Restoration of the Ikeda sum rule in self-consistent quasiparticle random-phase approximation

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The so-called self-consistent quasiparticle random phase approximation, accounting for a better treatment of ground-state correlations, is applied to a schematic Hamiltonian, describing the Fermi beta decay process. The self-consistent procedure coupling the BCS minimum with the quantum fluctuations yields an exact fulfillment of the Ikeda sum rule. The role of the ground-state correlations is analyzed in the case of the double beta decay process. [S0556-2813(97)02405-9]

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The interest in beta decay was renewed in the last decade mainly by the prediction of neutrinoless double beta decay ($0\nu\beta\beta$) in the frame of some grand unification models [1] and by new spectroscopy in the neutron-rich area [2]. An important test for nuclear current matrix elements (ME's) is given by the experimentally measured double beta decay process with emission of two neutrinos ($2\nu\beta\beta$). The main tool to estimate nuclear ME's of this process in medium and heavy nuclei is the random phase approximation in a quasiparticle representation (QRPA). The standard QRPA diagonalization procedure takes place in two steps. First one determines the static minimum, using the quasiparticle representation. In the second step one finds the eigenvalues, describing small vibrations around this minimum, by using different procedures to linearize the equations of motion. In the simplest quasiboson approximation (QBA) one considers bosonlike pairs of fermions, while different variants of the renormalized boson approximation (RBA) [3–6] account more exactly for the Pauli corrections.

Usually the two steps are considered separately both in the QBA and RBA. In spite of the fact that, for instance, the RBA corrects the collapse of the $2\nu\beta\beta$ amplitude versus particle-particle correlations [7,8] it was shown that the Ikeda sum rule [9] is violated [10]. Higher RPA corrections computed within the boson expansion technique also violate the sum rule [11] by a comparable amount.

In this paper we will remove this drawback by considering a simultaneous treatment of the BCS and QRPA vacua in applying the so-called self-consistent QRPA (SCQRPA), which better accounts for Pauli corrections. This is the generalization of the scheme proposed in Refs. [12,13] to proton-neutron systems. In this way one obtains a substantial correction of the collapse in the $2\nu\beta\beta$ transition rate with increasing particle-particle correlations.

For the sake of simplicity let us consider a schematic Hamiltonian, describing the gross properties of the decay processes in the simplest case of the monopole Fermi transitions. It describes a system of protons (π) and neutrons (ν), filling shells with the same spin j:

$$\begin{aligned}H=&(\epsilon_\pi-\lambda_\pi)N_{\pi\pi}+(\epsilon_\nu-\lambda_\nu)N_{\nu\nu}-\frac{G_\pi}{4}P^\dagger_{\pi\pi}P_{\pi\pi}\\&-\frac{G_\nu}{4}P^\dagger_{\nu\nu}P_{\nu\nu}+\frac{\chi}{2\Omega}[g_{ph}(N_{\pi\nu}N_{\nu\pi}+N_{\nu\pi}N_{\pi\nu})\\&-g_{pp}(P^\dagger_{\pi\nu}P_{\nu\pi}+P^\dagger_{\nu\pi}P_{\pi\nu})],\end{aligned}\tag{1}$$

where, by using single-particle operators $c^\dagger_{\alpha m}$, with $\alpha=\pi,\nu$ and $m=$spin projection, the following standard notations were introduced:

$$N_{\alpha\beta}=\sum_m c^\dagger_{\alpha m}c_{\beta m},\quad N_{\beta\alpha}=N^\dagger_{\alpha\beta},$$

$$P^\dagger_{\alpha\beta}=P^\dagger_{\beta\alpha}=\sum_m c^\dagger_{\alpha m}c^\dagger_{\beta\overline{m}}s_m,\quad P_{\beta\alpha}=(P^\dagger_{\alpha\beta})^\dagger,$$

$$\alpha,\beta=\pi,\nu,\quad \overline{m}=-m,\quad s_m=(-)^{j-m},\quad \Omega=j+1/2.\tag{2}$$

Here ϵ_α are single-particle energies and λ_α the Lagrange multipliers, adjusted by the particle number condition. Fermi beta decay operators are given by $\beta^-=N_{\pi\nu}$, $\beta^+=N_{\nu\pi}$, and χ is the overall strength of the beta decay process. A similar Hamiltonian describing the dipole Gamow-Teller beta decay process was proposed in Ref. [14]. In spite of its simplicity, it takes into account the main properties displayed also by realistic interactions. The factors g_{ph} and g_{pp} are the particle-hole and particle-particle strengths, respectively. In calculating double beta decay transition rates an important role is played by particle-particle correlations [15–17]. This is why in the case of Gamow-Teller transitions one usually studies the behavior versus particle-particle correlations by varying g_{pp} and keeping constant $g_{ph}=1$.

This Hamiltonian was extensively studied using group theoretical methods in Refs. [18–20]. The set of ten operators in Eq. (2) closes the commutation algebra of the O(5) group. In the general case the Hamiltonian can be diagonalized in the complete but nonorthogonal basis [19]

$$|N_\pi N_\nu N_0\rangle=(P^+_{\pi\pi})^{N_\pi}(P^+_{\nu\nu})^{N_\nu}(P^+_{\pi\nu})^{N_0}|0\rangle. \tag{3}$$

The Hamiltonian (1) is a quadratic Casimir of the O(5) group for $G_\pi=G_\nu=G$ and $\chi g_{pp}=G\Omega/2$. In this case the eigenstates can be labeled by the isospin quantum number. For g_{pp} values different from $G\Omega/2\chi$ the Hamiltonian violates isospin symmetry. Though an artifact of the model, this violation may simulate proton-neutron correlations coming from the other channels, like $T=0$ (isoscalar pairing), not included in the present model.

We will study the vibrations around the stationary point within the SCQRPA. In the quasiparticle representation given by single-particle operators $a^\dagger_{\alpha m}=U_\alpha c^\dagger_{\alpha m}-V_\alpha c_{\alpha\bar{m}}s_m$ the Hamiltonian (1) is given by

$$H=H_0+\sum_{\alpha=\pi\nu}[E_\alpha\mathcal{N}_{\alpha\alpha}+H^{(20)}_{\alpha\alpha}(A^\dagger_{\alpha\alpha}+A_{\alpha\alpha})]$$
$$+\sum_{\alpha\leqslant\beta}[H^{(22)}_{\alpha\beta}A^\dagger_{\alpha\beta}A_{\beta\alpha}+H^{(40)}_{\alpha\beta}(A^\dagger_{\alpha\beta}A^\dagger_{\alpha\beta}+A_{\beta\alpha}A_{\beta\alpha})], \tag{4}$$

where

$$\mathcal{N}_{\alpha\beta}=\sum_m a^\dagger_{\alpha m}a_{\beta m},\quad A^\dagger_{\alpha\beta}=(a^\dagger_\alpha a^\dagger_\beta)_0. \tag{5}$$

$H_0=H_{\rm BCS}$ is the expectation value of the Hamiltonian on the vacuum state, E_α are quasiparticle energies, and

$$H^{(20)}_{\alpha\alpha}=\epsilon_\alpha U_\alpha V_\alpha-\tfrac{1}{2}(U^2_\alpha-V^2_\alpha)G_\alpha\Omega U_\alpha V_\alpha,$$
$$H^{(22)}_{\alpha\beta}=2\chi[g_{ph}(U^2_\alpha V^2_\beta+V^2_\alpha U^2_\beta)-g_{pp}(U^2_\alpha U^2_\beta+V^2_\alpha V^2_\beta],$$
$$H^{(40)}_{\alpha\beta}=2\chi(g_{ph}+g_{pp})U_\alpha V_\alpha U_\beta V_\beta. \tag{6}$$

The SCQRPA state is written in terms of an excitation operator, acting on the vacuum state (in this work the generalization of the SCRPA excitation operator to include $\alpha^\dagger\alpha$ terms like proposed in [13] will not be considered, since it is not easily applied to schematic models such as the one treated here)

$$|\Psi\rangle=\Gamma^\dagger|0\rangle, \tag{7}$$

$$\Gamma|0\rangle=0, \tag{8}$$

where

$$\begin{pmatrix}\Gamma^\dagger\\ \Gamma\end{pmatrix}=\begin{pmatrix}\overline{X_\gamma} & -\overline{Y_\gamma}\\ -\overline{Y_\gamma} & \overline{X_\gamma}\end{pmatrix}\begin{pmatrix}\overline{A^\dagger_\gamma}\\ \overline{A_\gamma}\end{pmatrix}. \tag{9}$$

Here we introduced the normalized pair-creation operators

$$\overline{A^\dagger_\gamma}=T^{-1/2}_\gamma A^\dagger_\gamma,\quad \gamma=(\alpha\beta), \tag{10}$$

with a normalization factor given by

$$T_{\alpha\beta}=\langle 0|[A,A^\dagger]|0\rangle=\langle 0|1-\frac{\mathcal{N}}{2\Omega}|0\rangle,$$
$$\mathcal{N}=\mathcal{N}_{\alpha\alpha}+\mathcal{N}_{\beta\beta}. \tag{11}$$

The SCQRPA operators (9) obey boson commutation rules on the average and therefore the amplitudes $\overline{X_\gamma},\overline{Y_\gamma}$ are orthonormalized as follows:

$$\begin{pmatrix}\overline{X_\gamma} & -\overline{Y_\gamma}\\ -\overline{Y_\gamma} & \overline{X_\gamma}\end{pmatrix}\begin{pmatrix}\overline{X_\gamma} & \overline{Y_\gamma}\\ \overline{Y_\gamma} & \overline{X_\gamma}\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{12}$$

This relation also provides the inverse transformation expressing the operators $\overline{A^\dagger_\gamma},\overline{A_\gamma}$ in terms of $\Gamma^\dagger,\Gamma$. The SCQRPA equations for the renormalized amplitudes defined by Eq. (9) have then the standard form

$$\begin{pmatrix}\overline{\mathcal{A}_{\gamma\gamma'}} & \overline{\mathcal{B}_{\gamma\gamma'}}\\ \overline{\mathcal{B}_{\gamma\gamma'}} & \overline{\mathcal{A}_{\gamma\gamma'}}\end{pmatrix}\begin{pmatrix}\overline{X_{\gamma'}}\\ \overline{Y_{\gamma'}}\end{pmatrix}=\omega\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\overline{X_\gamma}\\ \overline{Y_\gamma}\end{pmatrix}, \tag{13}$$

with the usual expression for the ME's as expectation values of the following double commutators:

$$\overline{\mathcal{A}_{\gamma\gamma'}}=\langle 0|[\overline{A_\gamma},[H,\overline{A^\dagger_{\gamma'}}]]|0\rangle,$$
$$\overline{\mathcal{B}_{\gamma\gamma'}}=-\langle 0|[\overline{A_\gamma},[H,\overline{A_{\gamma'}}]]|0\rangle. \tag{14}$$

In the evaluation of these ME's, as proposed in Ref. [12], fermionic commutation relations are used and the SCQRPA vacuum is treated exactly by using Eq. (8). In order to find a self-consistent BCS minimum we will use the generalization of the gap equation [12,13], which corresponds to the minimization of the ground-state energy with respect to the BCS transformation amplitudes,

$$\langle 0|[H,A^\dagger_{\alpha\alpha}|0\rangle=0,\quad \alpha=\pi,\nu, \tag{15}$$

where H is given by Eq. (4). As in [13] for particle number equation one uses the exact expression

$$\langle 0|N_{\alpha\alpha}|0\rangle=2\Omega V^2_\alpha+(U^2_\alpha-V^2_\alpha)\langle 0|\mathcal{N}_{\alpha\alpha}|0\rangle=N_\alpha$$
$$=\begin{pmatrix}Z, & \alpha=\pi\\ N, & \alpha=\nu\end{pmatrix}. \tag{16}$$

By using Eqs. (8) and (12) it can be shown that the BCS equations have a standard structure with, however, a renormalized interaction. The particle number condition (16) is modified by the quasiparticle occupation numbers $\langle\mathcal{N}_{\alpha\alpha}\rangle\equiv\langle 0|\mathcal{N}_{\alpha\alpha}|0\rangle\neq 0$, accounting for ground state correlations. In the same way we obtain for the BCS amplitudes:

$$\begin{pmatrix}U^2_\alpha\\ V^2_\alpha\end{pmatrix}=\frac{1}{2}\left(1\pm\frac{\epsilon_\alpha-\lambda_\alpha}{E_\alpha}\right)=\frac{1}{2}\left(1\pm\frac{\Omega-N_\alpha}{\Omega-\langle\mathcal{N}_{\alpha\alpha}\rangle}\right),$$
$$E_\alpha=\frac{G_\alpha\Omega}{2},\quad \alpha=\pi,\nu. \tag{17}$$

It can also be shown that the SCQRPA matrices given by Eq. (14) split into two independent blocks, namely, a block connecting $\overline{A^\dagger_\pi}$ with $\overline{A^\dagger_\nu}$ and a single element $\overline{A^\dagger_{\pi\nu}}$. This last part is responsible for beta decay processes and we will analyze it separately, without any loss of generality. Thus the QRPA transformation (9) contains one component.

By using the inverse transformation of Eq. (9) and the property (8) one can exactly calculate the SCQRPA ME's by taking into account the fermion commutation relations

$$\overline{\mathcal{A}_{\pi\nu}}=E_{\pi}+E_{\nu}+H^{(22)}_{\pi\nu}\left[\frac{\langle(1-\mathcal{N}/2\Omega)^2\rangle}{\langle 1-\mathcal{N}/2\Omega\rangle}-\frac{\overline{Y^2_{\pi\nu}}}{\Omega}\right],$$

$$\overline{\mathcal{B}_{\pi\nu}}=2H^{(40)}_{\pi\nu}\left[\frac{\langle(1-\mathcal{N}/2\Omega)^2\rangle}{\langle 1-\mathcal{N}/2\Omega\rangle}-\frac{1+2\overline{Y^2_{\pi\nu}}}{2\Omega}\right]. \tag{18}$$

At this point some comments on the form of the SCQRPA matrices are necessary. The first terms in square brackets of Eq. (18) are taken into account already by the above-mentioned RBA. The other terms are obtained by considering the exact commutation fermionic rules. In this way, up to now, no approximations in the SCQRPA diagonalization procedure have been introduced. The only unknowns are the norm $T_{\pi\nu}$, which contains the average quasiparticle occupation number $\langle\mathcal{N}\rangle$, and $\langle\mathcal{N}^2\rangle$. To find $\langle\mathcal{N}\rangle$ we will for simplicity use the prescription given by [5,6], which is consistent up to first order in $1/\Omega$ with fermionic commutation rules (a more elaborate scheme has been given in [13], but this extension is of no consequence for the fulfillment of the Ikeda sum rule (see below) and we will not consider it)

$$\mathcal{N}=2A^{\dagger}_{\pi\nu}A_{\nu\pi}. \tag{19}$$

By using the inverse transformation expressing $\overline{A_{\pi\nu}}$ in terms of QRPA operators one easily obtains

$$T_{\pi\nu}=1-\frac{\langle\mathcal{N}\rangle}{2\Omega}=\frac{1}{1+\overline{Y^2_{\pi\nu}}/\Omega}. \tag{20}$$

With the usual approximation $\langle\mathcal{N}^2\rangle\approx\langle\mathcal{N}\rangle^2$ the system of SCQRPA equations is closed and can be solved.

Now let us point out that in this approach the Ikeda sum rule is automatically fulfilled. Indeed, if one computes the transition ME's of the beta decay operators

$$\langle\Psi|\beta^-|0\rangle=T^{1/2}_{\pi\nu}\sqrt{2\Omega}(U_{\pi}V_{\nu}\overline{X_{\pi\nu}}+V_{\pi}U_{\nu}\overline{Y_{\pi\nu}}),$$

$$\langle\Psi|\beta^+|0\rangle=T^{1/2}_{\pi\nu}\sqrt{2\Omega}(U_{\nu}V_{\pi}\overline{X_{\pi\nu}}+V_{\nu}U_{\pi}\overline{Y_{\pi\nu}}), \tag{21}$$

and considering that we have only one intermediate state, then one obtains

$$|\langle\Psi|\beta^-|0\rangle|^2-|\langle\Psi|\beta^+|0\rangle|^2=T_{\pi\nu}2\Omega(V^2_{\nu}-V^2_{\pi}). \tag{22}$$

If we use for the BCS amplitudes the standard particle number condition $2\Omega V^2_{\alpha}=N_{\alpha}$, the above relation is different from $N-Z$, the value given by the Ikeda sum rule, because the normalization factor $T_{\pi\nu}$ is different from unity. If we use the renormalized expressions (17), the product on the right-hand side (rhs) of relation (22) gives $N-Z$ and the Ikeda sum rule is automatically fulfilled. (One should notice that in the strict sense the Ikeda sum rule [9] involves spin and isospin degrees of freedom, whereas in this model only isospin is restored since spin is absent. As other authors we will not make this distinction here and call it "Ikeda sum rule" also in this more restricted case.)

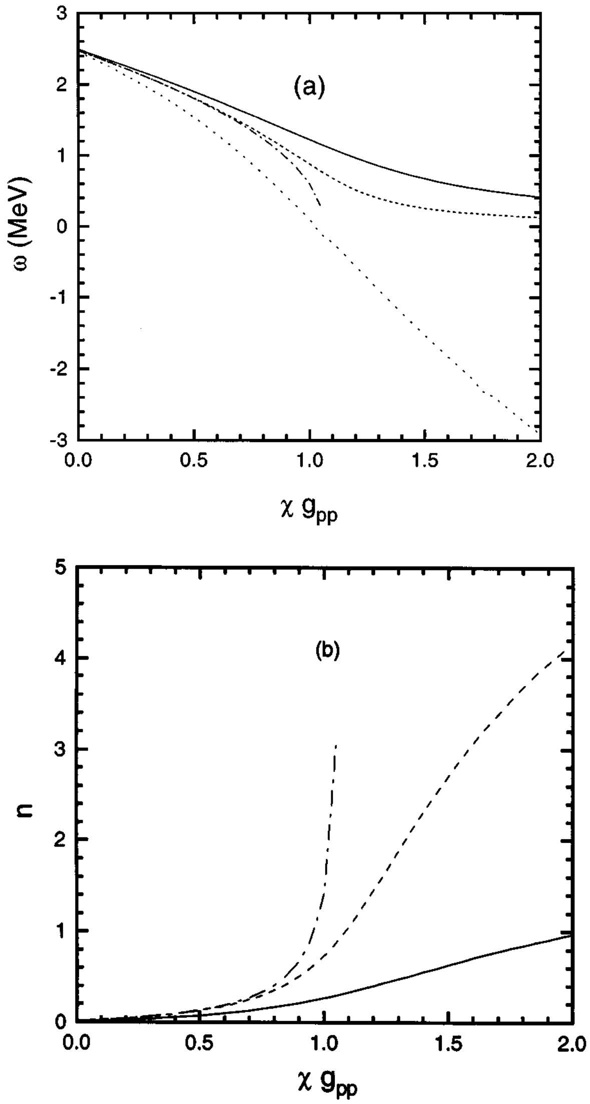

FIG. 1. (a) The RPA excitation energy as a function of χg_{pp} given by Eq. (13) in a quasiboson approximation (QBA) (dot-dashed line), renormalized boson approximation (RBA) (dashed line), self-consistent QRPA (SCQRPA) (solid line), and the exact solutions (dotted line). (b) The average quasiparticle occupation number versus χg_{pp} for QBA (dot-dashed line), RBA (dashed line), and SCQRPA (solid line).

An accurate prediction of the $0\nu\beta\beta$ amplitude depends on the quality of the nuclear ME's involved in $2\nu\beta\beta$, which can be compared with experimental measurements. To account for Pauli correlations in an optimal way, as is done in the SCQRPA, is therefore important. Let us consider $2\nu\beta\beta$ decay from an initial state $|i\rangle$ to a final state $|f\rangle$, through an intermediate state $|\Psi\rangle$ given by Eq. (7). One obtains the following expression for the transition amplitude:

$$M_{2\nu}=\frac{\langle f|\beta^-|\Psi\rangle\langle\Psi|\beta^-|i\rangle}{\omega+\Delta E}\approx\frac{\langle\Psi|\beta^+|0\langle\Psi|\beta^-|0\rangle}{\omega+\Delta E}, \tag{23}$$

where $\Delta E=m_ec^2+\frac{1}{2}Q_{\beta\beta}$ (m_e is electron mass and $Q_{\beta\beta}$ the Q value of the process).

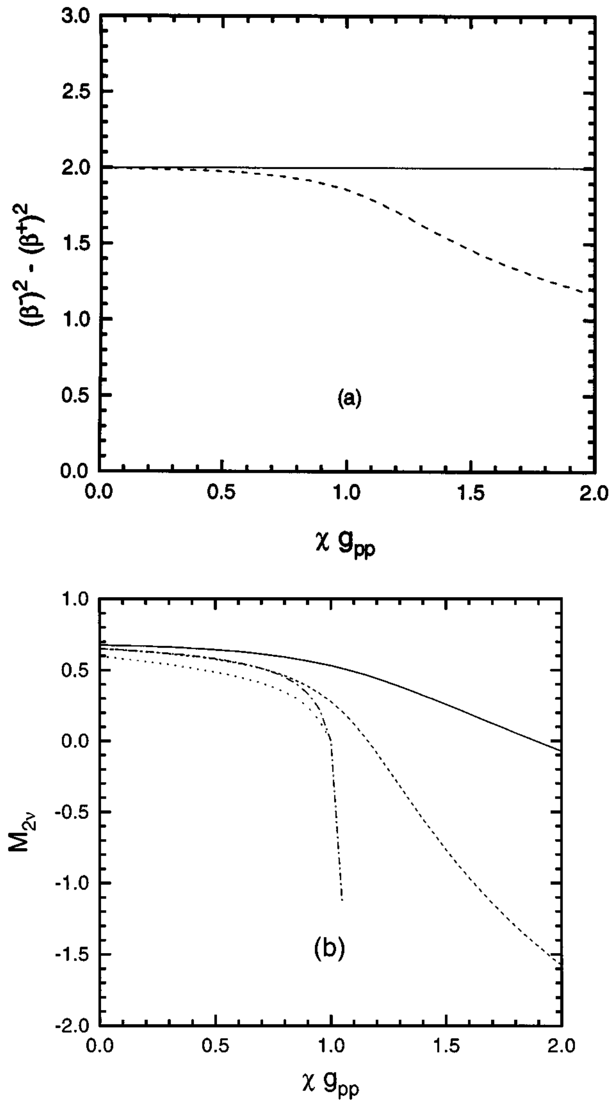

FIG. 2. (a) Ikeda sum rule versus χg_{pp} for RBA (dashed line) and SCQRPA (solid line). (b) $2\nu\beta\beta$ Fermi transition amplitude versus χg_{pp} for QBA (dot-dashed line), RBA (dashed line), SCQRPA (solid line), and exact solution (dotted line).

Here we approximated $\langle f|\beta^-|\Psi\rangle \approx \langle i|\beta^-|\Psi\rangle = \langle\Psi|\beta^+|0\rangle$ in order to better simulate the realistic situation where $M_{2\nu}$ is strongly suppressed.

The results of the calculations are presented in Figs. 1 and 2. We have chosen the following set of parameters

$$N=6, \quad Z=4, \quad j=9/2,$$

$$E_\pi = E_\nu = 1 \text{ MeV}, \quad \chi = 0.5 \text{ MeV},$$

$$g_{ph}=1, \quad \Delta E = 0.5 \text{ MeV}. \qquad (24)$$

We studied the behavior of different observables versus χg_{pp}, by changing the particle particle strength. First of all in Fig. 1(a) the energy given by the eigenvalue ω in Eq. (13) is plotted. The dot-dashed line presents the QBA result, which is obtained if one replaces in the SCQRPA matrices (18) the square brackets by unity. One can observe the breakdown of the solution around $\chi g_{pp}=1$. If one uses the RBA (first term in the square brackets), one obtains the dashed curve which avoids the breakdown. A similar result was also reported in Ref. [10]. If we use the SCQRPA, one obtains the solid line in this figure which smears out the phase transition even further. The exact result (lowest curve) is represented by dots.

To have an idea about the corrections induced by ground-state correlations we plotted in Fig. 1(b) the average quasiparticle occupation number $\langle\mathcal{N}\rangle$ versus χg_{pp}, using the same graphical representation. One can observe an important feedback behavior in the SCQRPA in comparison with the other two approaches.

Concerning the Ikeda sum rule we present in Fig. 2(a) the result given by Eq. (22) if one uses the RBA (dashed line). This shows the amount of violation in the sum rule when increasing g_{pp}. Of course for the SCQRPA the sum rule is automatically fulfilled (solid line).

Recent calculations [21] show for more realistic model describing the Gamow-Teller $2\nu\beta\beta$ process that the Ikeda sum rule is not fulfilled if one takes the exact expression (16), but within the above-mentioned RBA. Our hope is to fulfill the sum rule for realistic models by using the SCQRPA.

Finally in Fig. 2(b) we plotted the dependence of the $2\nu\beta\beta$ transition rate versus χg_{pp}. For the QBA the collapse around $\chi g_{pp}=1$ is induced by an overestimation of the ground-state correlations (dot-dashed line). The effect is partially removed by considering the RBA (dashed line). One can observe that in the SCQRPA case (solid line) the collapse is almost completely removed. By a dotted line we plotted the transition rate using the exact solution.

The conclusions extracted from this analysis can be summarized as follows. First of all a self-consistent treatment of the particle number condition, taking fully into account ground-state correlations, together with the coupling of the BCS transformation to the quantum fluctuations gives the necessary ingredients to fulfill the Ikeda sum rule. A similar treatment becomes very important for any sum rule connected with some procedure to renormalize RPA calculations [22].

Second, Pauli corrections and ground-state correlations are treated in an optimal way within the SCQRPA. The situation with respect to the exact solution of the model [Figs. 1(a), 2(b)] is paradoxical, however. Indeed, seemingly the better the theory, the further the results get away from the exact solution. In spite of the exact fulfillment of the Ikeda sum rule, SCRPA results are the worst. A similar behavior was already noticed and discussed in [10]. It implies, first, that the relative good agreement of QRPA with the exact results might be accidental and, second, that QRPA together with its extension of RBA and SCRPA misses an important piece of physics. In this respect it should be realized that the crossing of the zero line of the exact solution in Fig. 1(a) simply means that from this value of g_{pp} on the ground state of the odd-odd system becomes lower than the one of the even-even system. However QRPA plus extensions treat the difference in ground state energies of the even-even and odd-odd systems as an excitation energy which by definition is $\geqslant 0$. So the QRPA schemes generally considered for the double β-decay seem intrinsically incapable of describing in a continuous way the crossing of the ground state energies of the even-even and odd-odd systems. At this point we would like to remark that a continuation of RBA or SCQRPA far beyond the phase transition point where QRPA breaks down [at $\chi g_{pp}>1$ in our case, see Fig. 1(a)] makes little sense, as we know from the treatment of other models [12,22]. On the contrary, from the phase transition point on one should change the single particle basis which in our case means that we have to consider a general Bogoliubov transformation which mixes nn, pp, and pn pairs (the phase transition signals instability with respect to proton-neutron pairing). Whether this generalization can cure the problem is an open question.

Further work on this point is needed to get a better control of the situation.

Note added in proof. The comparison of exact and approximate results in Fig. 1(a) is biased, since the latter ones must be corrected for the chemical potentials of protons and neutrons (see Refs. [13, 21]). Though the introduction of this correction allows the RBA (dashed) and SCQRPA (solid) lines to cross the horizontal axis of zero energy, it still cannot remedy to the fact that SCQRPA, contrary to expectation, gives the least satisfactory agreement with the exact solution. One reason for this failure may be the breaking of consistency on the SCQRPA level by Eqs. (19) and (20). Work to improve on this is in progress. Another possibility is that it may turn out that exact particle number projection is necessary to remove any residual particle number fluctuation in the subtle balance between even-even and odd-odd ground-state energies.

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