Renormalized Proton-Neutron Quasiparticle Random-Phase Approximation and Its Application to Double Beta Decay

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A self-consistent method of treating excitations of the proton-neutron quasiparticle random-phase approximation is presented. The non-self-consistent methods violate the Pauli exclusion principle and lead to an eventual collapse of the ground state. This behavior renders a reliable calculation of the nuclear matrix elements, relevant for the prediction of double-beta-decay half-lives, difficult. The present formalism promotes the Pauli exclusion principle and avoids the collapse of the double-beta-decay matrix elements. We have applied this formalism to the double beta decay of ^{100}Mo.

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At the moment, the neutrinoless double beta decay ($0\nu\beta\beta$) is the best probe for physics beyond the standard model of electroweak interactions. Its existence connects with many fundamental aspects of neutrino physics [1]. To date, only lower limits on half-lives of different nuclei have been obtained experimentally. These limits are used to deduce upper limits on the Majorana-neutrino mass, the right-handed-current admixture parameters, the Majoron–Majorana-neutrino coupling constant, etc. One particular source of uncertainty in the above analyses is the evaluation of the nuclear matrix elements involved. For the decay to the ground state of the daughter nucleus, the mass mechanism is the dominant one [1], leading to the need of evaluating the associated double Gamow-Teller matrix element (DGT) as reliably as possible.

It is important to note that in connection with the $0\nu\beta\beta$ decay, the detection of double beta decay with the emission of two neutrinos ($2\nu\beta\beta$), which is an allowed process of second order in the standard model, enables experimental determination of the magnitude of the DGT. This is because both modes of double beta decay require the same basic many-body nuclear-structure wave functions leading to the need of developing theoretical schemes of calculation in connection with both the $2\nu\beta\beta$ decays and the $0\nu\beta\beta$ decays. The improved theoretical methods yield better predictions for double-beta half-lives and stimulate new and better-focused double-beta experiments.

After its successful application to $2\nu\beta\beta$ decay [2], the proton-neutron quasiparticle random-phase approximation (pnQRPA) has been the most powerful tool in studies of double beta decay of medium-heavy and heavy open-shell nuclei. In these studies both schematic [2] and realistic [3] two-body matrix elements have been used. A shortcoming of these calculations is that they violate the Pauli exclusion principle and lead to an eventual collapse of the pnQRPA ground state. This collapse is caused by generation of too many ground-state correlations with increasing strength of the proton-neutron interaction. This means that in the region of realistic pn-interaction strengths, i.e., near $g_{pp} = 1.0$, where g_{pp} is the strength parameter of the particle-particle part of the pn interaction [2], the DGT may be very unstable, changing its magnitude very fast as a function of g_{pp}. Therefore, a reliable calculation of the nuclear matrix elements, relevant for the prediction of double-beta-decay half-lives, becomes difficult. In particular, this instability has been speculated [4,5] to hinder a reliable calculation of the DGT in connection with the $2\nu\beta\beta$ transition ^{100}Mo(g.s.) $\rightarrow$ ^{100}Ru(g.s.).

Several attempts [4,6–8] have been made to shift the collapse of the pnQRPA ground state to higher values of g_{pp}, possibly beyond the physically acceptable region. In Refs. [4,7] the method of particle-number-projected pnQRPA equations was used and in Ref. [6] the BCS self-energy corrections were included in the calculations. The authors of Ref. [8] tried to achieve a consistent determination of g_{pp} by invoking partial restoration of isospin and Wigner SU(4) symmetries. All these methods, however, disregard the main source of ground-state instability, namely, the increasing violation of the Pauli principle with building up of an excessive amount of ground-state correlations.

In this Letter we present an easy-to-apply method with which one can avoid the instability of the DGT and produce more reliable predictions for the double-beta half-lives. This method we call the renormalized pnQRPA, RQRPA for short. It is not restricted to any particular choice of the single-particle basis or form of the two-body interaction. To our knowledge, the RQRPA is the first attempt to retain the Pauli exclusion principle in the correlated ground state of the pnQRPA with increasing strength of the proton-neutron interaction. Below we summarize its basic ingredients and demonstrate its application by comparing its results with the results of the ordinary pnQRPA in the case of the previously mentioned ^{100}Mo decay. On one hand, this comparison is stimulated by the suggested [4,5] instability of the DGT, and on the other hand, by the present experimental efforts [9] being invested in the study of the ^{100}Mo double beta decay.

The first step in the RQRPA calculation, as in the ordinary pnQRPA, is the BCS calculation of the even-even

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ground state leading to the quasiparticle representation of the nuclear Hamiltonian. After that, one can derive the RQRPA equations in a straightforward way by using the equations-of-motion (EOM) method [10]. In the EOM one starts from the creation and annihilation operators of excited states, which, in the case of odd-odd nuclei, consist of proton-neutron two-quasiparticle components

$$Q^{\dagger}(m;JM) = \sum_{pn} [X^{m}_{pn} A^{\dagger}(pn;JM) - Y^{m}_{pn} \tilde{A}(pn;JM)], \tag{1}$$

where the notation is from [11]. Using the machinery of the EOM theory [10], one arrives at the matrix equation

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} X^{m} \\ Y^{m} \end{pmatrix} = \hbar\omega_{m} \begin{pmatrix} U & 0 \\ 0 & -U \end{pmatrix} \begin{pmatrix} X^{m} \\ Y^{m} \end{pmatrix}, \tag{2}$$

where the matrices A and B are defined as

$$A(pnp'n'J) = \langle \mathrm{RPA}|[A(pn;JM), \hat{H}, A^{\dagger}(p'n';JM)] \times |\mathrm{RPA}\rangle, \tag{3a}$$

$$B(pnp'n'J) = \langle \mathrm{RPA}|[A(pn;JM), \hat{H}, A(p'n';JM)] \times |\mathrm{RPA}\rangle, \tag{3b}$$

Here the double commutators are defined as $[A,B,C] = \frac{1}{2}[A,[B,C]] + \frac{1}{2}[[A,B],C]$. The matrices A and B in (2) carry contributions from one-body and two-body ground-state densities [10]. These contributions go beyond the ordinary pnQRPA level and take into account the Pauli exclusion principle [10]. They are nonzero because in the EOM one takes the intrinsic fermion structure of the pair operators $A(pn;JM)$ and $A^{\dagger}(pn;JM)$ fully into account when deriving Eq. (2.)

Keeping only the diagonal parts of the one-body densities, the overlap matrix U on the right-hand side of (2) becomes

$$U(pnp'n') = \langle \mathrm{RPA}|[A(pn;JM), A^{\dagger}(p'n';JM)]|\mathrm{RPA}\rangle = \delta_{pp'}\delta_{nn'}(1 - \hat{j}_{p}^{-1}\langle \mathrm{RPA}|[a^{\dagger}_{p}\tilde{a}_{p}]_{00}|\mathrm{RPA}\rangle - \hat{j}_{p}^{-1}\langle \mathrm{RPA}|[a^{\dagger}_{n}\tilde{a}_{n}]_{00}|\mathrm{RPA}\rangle) \equiv \delta_{pp'}\delta_{nn'}D_{pn}, \tag{4}$$

where $\hat{j} = \sqrt{2j+1}$. This form of overlap matrix is exact if the single-particle valence space contains at most two major oscillator shells (which is the case in the present calculation). This approximation leads to a diagonal overlap matrix U, and Eq. (2) can be transformed to standard RPA form [1]. After this transformation, and omitting the two-body densities (supposed to act incoherently with random phases, see Ref. [10]), one obtains the RQRPA equations with new matrices $\overline{A}$ and $\overline{B}$

$$\begin{pmatrix} \overline{A} & \overline{B} \\ \overline{B} & \overline{A} \end{pmatrix} \begin{pmatrix} \overline{X}^{m} \\ \overline{Y}^{m} \end{pmatrix} = \hbar\omega_{m} \begin{pmatrix} \overline{X}^{m} \\ -\overline{Y}^{m} \end{pmatrix}, \tag{5}$$

where now the matrices $\overline{A}$ and $\overline{B}$ read

$$\begin{aligned} \overline{A}(pnp'n'J) &= (E_{p} + E_{n})\delta_{pp'}\delta_{nn'} - D^{1/2}_{pn}[2G(pnp'n'J)(u_{p}u_{n}u_{p'}u_{n'} + v_{p}v_{n}v_{p'}v_{n'}) \\ &\quad + 2F(pnp'n'J)(u_{p}v_{n}u_{p'}v_{n'} + v_{p}u_{n}v_{p'}u_{n'})]D^{1/2}_{p'n'}, \\ \overline{B}(pnp'n'J) &= D^{1/2}_{pn}[2G(pnp'n'J)(u_{p}u_{n}v_{p'}v_{n'} + v_{p}v_{n}u_{p'}u_{n'}) \\ &\quad - 2F(pnp'n'J)(u_{p}v_{n}v_{p'}u_{n'} + v_{p}u_{n}u_{p'}v_{n'})]D^{1/2}_{p'n'}. \end{aligned} \tag{6}$$

The amplitudes $\overline{X}^{m}_{pn} = D^{1/2}_{pn}X^{m}_{pn}$ and $\overline{Y}^{m}_{pn} = D^{1/2}_{pn}Y^{m}_{pn}$ fulfill the usual RPA orthogonality relations, as one can easily check using Eqs. (1) and (4).

So far nothing has been said about the calculation of the overlap matrix elements D_{pn}. We adopt the method of Ref. [12] where the one-body densities are expressed in terms of fermion-pair creation and annihilation operators $A^{\dagger}$ and A. One can expand the product of the fermion-pair operators [12] by using completeness of the intermediate states and then apply Eq. (4) to yield

$$D_{pn} = 1 - \hat{j}_{p}^{-2}\sum_{n'} D_{pn'}\left(\sum_{Jm} \hat{J}^{2}|\overline{Y}^{Jm}_{pn'}|^{2}\right) - \hat{j}_{n}^{-2}\sum_{p'} D_{p'n}\left(\sum_{Jm} \hat{J}^{2}|\overline{Y}^{Jm}_{p'n}|^{2}\right). \tag{7}$$

The above equation cannot be converted into an ordinary matrix-inversion problem and must therefore be solved by iteration. Equations (5) and (7) together form a doubly iterative problem. When the coefficients D_{pn} on the right-hand side of Eq. (7) are put equal to unity, we obtain the usual pnQRPA expression of ground-state correlations, which is valid as long as ground-state correlations are small. In this case no double iteration is needed. To access the difference between these two approximations of D_{pn}, we have used them both in our calculations.

To be able to calculate beta-decay and double-beta-decay transition amplitudes, one has to know the renormalized charge-changing transition densities of the RQRPA, namely,

$$(\mathrm{RPA}||[c^{\dagger}_{p}\tilde{c}_{n}]_{L}||J_{m}) = \hat{L}\delta_{LJ}[v_{p}u_{n}\overline{X}^{Jm}_{pn} + u_{p}v_{n}\overline{Y}^{Jm}_{pn}]D^{1/2}_{pn}, \tag{8a}$$

$$(\mathrm{RPA}||[c^{\dagger}_{n}\tilde{c}_{p}]_{L}||J_{m}) = \hat{L}\delta_{LJ}[u_{p}v_{n}\overline{X}^{Jm}_{pn} + v_{p}u_{n}\overline{Y}^{Jm}_{pn}]D^{1/2}_{pn}\eta_{J_{pn}}, \tag{8b}$$

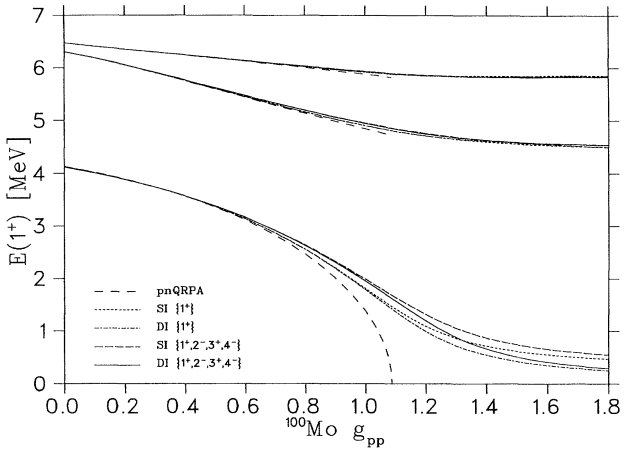

FIG. 1. Energies of the three lowest 1^+ states of ^{100}Tc calculated using the pnQRPA and four different approximations of the RQRPA as a function of the particle-particle interaction strength g_{pp}. Short-dashed line: single-iterative (SI) with intermediate 1^+ states only. Dot-dashed line: double-iterative (DI) with intermediate 1^+ states only. Long-dashed line: SI using intermediate 1^+, 2^-, 3^+, and 4^- states. Solid line: DI using intermediate 1^+, 2^-, 3^+, and 4^- states.

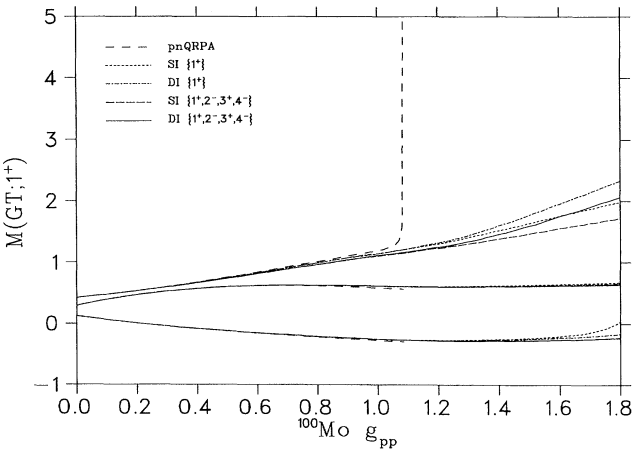

FIG. 2. β^- transition amplitudes M(GT) for the decay of ^{100}Mo(g.s.) to the three lowest 1^+ states of ^{100}Tc as functions of the particle-particle interaction strength g_{pp}. Highest group of lines: M(GT) for the state 1_1^+. Middle group of lines: M(GT) for the state 1_2^+. Lowest group of lines: M(GT) for the state 1_3^+. For the meaning of the various line types, see the caption of Fig. 1.

where $\eta_{J_{pn}} \equiv (-1)^{j_p+j_n+J+1}$. These transition matrix elements can be inserted into the standard expressions of the Gamow-Teller beta-decay [11] and double-beta-decay [1–3] amplitudes.

We demonstrate the use of the RQRPA by calculating the $2\nu\beta\beta$ transition amplitude ^{100}Mo(g.s.) $\rightarrow$ ^{100}Ru(g.s.). Both the pnQRPA and RQRPA calculations follow the scheme of Ref. [5]. Our single-particle valence space consists of major shells $3\hbar\omega$, $4\hbar\omega$, and the $0h_{11/2}$ intruder orbital from the $5\hbar\omega$ major shell. The adopted single-particle energies and the two-body G-matrix interaction are the ones of Ref. [5].

Our results are summarized in Figs. 1–3. Figures 1 and 2 show the three lowest energies of the intermediate 1^+ states and the β^- transition amplitudes to these states from ^{100}Mo(g.s.) as functions of the proton-neutron interaction strength g_{pp}. Corresponding results for ^{100}Ru are qualitatively similar. Finally, in Fig. 3 we summarize the calculated results for the $2\nu\beta\beta$ decay ^{100}Mo(g.s.) $\rightarrow$ ^{100}Ru(g.s.) as a function of g_{pp}.

In all figures we call those results where Eq. (7) is simplified noniterative as "SI" and those results where we take Eq. (7) fully iterative as "DI". The full RQRPA calculation needs fairly big computational effort because in each step of the singly or doubly iterative procedure of solving Eqs. (5) and (7), for a given g_{pp}, we must, in principle, find eigenstates for all intermediate multipolarities J^π. To study the effects of different numbers of intermediate multipolarities, we have performed the calculations using two sets of J^π: either only 1^+ states (denoted $\{1^+\}$ in the figures) or states 1^+, 2^-, 3^+, and 4^- ($\{1^+, 2^-, 3^+, 4^-\}$ in the figures) which, in this case, are the only important multipoles affecting the solution of Eq. (7).

As can be seen from the figures, for part of the physically acceptable values of particle-particle interaction strength, e.g., $0.8 \leq g_{pp} \leq 1.0$, the results of different approximation schemes differ only little from each other. For larger values of g_{pp} the lowest 1^+ state vector, which in ordinary pnQRPA collapses at some critical particle-particle interaction strength, in this case at $g_{pp} = 1.03$, behaves smoothly in the RQRPA. Thus the pnQRPA collapses in the physically acceptable region of g_{pp} and may lead

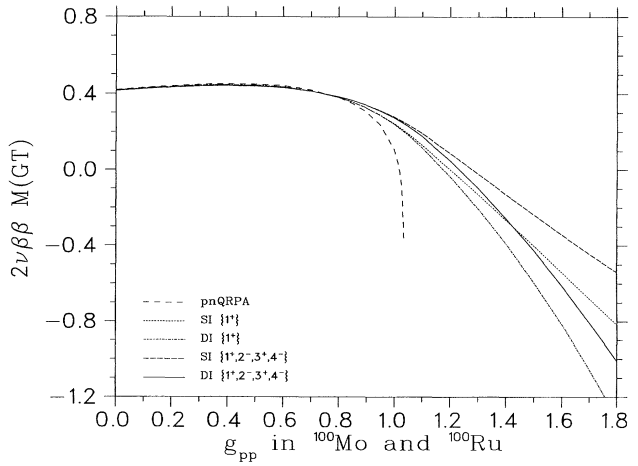

FIG. 3. The $2\nu\beta\beta$ transition amplitude ^{100}Mo(g.s.) $\rightarrow$ ^{100}Ru(g.s.) as a function of the particle-particle interaction strength g_{pp}. For the meaning of the various line types, see the caption of Fig. 1.

to ambiguous determination of the beta-decay and double-beta-decay Gamow-Teller matrix elements. This is further demonstrated in Fig. 2 where one observes that near $g_{pp} = 1.0$ the decay amplitude to the lowest intermediate 1^+ state becomes unphysically large for the pnQRPA, whereas in the RQRPA the corresponding amplitude remains stable. Figure 3, in turn, indicates that the $2\nu\beta\beta$ amplitude remains rather stable at $g_{pp} = 1.0$ for the pnQRPA and does not differ drastically from the result of the RQRPA, establishing the validity of the results of Ref. [5]. In some other cases [3], especially for some double β^+ and electron capture decays, the situation may not be that fortunate and severe difficulties can arise in the pnQRPA.

For higher 1^+ states both energies and beta-decay amplitudes are well described by the pnQRPA, even beyond the physical region of g_{pp}. As a general observation, the RQRPA amplitudes calculated with Eq. (7) tend to diminish faster than the corresponding amplitudes calculated using the noniterative approximation of D_{pn}. This is in keeping with the observations of Ref. [12]. However, for all shown values of g_{pp} the different RQRPA approaches yield amplitudes of the same order of magnitude.

In conclusion, we have developed a straightforward method, the renormalized proton-neutron QRPA, for a reliable calculation of beta and double-beta transition matrix elements in a region of two-body interactions where the ordinary pnQRPA becomes unstable. This method is not restricted to any particular choice of the single-particle basis or form of the two-body interaction. It simply promotes the Pauli exclusion principle violated by the excessive ground-state correlations of the pnQRPA in the physically interesting region of the proton-neutron interaction. This aspect has been neglected in all previous attempts to overcome the eventual collapse of the pnQRPA. We demonstrate the RQRPA method by comparing its results with the pnQRPA results in the case of the $2\nu\beta\beta$ transition ^{100}Mo(g.s.) $\rightarrow$ ^{100}Ru(g.s.).

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