagger_{(pn)J,-M}(-1)^M, [\hat{H}, \bar{A}^\dagger_{(p'n')J,M}]]|0^+_{\mathrm{QRPA}}\rangle, \quad (10)$$

where $\bar{A}_{(pn)J,M} = D^{-1/2}_{pn} A_{(pn)J,M}$. The resulting matrices are independent of the angular momentum projection M.

In RQRPA and SRQRPA the nonvanishing values of $\mathcal{D}_{pn} - 1$ is taken into account by using the amplitudes

$$\overline{X}^m_{(pn,J^\pi)} = \mathcal{D}^{1/2}_{pn} X^m_{(pn,J^\pi)}, \quad \overline{Y}^m_{(pn,J^\pi)} = \mathcal{D}^{1/2}_{pn} Y^m_{(pn,J^\pi)}, \quad (11)$$

instead of the standard X and Y, everywhere and also in the QRPA equations of motion.

By doing all of this an inconsistency appears between the BCS, with the ground state $|0^+_{\mathrm{BCS}}\rangle$, and QRPA (as well as RQRPA) with the ground state $|0^+_{\mathrm{QRPA}}\rangle$. In SRQRPA this inconsistency is overcome by reformulating the BCS equations. This is achieved by recalculating the u and v amplitudes. In SRQRPA the state around which the vibrational modes occur is no longer the quasiparticle vacuum, but instead the Bogoliubov transformation is chosen is such a way that provides the optimal and consistent basis while preserving the form of the phonon operator, Eq. (8). The modified coefficients of the Bogoliubov transformation still fulfill the basic requirement that the so-called dangerous graphs, terms in the Hamiltonian with only two quasiparticle creation or annihilation operators, vanish.

In practice, the SRQRPA equations are solved iteratively. One begins with the standard BCS u, v amplitudes, solves the RQRPA equations of motion and calculates the factors D_{pn}. The u, v amplitudes are recalculated and the procedure is repeated until the self-consistency is achieved.

The SRQRPA was applied initially to the evaluation of $2\nu\beta\beta$ matrix elements in Ref. [14] and to the evaluation of $0\nu\beta\beta$ matrix elements in Ref. [15]. Numerically, the double iteration procedure represents a challenging problem. To simplify it, in Refs. [14,15] the bare interaction was used, and no attempt was made to fit the odd-even mass differences. In addition, no adjustment of the particle-particle coupling constant g_{pp} was made, and $g_{pp} = 1$ was used. Consequently, the numerical values disagreed noticeably with the experiment in the $2\nu\beta\beta$ case, and with calculations by other authors in the $0\nu\beta\beta$ case.

The numerical problems were resolved in Ref. [16] where instead of the G-matrix based interaction the pairing part (and

TABLE I. The expectation values of the particle number operator. The mean field energies as in Ref. [3]. For QRPA, RQRPA, and SRQRPA the particle-particle interaction renormalization constant g_{pp} is chosen from the requirement that the $2\nu\beta\beta$-decay rate is correctly reproduced.

System:	BCS	QRPA	RQRPA	SRQRPA
Initial protons	12.00	13.05	12.05	12.00
Final protons	14.00	14.61	14.01	14.00
Initial neutrons	24.00	23.86	23.98	24.00
Final neutrons	22.00	22.16	21.95	22.00

only that part) of the problem was replaced by a pairing interaction that uses a constant matrix element whose value was adjusted to reproduce the experimental odd-even mass differences. This is the procedure that we adopt also here, after showing that within the QRPA the replacement of the G-matrix by a constant pairing matrix element makes little difference (see below). Thus, in the iterative procedure only the chemical potentials λ_n and λ_p are changed.

Adopting this simplification, and using the usual requirement, as in [3], namely that the $2\nu\beta\beta$ decay rate is correctly reproduced by renormalizing the coupling constant g_{pp} correspondingly, the authors of Ref. [16] have shown that the $0\nu\beta\beta$ matrix elements evaluated with SRQRPA agree quite well with the matrix elements of Ref. [3]. The requirement of conserving the particle number have not caused substantial changes in the value of the $0\nu\beta\beta$ matrix elements in that case.

In Table I we illustrate the problem of the particle number nonconservation within QRPA and to some extent also in RQRPA, and its restoration in SRQRPA. The case of $^{76}\mathrm{Ge} \rightarrow$ $^{76}\mathrm{Se}$ is chosen, with $^{40}\mathrm{Ca}$ as a core, and with the p, f and s, d, g shells (nine single particle orbits) for both neutrons and protons included. Note that in Ref. [10], as noted above, only the BCS occupancies were considered. We believe, contrary to the arguments there, that the effect of average particle number nonconservation in the QRPA vacuum need to be considered. Using SRQRPA, which does conserve the average particle number, is certainly more consistent when the problem of individual orbit occupancies is addressed.

Even though the conservation of the average particle number is almost restored in RQRPA and, as we will show below, the numerical values of the $M^{0\nu}$ are very similar in RQRPA and SRQRPA, we still prefer to use the self-consistent method. Among other things, the violation of the Ikeda sum rule, which in the RQRPA is as large as 20%, is reduced substantially (but not eliminated completely) when SRQRPA is employed.

Finally, to see the difference in treating the pairing part of the problem using the realistic G-matrix based interaction (but adjusting its strength so that the experimental pairing gaps are correctly reproduced, as was done in Ref. [3]) and calculation performed with the schematic pairing force (a constant matrix element adjusted similarly) we quote the QRPA and RQRPA values of the $M^{0\nu}$ matrix element, again for the $^{76}\mathrm{Ge} \rightarrow {}^{76}\mathrm{Se}$ case. With realistic pairing interaction we obtain $M^{0\nu} = 4.3(3.8)$ with QRPA(RQRPA) while with

the schematic pairing interaction the result is 4.4(3.9). Using the schematic pairing makes little difference in this case.

III. THE ROLE OF ORBIT OCCUPANCIES

The occupancies of the neutron and proton valence orbits in ^{76}Ge and ^{76}Se were determined experimentally in Refs. [5,6]. As shown in Sec. I, within QRPA and its generalizations, the occupancies of individual orbits, corresponding to the summed spectroscopic strength measured in Refs. [5,6], are determined not only by the BCS amplitudes u and v but also by the quasiparticle content of the correlated ground state $|0^+_{\rm QRPA}\rangle$. In turn, the BCS amplitudes u and v depend on the nuclear mean field energies, on pairing gaps Δ that are fitted to agree with the known odd-even mass differences, on the chemical potentials λ that are determined by the requirement that the particle number is conserved on average and, within SRQRPA that we adopt, indirectly on the solutions of the phonon equations of motion.

In Ref. [3] the mean field was based on Coulomb corrected Woods-Saxon potential using the globally fitted parameters quoted in [7]. The resulting valence orbits occupancies do not agree very well with experiment in that case. In order to describe the experimental occupancies better, we modify the input mean field energies to some extent, mainly for the valence orbits. Since our primary goal is to evaluate the nuclear matrix elements for the $0\nu\beta\beta$ decay which depend on the quasiparticle energies only weakly, modifying the mean field energies essentially means that, through the u and v, the occupancies are adjusted.

On the other hand, we use the known rate of the $2\nu\beta\beta$-decay to fix the renormalization constant g_{pp}, the strength of the neutron-proton particle-particle force. The matrix element for the $2\nu\beta\beta$ decay, in turn, depends on the energies of the 1^+ states significantly. In the intermediate nucleus ^{76}As the energies of a few low-lying 1^+ states are known. In calculation that used the global Woods-Saxon potential [3] these energies were not described well either, indicating again that the global single-particle potential is not optimal for the $A = 76$ system.

Guided by such considerations we modified the mean field energy input, determining a set of effective single-particle energies for ^{76}Ge and ^{76}Se that gives, essentially within errors, the measured valence orbit occupancies calculated using the SRQRPA. This effective set, at the same time, improves the description of the energies of low-lying 1^+ states in ^{76}As. In constructing the effective single-particle energies, we kept, unlike in Ref. [10], the globally fitted spin-orbit splittings of all orbits intact. The neutron and proton mean field energies used previously in Ref. [3] are compared with the adjusted set used further here in Figs. 1 and 2.

As one could see, the main difference is the overall shift of the neutron gds shell closer to the fp shell. The proton levels are shifted less, with the gds shell lifted further away from the chemical potential λ and from the fp shell, i.e., an opposite tendency than in the case of neutrons. The resulting occupancies of the valence subshells are shown in Table II and compared with the measured values [5,6] (in columns 5 and 9). The occupancies in columns 2 and 6 are those of Ref. [3]
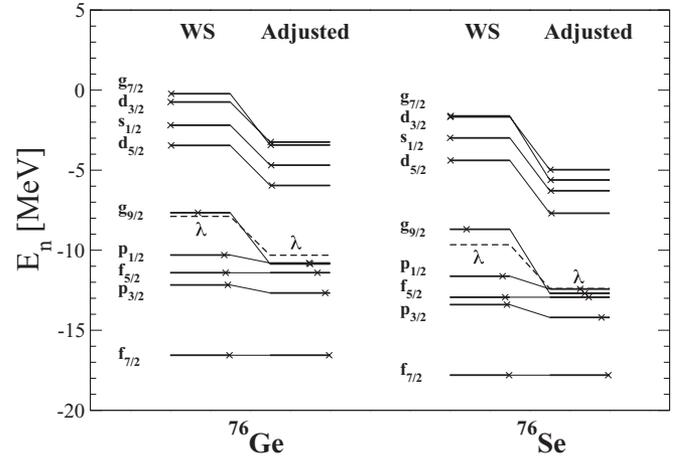

FIG. 1. Comparison of the neutron levels in the Woods-Saxon potential used in Ref. [3] (WS) and the adjusted mean field energies used here and described in the text. Symbols λ indicate the chemical potential and the crosses indicate the occupancy of the individual orbits.

evaluated from the BCS expression, Eq. (2), with the standard Woods-Saxon potential as input. Those are the values quoted in the experimental papers [5,6]. The values in columns 3 and 7 are the $n^{\rm QRPA}_{n(p)}$ evaluated with the standard QRPA and using the standard Woods-Saxon potential. We display them in order to stress the importance of proper theoretical treatment, and to show how much difference the ground state correlations make. Finally, in columns 4 and 8 are the occupancies that we use further here and which are evaluated in the correlated ground state using the SRQRPA and the adjusted set described above. Note that the entries in columns 3, 4, 7, and 8 were evaluated with the correlated QRPA state obtained with the coupling constant g_{pp} determined in the usual way, i.e., so that the $2\nu\beta\beta$ rate is correctly reproduced. The sum of the corresponding entries, i.e., the total calculated number of neutrons and protons above the ^{40}Ca core were already given in Table I.
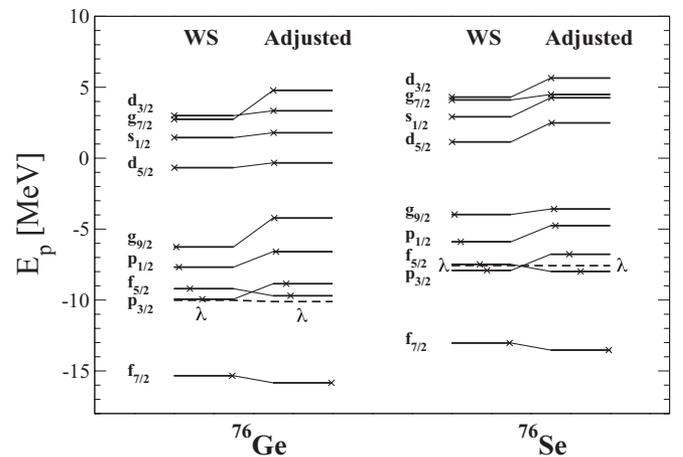

FIG. 2. Comparison of the proton levels of the Woods-Saxon potential used in [3] and the adjusted mean field energies used here and described in the text. Notation as in Fig. 1.

The overall improvement in describing the occupancies is clearly visible. For neutrons, the total calculated occupancy of the valence shells is calculated to be 15.3 and 13.4 for ^{76}Ge and ^{76}Se, respectively, with 0.4(0.6) neutron vacancies in the $f_{7/2}$ and 1.0(1.2) neutrons occupying the rest of the gds shell. In particular, in the $d_{5/2}$ there should be 0.35(0.39) neutrons according to our calculation, while Ref. [5] tentatively assigns 0.2 neutrons to $d_{5/2}$ in ^{76}Se. For protons the total occupancy of valence shell is calculated to be 4.4 and 6.3, respectively, with 0.8(0.9) proton vacancies in $f_{7/2}$ and 0.4(0.6) protons in the rest of the gds shell.

To further test the adequacy of the adjusted effective mean field, the running sum of the contributions to the $M^{2\nu}$, the nuclear matrix element for the $2\nu\beta\beta$-decay mode, is shown in Fig. 3 and compared with the available data. The quantity displayed is

$$M^{2\nu} = \Sigma_{k,m,\omega_m \leq \Omega} \frac{\langle f||\vec{\sigma}\tau^+||1_k^+\rangle\langle 1_k^+|1_m^+\rangle\langle 1_m^+||\vec{\sigma}\tau^+||i\rangle}{\omega_m - (M_i + M_f)/2}, \quad (12)$$

where on the x-axis in Fig. 3 we use the excitation energy $E_{\rm ex}$ in the intermediate nucleus ^{76}As instead of the Ω the largest included eigenvalue of the QRPA equation of motion.

We adopted the adjusted effective mean field energies shown in Figs. 1 and 2 for ^{76}Ge and ^{76}Se together with the SRQRPA method for the evaluation of the $2\nu\beta\beta$ nuclear matrix element. Again, the adjusted effective mean field describes much better the energies and amplitudes of the states for excitation energies below ~4 MeV where experimental data are available. We should point out, however, that the good agreement for the product of the two weak amplitudes [the numerator of Eq. (12)] does not mean that our calculation
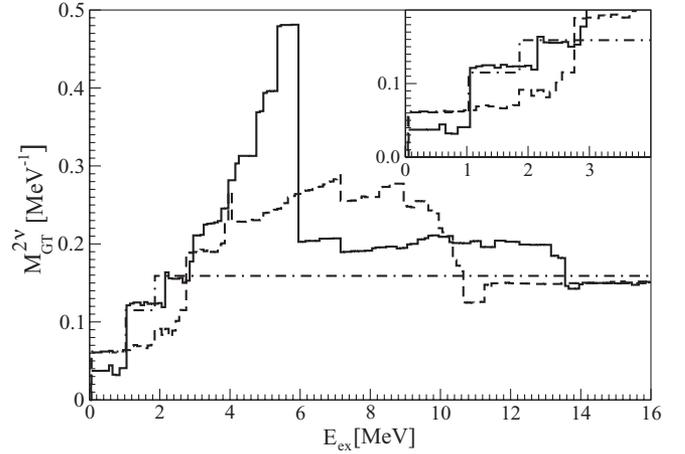

FIG. 3. The running sum of $M^{2\nu}$, Eq. (12). The dashed line corresponds to Ref. [3], the full line is the present result, and the dot-and-dashed line is the experimental result [17]. In the insert the first 4 MeV of excitation energy are shown in detail.

is free from the general problem of QRPA calculations, namely that the β^- strength corresponding to the GT transition ^{76}Ge → ^{76}As is too large while the β^+ strength ^{76}Se → ^{76}As is too small, as stressed, e.g., in Ref. [18]. Based on Fig. 3 one can conclude that the reasonable agreement between the experimental value of $M^{2\nu}$ and the value based on the few low-lying states (the so-called low-lying states dominance) appears to be accidental, at least in this case; if measurements could be extended to ~5–6 MeV and stopped there, that

TABLE II. The calculated occupancies of individual neutron and proton orbits for the two considered nuclei and using BCS only in columns 2 and 6, standard QRPA in columns 3 and 7 (labeled Q, these entries were obtained with the standard Woods-Saxon potential) and the average nucleon number conserving SRQRPA in columns 4 and 8 (labeled S, these entries were obtained with adjusted single particle energies). In columns 5 and 9 are the experimental occupancies of valence orbits [5,6]. The first entry, for the p orbit, is the sum of occupancies of $p_{1/2}$ and $p_{3/2}$ orbits.

	^{76}Ge				^{76}Se			
Neutrons	BCS	Q	S	exp	BCS	Q	S	exp
p	5.65	5.27	4.64	4.9 ± 0.2	5.57	5.05	4.12	4.4 ± 0.2
$f_{5/2}$	5.54	5.12	4.34	4.6 ± 0.4	5.53	5.00	3.63	3.8 ± 0.4
$f_{7/2}$	7.91	7.67	7.62	–	7.90	7.54	7.37	–
$s_{1/2}$	0.01	0.05	0.07	–	0.01	0.04	0.08	–
$d_{3/2}$	0.03	0.14	0.15	–	0.02	0.14	0.16	–
$d_{5/2}$	0.09	0.30	0.36	–	0.07	0.27	0.39	–
$g_{7/2}$	0.14	0.53	0.48	–	0.12	0.56	0.58	–
$g_{9/2}$	4.63	4.78	6.35	6.5 ± 0.3	2.78	3.55	5.66	5.8 ± 0.3
Protons								
p	2.23	2.34	1.75	1.77 ± 0.15	2.77	2.76	2.28	2.08 ± 0.15
$f_{5/2}$	1.61	2.27	2.08	2.04 ± 0.25	2.95	2.97	3.03	3.16 ± 0.25
$f_{7/2}$	7.83	7.19	7.13	–	7.76	7.12	7.06	–
$s_{1/2}$	0.00	0.02	0.03	–	0.00	0.03	0.04	–
$d_{3/2}$	0.01	0.07	0.07	–	0.01	0.09	0.09	–
$d_{5/2}$	0.01	0.12	0.15	–	0.02	0.17	0.18	–
$g_{7/2}$	0.02	0.19	0.16	–	0.03	0.31	0.27	–
$g_{9/2}$	0.29	0.85	0.62	0.23 ± 0.25	0.46	1.15	1.04	0.84 ± 0.25

agreement would be lost, particularly when the adjusted energies are used.

While the chosen procedure is not ideal, since the effective single-particle energies are chosen ad hoc, it is clearly an improvement when compared to our previous work [3]. First, the adopted method, SRQRPA, conserves the mean particle number in the correlated ground state, unlike the QRPA. Second, the occupancies of the valence orbits, in both protons and neutrons, agree now within errors with the experimental data [5,6].

IV. RESULTS

We are now in the position to ascertain to what degree the $0\nu\beta\beta$-decay nuclear matrix element $M^{0\nu}$ for the ^{76}Ge $\rightarrow$ ^{76}Se transition change with the modification of the effective mean field energies in combination with the application of the SRQRPA method. In Table III we show the sequence of the $M^{0\nu}$ values, together with the fitted renormalization constants g_{pp} as well as the calculated half-life for the nominal neutrino mass $\langle m_{\beta\beta} \rangle = 50$ meV. The table entries were obtained using ^{40}Ca as a core, with the p, f and s, d, g shells (nine single particle orbits) for both neutrons and protons included, with unrenormalized value $g_A = 1.25$, CD-Bonn based G-matrix interaction, and with Jastrow-like function included [19] in order to include the effect of the short range correlations. (We will discuss the dependence on these assumptions below. Note that since we use $g_A = 1.25$ everywhere in this work, we denote the $0\nu\beta\beta$ nuclear matrix element as $M^{0\nu}$ and do not use the notation $M'^{0\nu} = (g_A/1.25)^2 M^{0\nu}$ of Ref. [3].)

The last, and thus our final entry for this variant in Table III, $M^{0\nu} = 3.27$, was obtained when, in addition, the lowest energy denominator in the expression for $M^{2\nu}$, Eq. (12), was shifted in such a way that it agreed with the known energy of the first 1^+ state in ^{76}As. All other energy denominators were then shifted by the same amount as the first one. (The entry in line 5 was obtained this way as well.) This procedure is commonly used when $M^{0\nu}$ are evaluated, but was not employed previously in Ref. [3]. This value, $M^{0\nu} = 3.27$, can be compared now with the same quantity calculated by other methods. To make the comparison meaningful one has to keep in mind that

$M^{0\nu}$ contain R, the nuclear radius, as a factor. Unfortunately, different authors use different conventions for $R = r_o \times A^{1/3}$. In our work we use $r_0 = 1.1$ fm. Presumably the same is used in Ref. [10], even though the r_0 value is not explicitly quoted there, while in the shell model works [11] $r_o = 1.2$ fm.

With this correction included, the shell model value [11] of $M^{0\nu}$ is 2.11, and the QRPA result of Ref. [10] with the adjusted single-particle energies chosen there, is 2.8. All these calculations use the same method, namely the Jastrow function [19] for the treatment of short range correlations. It, therefore, appears that the adjustment of mean field energies, in order to correctly reproduce the measured occupancies of the valence orbits [5,6], results in reduction of $M^{0\nu}$ when QRPA or its generalizations are used. The discrepancy with respect to the shell model result [11] is reduced, in our work, to about half of its previous magnitude.

The value $M^{0\nu} = 2.8$ of Ref. [10] appears to be even closer to the shell model result than our preferred value $M^{0\nu} = 3.27$. It is worthwhile to point out, however, that as stated above, in Ref. [10] the BCS occupancies were used instead of the more realistic values used here which are based on the SRQRPA that conserves the average nucleon number. Moreover, Ref. [10] appeared before the experimental occupancies of the proton orbits, Ref. [6], became available, and those data were not used there.

As in Ref. [3] we would like to estimate the possible range of the $M^{0\nu}$ values taking into account changes corresponding to the variation in the number of single particle states included and to different treatment of the short range repulsion. Accordingly, we repeated the $M^{0\nu}$ evaluation with three and five oscillator shells included, in addition to the two oscillator shell result described above. The single particle energies in these additional shells were kept at their original Woods-Saxon potential values. For all these three variants we performed the calculations using the Jastrow function [19] for the treatment of short range correlations as well as the unitary correlation operator method (UCOM) [20]. We kept the axial current coupling constant g_A at its unrenormalized value 1.25 in all cases. The previous, Ref. [3], and the new results are compared in Table IV.

V. APPLICATION TO THE ^{82}Se $0\nu\beta\beta$ DECAY

It is reasonable to expect that the modifications of the mean field energies, described above, that were relevant to the ^{76}Ge $\rightarrow$ ^{76}Se decay, will also apply, at least approximately,

TABLE III. The values of g_{pp}, $M^{0\nu}$, and $T^{0\nu}_{1/2}$ for $\langle m_{\beta\beta} \rangle =$ 50 meV in units of 10^{26} yr, for different variants of the calculations. For further explanations, see text.

Variant	g_{pp}	$M^{0\nu}$	$T^{0\nu}_{1/2}(10^{26}$ yr)
QRPA, WS mean field [3]	0.849	4.34	7.0
RQRPA, WS mean field [3]	0.990	3.81	9.1
QRPA, effective mean field	0.903	4.23	7.4
RQRPA, effective mean field	1.170	3.44	11.1
RQRPA, effective mean field and adjusted $M^{2\nu}$ denominators	1.206	3.18	13.0
SRQRPA, effective mean field	1.125	3.66	9.8
SRQRPA, effective mean field and adjusted $M^{2\nu}$ denominators	1.184	3.27	12.3

TABLE IV. The calculated $M^{0\nu}$ matrix elements for the ^{76}Ge$0\nu\beta\beta$ decay; the mean value and its range are shown for the two alternative treatments of the short range correlations. In column 2 are the previous values obtained with (R)QRPA method and with the Woods-Saxon potential single particle energies [3], and in column 3 are the values obtained with the SRQRPA method and the adjusted energies described above.

	Prev.	New
Jastrow s.r.c.	4.24(0.44)	3.49(0.23)
UCOM s.r.c.	5.19(0.54)	4.60(0.39)

TABLE V. The calculated occupancies of valence neutron and proton orbits for ^{82}Se and ^{82}Kr. See the text for explanation.

	^{82}Se		^{82}Kr	
	Prev.	New	Prev.	New
Neutrons				
p	5.5	5.2	5.4	4.8
$f_{5/2}$	5.4	5.2	5.4	4.9
$g_{9/2}$	7.2	8.5	6.1	7.3
Protons				
p	2.7	2.2	3.2	2.8
$f_{5/2}$	3.0	3.2	3.6	4.0
$g_{9/2}$	1.0	0.9	1.3	1.2

to the ^{82}Se $\rightarrow$ ^{82}Kr decay, since in that case there are just two more protons and four more neutrons compared to the $A = 76$ case. Guided by such considerations we modified the Woods-Saxon potential energies used previously in Ref. [3] for $A = 82$ for the protons in both ^{82}Se and ^{82}Kr as for the proton energies for ^{76}Se, and for the neutrons as in the ^{76}Ge that is closer to them in the number of neutrons. The resulting valence orbit occupancies are shown in Table V. In columns 2 and 4 are the $n_{n(p)}^{\text{QRPA}}$ values evaluated with the standard Woods-Saxon potential and in columns 3 and 5 are the $n_{n(p)}^{\text{SRQRPA}}$ values evaluated with the adjusted energies. In the neutron system the present treatment predicts that the valence shells contain only $\sim$19(17) neutrons compared with the naive expectation of 20(18) neutrons.

Performing the same set of calculations as described previously for the ^{76}Ge decay, we conclude that the $0\nu\beta\beta$ nuclear matrix element for the ^{82}Se decay is also reduced from the previous (R)QRPA value of 3.76(0.40) for Jastrow s.r.c. and 4.59(0.39) for UCOM s.r.c. to the SRQRPA values (with modified mean field energies and shifted energy denominators for the $2\nu\beta\beta$ decay) of 3.50(0.24) for Jastrow s.r.c. and 4.54(0.40) for UCOM s.r.c., again reducing somewhat the difference between this value and the shell model result of 2.0 [11] (adjusted for the different values of r_0 and with Jastrow s.r.c.).

VI. CONTRIBUTION OF INDIVIDUAL ORBITS TO $M^{0\nu}$

In the QRPA, RQRPA, and SRQRPA the $M^{0\nu}$ is written as the sum over the virtual intermediate states, labeled by their angular momentum and parity J^{π} and indices k_i and k_f:

$$
\begin{aligned}
M_K \\
= \sum_{J^{\pi}, k_i, k_f, \mathcal{J}} \sum_{pnp'n'} (-1)^{j_n + j_{p'} + J + \mathcal{J}} \sqrt{2\mathcal{J}+1}
\begin{Bmatrix} j_p & j_n & J \\ j_{n'} & j_{p'} & \mathcal{J} \end{Bmatrix} \\
\times \langle p(1), p'(2); \mathcal{J} \parallel \bar{f}(r_{12}) O_K \bar{f}(r_{12}) \parallel n(1), n'(2); \mathcal{J} \rangle \\
\times \langle 0_f^+ || [c_{p'}^+ \tilde{c}_{n'}]_J || J^{\pi} k_f \rangle \langle J^{\pi} k_f | J^{\pi} k_i \rangle \langle J^{\pi} k_i || [c_p^+ \tilde{c}_n]_J || 0_i^+ \rangle.
\end{aligned}
$$
(13)

The operators O_K, $K =$ Fermi (F), Gamow-Teller (GT), and tensor (T), contain neutrino potentials and spin and isospin
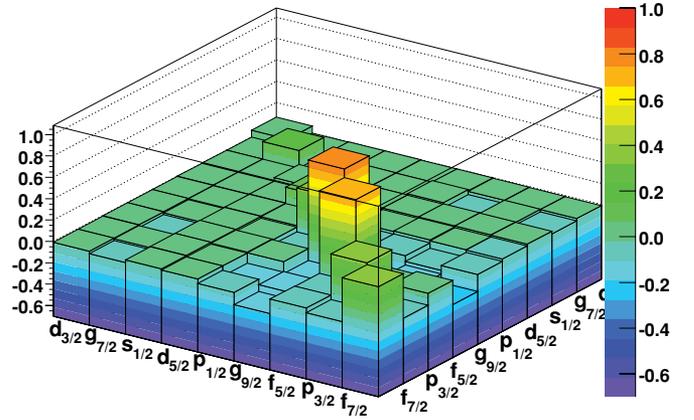

FIG. 4. (Color online) The contribution of individual neutron orbit pairs to $M^{0\nu}$. The entries are normalized so that their sum is unity.

operators, and RPA energies $E_{J^{\pi}}^{k_i, k_f}$. The $\mathcal{J}^{\pi}$ labels angular momentum and parity of the pairs of neutrons that are transformed into protons with the same $\mathcal{J}^{\pi}$.

The nucleon orbits are labeled in Eq. (13) by p, p', n, n'. We can isolate the contribution of, say, neutron orbits n, n' by fixing these two labels, but performing the summation over all other indices. The resulting two-dimensional array $f(n, n')$ obviously must obey $\Sigma_{nn'} f(n, n') = M^{0\nu}$; the individual contributions can be positive or negative. It is interesting to visualize such contributions in order to see which orbits are important and which are not, and to gain a better understanding of the various physics effects affecting the $M^{0\nu}$ values.

We show a lego plot of such contributions to the $M^{0\nu}$ for the ^{76}Ge decay, normalized to unity, in Figs. 4 and 5. The large positive contributions along the diagonals, stemming dominantly, but not exclusively, from the $\mathcal{J}^{\pi} = 0^+$ pairing part of $M^{0\nu}$, contribute +2.97 when added together. The off-diagonal entries, related to the 'broken pairs' or higher seniority parts of $M^{0\nu}$, give −1.97 when added. The well known opposite tendencies of the pairing and broken pairs contributions is thus clearly visible. In addition, one can also see that the valence orbits $g_{9/2}, p_{3/2}, f_{5/2}, p_{1/2}$ contribute
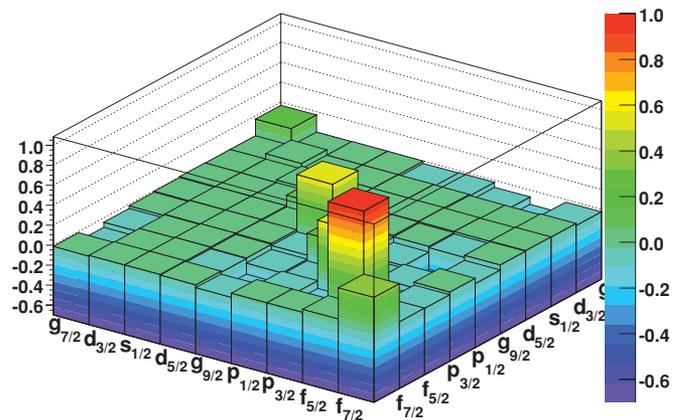

FIG. 5. (Color online) The contribution of individual proton orbit pairs to $M^{0\nu}$. The entries are normalized so that their sum is unity.
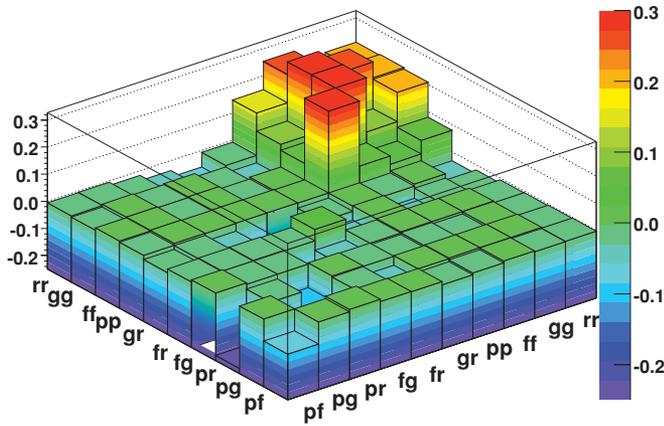
FIG. 6. (Color online) The contribution of the initial neutron orbits (combination n, n') (along the y axis) plotted against the analogous combinations p, p' (along the x axis) of the final proton orbits. The entries are again normalized to unity. For notation along the axes, see text.

considerably more than the orbits further away from the Fermi level, even though the $f_{7/2}$ and $g_{7/2}$ give non-negligible contributions.

In order to better visualize which combinations of neutron and proton orbits contribute one could, in principle, isolate in Eq. (13) the pieces corresponding to the combination n, n' of neutron orbits from which the neutrons disappear in the initial nucleus and plot them against the combination p, p' of proton orbits in which the protons appear in the final nucleus. Such a plot, however, would be difficult to visualize since it would represent a 81×81 matrix even with our minimal space of nine orbits. Instead, we consider just the three valence orbits p (representing both $p_{1/2}$ and $p_{3/2}$), $f_{5/2}$ and $g_{9/2}$, and lump all the other orbits further removed from the Fermi level into one combination r (for remote). This allows us to reduce the dimension of the matrix and the corresponding plot to 10×10, shown in Fig. 6. Again the entries are normalized so that their sum is unity, and the labels along the x and y axes are arranged in such a way that most of the negative entries are in the front (total, naturally, again -1.97) and most of the positive entries are near the far corner, in order to enhance visibility.

In Fig. 6 the contribution of the r nonvalence remote orbits is sizable, and for the negative entries, in fact, dominating. However, the positive and negative contributions from combinations that include the r orbits cancel each other to a large extent (positive contributions total 1.29 and negative ones

-1.45) so that the net effect on $M^{0\nu}$ of the remote orbits is only $\sim 15\%$.

However, in QRPA and its generalizations the inclusion of orbits of at least two oscillator shells, i.e. the set that obeys the full Ikeda sum rule, is essential. Without it, the description of the $2\nu\beta\beta$ decay is impossible with a reasonable value of the effective particle-particle coupling constant g_{pp}.

VII. CONCLUSION

The occupancies of valence neutron and proton orbits, determined experimentally in Refs. [5,6], represent important constraints for nuclear models used in the evaluation of the $0\nu\beta\beta$ nuclear matrix element. In the present work we have modified the input mean field in such a way that the valence orbits in the model obey these constraints. Within QRPA and its generalizations we found that it is important to also choose the variant of the basic method that makes such comparison meaningful by conserving the average particle number in the correlated ground state. When following this procedure, but otherwise keeping the same steps as in our previous evaluation of $M^{0\nu}$ within QRPA, we find that for the $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$ transition the matrix element is smaller by $\sim 25\%$, reducing the previously bothersome difference with the shell model prediction noticeably. Moreover, when we assume that analogous changes in the mean field should be applied also to the $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$ $0\nu\beta\beta$ decay, that differs from the ^{76}Ge decay by only two additional protons and four additional neutrons, we find similar reduction in $M^{0\nu}$ as well. Clearly, having the experimental orbit occupancies available, and adjusting the input to fulfill the corresponding constraint, makes a difference. It would be very useful to have similar constraints available also in other systems, in particular for ^{130}Te and/or ^{136}Xe.

ACKNOWLEDGMENTS

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