

New BCS and renormalized QRPA formalism with application to double beta decay

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Abstract. A new analysis of the renormalized proton–neutron quasiparticle random phase approximation based on simultaneous recalculation of the one-body density matrix and the pairing tensor has been used to study the double beta decay. We demonstrated that inclusion of the quasiparticle correlations at the BCS level reduces ground state correlations in the particle–particle channel of the proton–neutron interaction. We also simplified the RQRPA equations significantly obtaining a low-dimensioned set of linear equations for the quasiparticle densities. The formalism was applied to the double beta decay of ^{76}Ge .

PACS. 21.60Jz HartreeFock and random-phase approximations – 23.40.Bw Weak-interaction and lepton (including neutrino) aspects – 23.40.Hc Relation with nuclear matrix elements and nuclear structure

1 Introduction

The proton–neutron quasiparticle random phase approximation (pn–QRPA) has been considered the most powerful method for beta and double beta transition calculations of nuclear systems which are far away from closed shells [1–8]. Especially, a remarkable success was achieved by the QRPA approach in revealing the suppression mechanism of the neutrino accompanied double beta decay, a long-standing problem of the theoretical treatment of this process. Further development of the approach went beyond many shortcomings and refined calculations of nuclear matrix elements involved in the double beta decay. Among others the following problems were set and solved: particle number non-conservation [9, 10], a role of the proton–neutron pairing [11], the higher-order corrections to the ordinary QRPA [12–15], treatment of transitions to final excited states [16–19], extension of the definition of phonon operators by means of the so-called scattering terms [20–23], etc.

Most of such improvements disregarded, however, the main source of the formalism instability connected with violation of the Pauli exclusion principle by using commutation relations for the QRPA phonon operators. To overcome this shortcoming of the pn–QRPA framework the renormalization technique has been proposed [24] and extended to include proton–neutron pairing [25]. This approach has been based on the early works by Hara [26], Ikeda [27], Rowe [28] and Schuck and Ethofer [29] in the

context of RPA and QRPA. The main goal of the method called in the literature the renormalized QRPA (RQRPA) is to use of a self-iteration of the QRPA equation to take into account additional one-quasiparticle scattering terms in the commutation relations. But this procedure results in non-vanishing quasiparticle content of the ground state and what follows some inconsistency between RQRPA and the BCS approach since the ground state approximated by the BCS state is chosen to be the quasiparticle vacuum. To minimize an influence of such a discrepancy one needs to reformulate the BCS equations in a way proposed in [30]. Combining both RQRPA and so modified BCS one obtains the self-consistent BCS+RQRPA approach (SRQRPA) which we study in more detail in this paper.

2 Formalism

This section recapitulates shortly the QRPA formalism and its extensions. In the QRPA (either ordinary or renormalized) approach one assumes the harmonicity of the nuclear motion and starts with the excited-state creation phonon operators of the form [28, 31]:

$$Q_{J^\pi M}^{m\dagger} = \sum_{pn} \left[X_{(pn)J^\pi}^m A_{(pn)J^\pi M}^\dagger - Y_{(pn)J^\pi}^m \tilde{A}_{(pn)J^\pi M} \right], \quad (1)$$

where $X_{(pn)J^\pi}^m$ and $Y_{(pn)J^\pi}^m$ are respectively, the forward-going and backward-going variational amplitudes. The operators $A_{(pn)J^\pi M}^\dagger \equiv [a_p^\dagger a_n^\dagger]_{J^\pi M}$ are the angular-momentum coupled two-quasiparticle creation operators.

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Since they do not fulfill the bosonic commutation relations exactly, in the quasiboson approximation (QBA), that is used to derive the usual QRPA equations, the Pauli principle is violated. To avoid this serious drawback in the improved version of the theory one introduces the renormalized operators [32]:

$$\mathcal{A}_{(pn)J^\pi M}^\dagger \equiv D_{pn}^{-1/2} A_{(pn)J^\pi M}^\dagger, \quad (2)$$

along with the renormalized amplitudes:

$$\mathcal{X}_{(pn)J^\pi}^m \equiv D_{pn}^{1/2} X_{(pn)J^\pi}^m, \quad (3)$$

$$\mathcal{Y}_{(pn)J^\pi}^m \equiv D_{pn}^{1/2} Y_{(pn)J^\pi}^m, \quad (4)$$

where D_{pn} matrix is defined by the expectation value in the RPA ground-state of the commutator:

$$D_{pn} \equiv \langle 0 | [A_{(pn)J^\pi M}, A_{(pn)J^\pi M}^\dagger] | 0 \rangle = (1 - n_p - n_n) \quad (5)$$

together with the quasiparticle densities ($\hat{j}_a \equiv \sqrt{2j_a + 1}$):

$$n_p \equiv \hat{j}_p^{-1} \langle 0 | [a_p^\dagger \tilde{a}_p]_{00} | 0 \rangle, \quad (6)$$

$$n_n \equiv \hat{j}_n^{-1} \langle 0 | [a_n^\dagger \tilde{a}_n]_{00} | 0 \rangle. \quad (7)$$

The above equation has been derived using exact fermionic commutation relations and thus goes beyond the ordinary quasiboson approximation. One can prove easily that now the following relation holds:

$$\langle 0 | [\mathcal{A}_{(pn)J^\pi M}, \mathcal{A}_{(p'n')J'^\pi M'}^\dagger] | 0 \rangle = \delta_{pp'} \delta_{nn'} \delta_{JJ'} \delta_{\pi\pi'} \delta_{MM'}, \quad (8)$$

i.e. the renormalized operators behave as bosons, at least in the sense of the ground-state expectation value of their commutator. The phonon operator now reads:

$$Q_{J^\pi M}^{m\dagger} = \sum_{pn} [\mathcal{X}_{(pn)J^\pi}^m \mathcal{A}_{(pn)J^\pi M}^\dagger - \mathcal{Y}_{(pn)J^\pi}^m \tilde{\mathcal{A}}_{(pn)J^\pi M}], \quad (1')$$

and using e.g. the equation of motion (EOM) method [28] one gets the RQRPA equations of the usual form:

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B} & \mathcal{A} \end{pmatrix}_{J^\pi} \begin{pmatrix} \mathcal{X}^m \\ \mathcal{Y}^m \end{pmatrix}_{J^\pi} = \Omega_{J^\pi}^m \begin{pmatrix} \mathcal{X}^m \\ -\mathcal{Y}^m \end{pmatrix}_{J^\pi}, \quad (9)$$

with the new renormalized RPA matrices \mathcal{A} and \mathcal{B} defined in [24]. Here $\Omega_{J^\pi}^m \equiv E_{J^\pi}^m - E_0$ is the RPA excitation energy with respect to the ground state.

Although the renormalized RPA takes into account the important coherent contributions that are connected to the one-quasiparticle densities in the ground-state, it misses other terms due to the restricted form of the phonon operator (1). We namely dispose of the so-called scattering terms, that are on the other hand retained in the RQRPA. Inclusion of such terms, however, is not conceptually straightforward and leads to much more elaborate theory [20–23], reaching beyond the RPA scheme. Also no detailed calculation, trying to estimate the contribution of the higher-order correlation terms associated

with the two-quasiparticle densities, has ever been performed. There is, however, the widely accepted hope that the corresponding corrections will be small due to a random phase cancellation [28].

Now comes the question of the calculation of the D_{pn} matrix entering the expressions for the RPA matrices \mathcal{A} and \mathcal{B} . Using the mapping¹

$$[a_p^\dagger \tilde{a}_p]_{00} \mapsto \hat{j}_p^{-1} \sum_{J^\pi M n} A_{(pn)J^\pi M}^\dagger A_{(pn)J^\pi M}, \quad (10)$$

$$[a_n^\dagger \tilde{a}_n]_{00} \mapsto \hat{j}_n^{-1} \sum_{J^\pi M p} A_{(pn)J^\pi M}^\dagger A_{(pn)J^\pi M}, \quad (11)$$

that preserves the commutation relations up to the second order in the A and A^\dagger operators [32] and inverting (1) one derives the following equations for the quasiparticle densities:

$$n_p = \hat{j}_p^{-2} \hat{j}^2 \sum_{J^\pi m n} D_{pn} |\mathcal{Y}_{(pn)J^\pi}^m|^2, \quad (12)$$

$$n_n = \hat{j}_n^{-2} \hat{j}^2 \sum_{J^\pi m p} D_{pn} |\mathcal{Y}_{(pn)J^\pi}^m|^2. \quad (13)$$

Inserting (5) into (13) one gets the following system of linear equations for n_p and n_n :

$$\begin{aligned} \mathcal{Y}'_p n_p + \sum_n \mathcal{Y}_{pn} n_n &= \mathcal{Y}_p, \\ \mathcal{Y}'_n n_n + \sum_p \mathcal{Y}_{pn} n_p &= \mathcal{Y}_n, \end{aligned} \quad (14)$$

or, in the matrix form:

$$\begin{pmatrix} \text{diag}(\mathcal{Y}'_{(p)}) & \mathcal{Y} \\ \mathcal{Y}^T & \text{diag}(\mathcal{Y}'_{(n)}) \end{pmatrix} \begin{pmatrix} n_{(p)} \\ n_{(n)} \end{pmatrix} = \begin{pmatrix} \mathcal{Y}_{(p)} \\ \mathcal{Y}_{(n)} \end{pmatrix}, \quad (14')$$

where

$$\begin{aligned} \mathcal{Y}_{pn} &\equiv \sum_{J^\pi m} \hat{j}^2 |\mathcal{Y}_{(pn)J^\pi}^m|^2, \\ \mathcal{Y}_p &\equiv \sum_n \mathcal{Y}_{pn}, \quad \mathcal{Y}'_p \equiv \hat{j}_p^2 + \mathcal{Y}_p, \\ \mathcal{Y}_n &\equiv \sum_p \mathcal{Y}_{pn}, \quad \mathcal{Y}'_n \equiv \hat{j}_n^2 + \mathcal{Y}_n. \end{aligned} \quad (15)$$

It is worth mentioning, that the dimension of our linear problem is only $2n \times 2n$, where n is the dimension of the single-particle basis. This is of much advantage, since (14) has to be solved many times as one should iterate between (9) and (14) until convergence is achieved. The other way round, inserting (13) into (5), as it is done by several authors, e.g. [24, 25], one obtains the equation:

$$D_{pn} = 1 - \hat{j}_p^{-2} \sum_{n'} D_{pn'} \mathcal{Y}_{pn'} - \hat{j}_n^{-2} \sum_{p'} D_{p'n} \mathcal{Y}_{p'n}, \quad (16)$$

¹ An alternative way to derive the equations presented below has been elaborated by Hara [26] and Rowe [28].

that, on the contrary to the claim expressed in [24], can be transformed into $n^2 \times n^2$ linear system:

$$\sum_{p'n'} W_{pn,p'n'} D_{p'n'} = U, \quad (17)$$

where

$$W_{pn,p'n'} \equiv \delta_{pp'} \delta_{nn'} + \delta_{pp'} \hat{J}_p^{-2} \mathcal{Y}_{pn'} + \delta_{nn'} \hat{J}_n^{-2} \mathcal{Y}_{p'n}, \quad (18)$$

and U is the vector of 1's. In practice however, it takes much less time to solve this system using standard linear algebra procedures than following iteration methods, as in [24,25]. But further reduction of the complexity of the problem to the form of (14) allows us to take all possible multiplicities into account for the calculation of the D_{pn} renormalization factors. Although some of them are less important and are neglected in [24,25], when one leaves only a few, the J-coupling scheme breaks, since the basis becomes uncomplete and the validity of the mapping (10)–(11) is questionable. As we will see further, this reflects itself in the results.

With non-vanishing quasiparticle content of the ground state one arrives at the inconsistency between RQRPA and BCS, since in the latter one assumes the ground state to be the quasiparticle vacuum. One thus needs to reformulate the BCS equations [30], namely by recalculating the density matrix ρ and the pairing tensor κ . With standard Bogoliubov–Valatin transformation [31] they read now:

$$\rho_a \equiv \langle 0 | c_\alpha^\dagger c_\alpha | 0 \rangle = v_a^2 + (u_a^2 - v_a^2) n_a, \quad (19)$$

$$\kappa_a \equiv \langle 0 | \tilde{c}_\alpha c_\alpha | 0 \rangle = u_a v_a (1 - 2n_a), \quad (20)$$

and depend on the quasiparticle densities n_a , where a runs over proton or neutron indices. The u and v coefficients are obtained now by minimizing the RQRPA ground-state energy, that by virtue of the Wick's theorem is expressed as [31,33]:

$$\begin{aligned} \langle 0 | \hat{H} | 0 \rangle &= \sum_a \hat{J}_a^2 \varepsilon_a \rho_a \\ &+ \frac{1}{4} \sum_{ab} \hat{J}_a \hat{J}_b \langle (aa)_{J^\pi=0^+}^{T=1} | V | (bb)_{J^\pi=0^+}^{T=1} \rangle \kappa_a \kappa_b \end{aligned} \quad (21)$$

with the particle-number constraint:

$$N_0 = \langle 0 | \hat{N} | 0 \rangle = \sum_a \hat{J}_a^2 \rho_a. \quad (22)$$

In the above equation ε_a are the single-particle energies and $\langle (aa)_{J^\pi=0^+}^{T=1} | V | (bb)_{J^\pi=0^+}^{T=1} \rangle$ are the matrix elements of the two-body interaction.

This minimization is equivalent to solving a very natural equation from the EOM point of view [34]:

$$\langle 0 | [\hat{H} - \lambda_p \hat{Z} - \lambda_n \hat{N}, Q_{JM}^\dagger] | 0 \rangle = 0. \quad (23)$$

We therefore dispose of the ground-state to be a quasiparticle vacuum but rather choose such a Bogoliubov–Valatin

transformation that provides the optimal (i.e. consistent) basis for RQRPA calculations, preserving the form of the phonon operator (1). As already mentioned, inclusion of e.g. scattering terms or higher-order terms in the QRPA operator is possible but certainly beyond the scope of the present study.

It is worth mentioning, that in our approach we avoided an explicit construction of the ground-state wave function. It can be feasible in some simple algebraic models [34], but in general approximations must be used to close the system of coupled BCS+RQRPA equations. We dropped the terms of order higher than quadratic in n_a when evaluating (19)–(22), since these quantities are considered to be small. Indeed, our numerical calculations support this claim.

The general scheme to solve the SRQRPA equations is therefore to start from the ordinary BCS equations, putting $n_p = n_n = 0$, solve the corresponding RQRPA problem (inner iteration), that gives us new quasiparticle densities and loop with them back to BCS until the convergence is achieved (outer iteration). We arrive thus at the doubly-iterative problem and the question of efficient and accurate getting through all the calculation steps becomes very important. We then stress again, that without showing that the problem of calculating the D matrix can be reduced to the linear system (14) of acceptable size the realization of this task would be hardly possible.

The ground state to ground state $2\nu\beta\beta$ Gamow–Teller matrix elements are expressed as follows:

$$M_{GT}^{2\nu} = \sum_{mm'} \frac{2 \langle 0_{f,gs}^+ | \sigma \tau_+ | 1_{m'}^+ \rangle \langle 1_{m'}^+ | 1_m^+ \rangle \langle 1_m^+ | \sigma \tau_+ | 0_{i,gs}^+ \rangle}{\Omega_{1^+}^m + \Omega_{1^+}^{m'} + Q_{\beta^-}(A, Z+1) - Q_{\beta^-}(A, Z)}, \quad (24)$$

where the charge-changing transition densities are:

$$\langle 0_{f,gs}^+ | \sigma \tau_+ | 1_{m'}^+ \rangle = \quad (25)$$

$$\sum_{pn} \langle p || \sigma || n \rangle (v'_p u'_n \mathcal{X}_{(pn)1^+}^{m'} + u'_p v'_n \mathcal{Y}_{(pn)1^+}^{m'}) \sqrt{D_{pn}^m},$$

$$\langle 1_m^+ | \sigma \tau_+ | 0_{i,gs}^+ \rangle = \quad (26)$$

$$\sum_{pn} \langle p || \sigma || n \rangle (u_p v_n \mathcal{X}_{(pn)1^+}^m + v_p u_n \mathcal{Y}_{(pn)1^+}^m) \sqrt{D_{pn}^m}$$

and the overlap of intermediate excited states is assumed to be expressed as:

$$\langle 1_{m'}^+ | 1_m^+ \rangle = \sum_{pn} \left(\mathcal{X}_{(pn)1^+}^{m'} + \mathcal{X}_{(pn)1^+}^m - \mathcal{Y}_{(pn)1^+}^{m'} - \mathcal{Y}_{(pn)1^+}^m \right). \quad (27)$$

In the above the non-primed (primed) quantities result from SRQRPA calculation based on initial (final) ground state, respectively.

3 Results

To show the differences between the QRPA, the RQRPA and the SRQRPA and to illustrate much better stability of the SRQRPA solutions we plot in Figs. 1–3

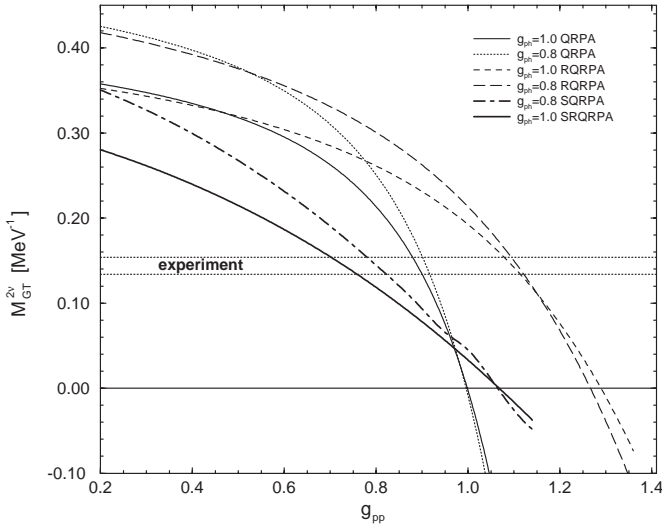


Fig. 1. The dependence of the double Gamow–Teller matrix element $M_{GT}^{2\nu}$ on the renormalization factor in the particle–particle channel g_{pp} . Two different cases for $g_{ph} = 0.8$ and 1.0 and for three different QRPA approaches are shown. Magnitude of the experimental estimate is marked by two parallel dotted lines [35]

the results of our calculations as a function of particle–particle (g_{pp}) and particle–hole (g_{ph}) factors, renormalizing the bare two-body NN interaction. This commonly used renormalization is necessary due to finite size of the nucleus (the bare NN matrix elements are calculated for the infinite nuclear matter) and due to the limited dimension of the single-particle basis. In our calculations we used the two-body matrix elements calculated from the Bonn–B nucleon–nucleon one boson exchange potential. The single-particle energies are calculated from the Coulomb-corrected Woods–Saxon potential with Bertsch parametrization. We used several sets of single-particle levels to see how the choice of the basis influences the results. We find weak dependence of the RQRPA and the SRQRPA results on the dimension of the single-particle basis. On the other hand the QRPA shows no stability with respect to the chosen basis. The conclusion is that the most suitable basis for the calculations of $2\nu\beta\beta$ decay of ^{76}Ge consists of 16 levels with ^{16}O as a core. Therefore we used this basis in all the further studies described below. To compare with the experiment we have adopted the experimental half-life of $T_{1/2}^{2\nu} = (1.42 \pm 0.03 \pm 0.13) \times 10^{21}$ yr from the latest measurement by the Heidelberg–Moscow $\beta\beta$ cooperation [35].

In Fig. 1 we plot the calculated double Gamow–Teller matrix elements $M_{GT}^{2\nu}$ as a function of g_{pp} for two different g_{ph} values and for three different QRPA approaches. We would like to stress that in these calculations in the self-consistent iterations of the RQRPA and the SRQRPA all the intermediate multipolarities were present. The comparison between the QRPA, the RQRPA and the SRQRPA results in the physically acceptable region of the g_{pp} parameter $0.8 \leq g_{pp} \leq 1.2$ shows two main features of the renormalized QRPA. First, the inclusion of

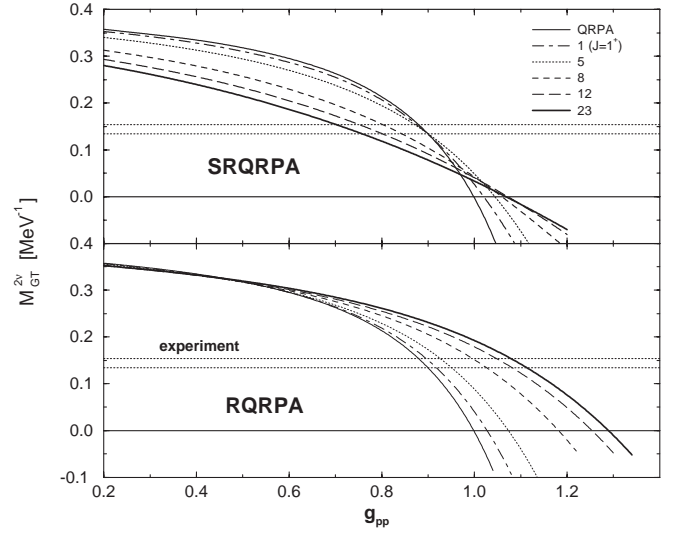


Fig. 2. The influence of the different number of the added multipolarities on $M_{GT}^{2\nu}$ for two types of the renormalization: RQRPA and SRQRPA. Full range of the strength factor g_{pp} is scanned for fixed $g_{ph} = 1.0$. SRQRPA shows less dependence on g_{pp} parameter than the RQRPA approach. The experimental values [35] are between two parallel dotted lines

the ground-state correlations beyond QRPA is not only improving the agreement between theoretical calculations and experimental data but also causes the stabilization of the dependence of $M_{GT}^{2\nu}$ as a function of g_{pp} . Second, the iteration procedure for quasiparticle densities which causes the treating RQRPA and BCS on the same footing stabilizes the results even further.

Some authors claim that only the limited set of these multipolarities plays a role in the evaluation of double Gamow–Teller matrix elements [24, 25]. In Fig. 2 there are shown the results of calculations of $M_{GT}^{2\nu}$ as a function of g_{pp} for different number of multipolarities for the RQRPA and the SRQRPA, respectively. The basis is the same as in Fig. 1, but the value of g_{ph} parameter is fixed to 1.0. It can be seen why the inclusion of all multipolarities is essential to obtain the reliable predictions of the RQRPA and the SRQRPA calculations. The solid line in Fig. 2 represents the QRPA calculations, dot-dashed line the calculations with only 1^+ multipolarity, dotted line with multipolarities up to 2^+ , dashed line up to 3^- , long-dashed up to 5^- and thick solid line all considered multipolarities up to 11^+ . The inclusion of higher multipolarities causes the shift of the collapse of the RQRPA and the SRQRPA beyond the value of $g_{pp} = 1.0$. The additional advantage of the SRQRPA solutions is that calculated matrix elements are less dependent on the g_{pp} parameter.

In Fig. 3 the effect of including more multipolarities J^π in the RQRPA and the SRQRPA calculations of $M_{GT}^{2\nu}$ for fixed $g_{ph} = 1.0$ is shown. Filled symbols represent the calculations for $g_{pp} = 0.8$ and open symbols for $g_{pp} = 1.0$. One can see the saturation effect for higher multipolarities. The explanation of this behaviour is that higher multipolarities J^π are less collective. Their contribution to the

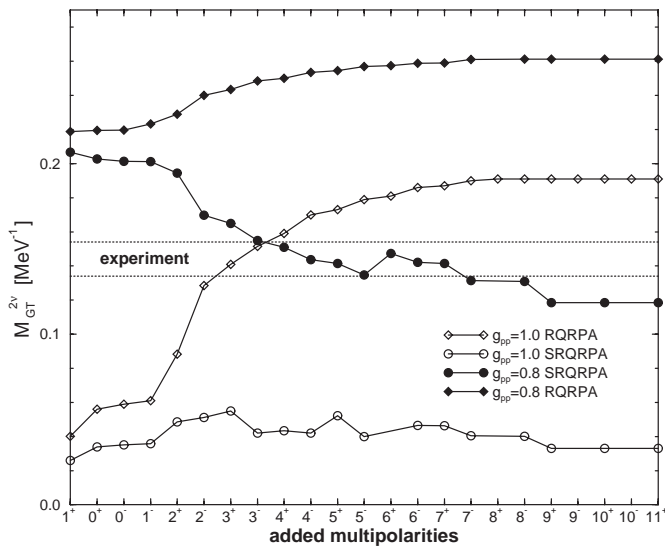


Fig. 3. Influence of addition of individual multipolarities (1^+ , 0^+ , \dots , 11^+) on magnitude of the double Gamow–Teller matrix element within two different RQRPA approaches. Calculations shown for $g_{pp} = g_{ph} = 1.0$. For details see text

ground-state correlations is much smaller than the lower ones. An interesting feature is the virtual independence of the matrix element on the number of multipolarities in SRQRPA around $g_{pp} = 1.0$. It is reflected in Fig. 2, where one can see that RQRPA “diverges” when going with g_{pp} from 0 to 1, while the SRQRPA “converges”. This, in our opinion, is a clear signal that the self-consistency between BCS and RPA, i.e. between ground-state and excited-state properties is being restored in SRQRPA.

Finally, we would like to address the question of the Ikeda sum rule violation. It is well known, that in the usual QRPA the Ikeda sum rule [27] is conserved exactly if all the spin-orbit partners of the single-particle orbitals are present in the basis, i.e.

$$S_- - S_+ \equiv \sum_m |\langle 0_{gs}^+ || \sigma \tau_+ || 1_m^+ \rangle|^2 - \sum_m |\langle 0_{gs}^+ || \sigma \tau_- || 1_m^+ \rangle|^2 = 3(N - Z). \quad (28)$$

The violation is marginal even if one or two of these partners are omitted. But this is not the case in RQRPA, where the Ikeda sum rule is violated up to 20% and is similar in the SRQRPA. One can conclude, that the inclusion of the ground-state correlations beyond RQRPA can not restore the Ikeda sum rule. As already pointed out [34, 36], the scattering terms present in the β -decay operators can be responsible for this effect. They appear to be very important to fulfill both the energy weighted and normal sum rules in the case of homogeneous infinite nuclear matter [22]. These terms give no contribution in QRPA, because they are of quasiparticle–quasihole character, but should be taken into account when the ground-state quasiparticle densities are not assumed to be zero, like in the RQRPA or SRQRPA. It is necessary to extend the form of the QRPA phonon operator (1) by including new excitation modes, the so-called B -modes [20–23]. The corresponding

extension of the theory is not straightforward and gives some conceptual problems. Such an analysis requires further discussion that is beyond the scope of the present paper.

4 Summary and conclusions

We calculated the nuclear matrix elements for the neutrino accompanied double beta decay to the ground state in a frame of the new self-iterative BCS+RQRPA approach. Using $2\nu\beta\beta$ decay of germanium ^{76}Ge as an example we demonstrated that the inclusion of the ground-state correlations beyond QRPA causes the stabilization of the dependence of the Gamow–Teller nuclear matrix element, but also weakens their influence on their magnitude because of additional change of the quasiparticle densities during the iteration procedure with the modified BCS solution.

Unlike orthodox QRPA which needs fine tuning of the g_{pp} parameter describing the particle–particle interaction strength as the matrix element collapses near the physical strength, RQRPA and BCS+RQRPA gives stable matrix elements over the whole range of physical strength and thus these last approaches allow for more predictive power than the old method.

Due to the development of the method of calculation the D_{pn} normalization factors we could take all possible multipolarities into account. Then we were able to avoid the possibility of the J-scheme breaking, because by neglecting some of the multipolarities the basis becomes incomplete and the validity of mappings (10)–(11) is under question. Our calculations are the first ones that include the full spectrum of the intermediate states in both RQRPA and the BCS+RQRPA approaches.

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