Fully-Renormalized QRPA fulfills Ikeda sum rule exactly

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Abstract

The renormalized quasiparticle-RPA is reformulated for even-even nuclei using restrictions imposed by the commutativity of the phonon creation operator with the total particle number operator. This new version, Fully-Renormalized QRPA (FR-QRPA), is free from the spurious low-energy solutions. Analytical proof is given that the Ikeda sum rule is fulfilled within the FR-QRPA.

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The well-known Random Phase Approximation (RPA) has found many applications in different fields of physics, from chemistry and condensed matter to relativistic field theory. In nuclear physics RPA has been extensively exploited to model properties of the excited nuclear states that allows to calculate intensities of various nuclear reactions, including the double beta decay (see reviews).

The neutrinoless double beta decay (0νββ-decay), which violates the total lepton number by two units, is a sensitive low-energy probe for new physics beyond the Standard Model. The observation of the 0νββ-decay would give unambiguous evidence that at least one of the neutrinos is a Majorana particle with non-zero mass. The current experimental upper limits on the 0νββ-decay half-life impose stringent constraints, e.g., on the parameters of Grand Unification and supersymmetric extensions of the Standard Model.

It is important that the same nuclear structure methods can be applied to calculate intensities of 2νββ-decay, which is a second order process allowed within the Standard Model. In this case the quality of the RPA calculations can be directly checked by comparison with the corresponding experimental data available at the moment for a number of nuclei. Most of the nuclei are open-shell ones and one uses the quasiparticle version of RPA (QRPA) which takes into account nucleon pairing correlations.

The QRPA is able to reproduce the experimental data, but with the strength of a particle-particle interaction which is very close to the point where QRPA collapses. This well-known drawback of the RPA is due to overestimation of ground state correlations when one uses the quasiboson approximation (QBA) for the bifermionic operators and the Pauli exclusion principle (PEP) is violated. The proximity to the collapse makes the entire QRPA scheme unstable and calculation results unreliable. To cure this problem, the so-called renormalized QRPA (RQRPA) was invented, which takes into account PEP in an approximate way. Namely, the expectation values of the quasiparticle number operators are consistently treated to be non-vanishing in the RQRPA vacuum. The RQRPA does not collapse for physical values of the particle-particle interaction strength. It has been shown within schematic models that by including PEP in the QRPA good agreement with the exact solution of the many-body problem can be achieved even beyond the critical point of the standard QRPA (see, e.g. and references therein). The RQRPA has been used in previous studies of the double beta decay.

Nevertheless, it has been shown within the modern versions of RQRPA that the model-independent Ikeda sum rule (ISR) is violated. The Ikeda sum rule states that the difference between the total Gamow-Teller strengths in the β− and β+ channels is 3(N − Z). This drawback of the model is quite serious, because the derivation of the ISR is based just upon two principles: closure relation and average conservation of the particle number. Violation of the ISR immediately means violation of one (or both) of these important principles. The drawback has not been cured neither in the self-consistent QRPA nor in second-QRPA. The restoration of the ISR claimed in the Ref. actually works only for a special one-level model and can not be generalized for the realistic case as shown in Ref. At the moment, the second-QRPA is able to reduce the violation of the ISR to the level of few percents only when contributions from the three (and more) boson states are neglected in the boson expansion of the bifermionic operators.

It can be conjectured that the closure relation is not fulfilled within the standard formulation of the RQRPA. The vacuum of the RQRPA contains quasiparticles. The RQRPA
takes into account the fact that the quasiparticles block creation of the bifermionic QRPA bosons but does not consider the possibility, that the quasiparticles in the ground state take part in the transitions. This leads to violation of the unitarity and underestimates the ISR which should be fulfilled exactly.

In view of these remarks, modification of the phonon operator in order to include so-called scattering terms (describing transitions of the quasiparticles) is unavoidable if one wants to restore the ISR within RQRPA. This has been understood for some time and attempts have been undertaken to treat the terms as additional independent constituents of the phonon operator \[17\], in spirit of the thermal extensions of RPA \[18\] for description of the particle-hole excitations in heated nuclei. That leads to increasing of the dimension of the QRPA equation system and the appearance of low-lying energy roots originating from the transitions of the quasiparticles. Although such a consideration has allowed to restore the ISR for finite temperatures \[19\], the low-lying spectrum has no physical interpretation when the even-even nuclei are considered. For instance, the model would predict a number of \(2^+\) excitations below the first quadrupole state, that have never been observed in experiments (see also the discussion in Ref. \[20\]). Authors of a recent paper \[20\] have succeeded in removing these spurious states by introducing new quasiparticles but they have again used the QBA in terms of the new quasiparticles and formulated the QRPA with respect to the HFB vacuum.

The above-mentioned examples show that a correct formulation of the RQRPA is quite a delicate task. The goal of this Letter is to introduce a version of the RQRPA for even-even nuclei which is able to overcome mentioned difficulties, i.e. it fulfills the ISR and at the same time is free from the spurious solutions.

Let us start from the general basis of the RPA, which assumes that an excited state of the nucleus in question, with the angular momentum \(J\) and the projection \(M\), is created by applying the phonon-operator \(Q^\dagger_{JM}\) to the vacuum state \(|0^+_{RPA}\rangle\) of the initial, even-even, nucleus with the same nucleon number \(A\):

\[
|JM\rangle = Q^\dagger_{JM}|0^+_{RPA}\rangle \quad \text{with} \quad Q_{JM}|0^+_{RPA}\rangle = 0. \quad (1)
\]

At this point one usually introduces the following ansatz for the phonon-operator \(Q^\dagger_{JM}\):

\[
Q^\dagger_{JM} = \sum_{\tau \tau'} \left[ X_{(\tau \tau', J)} A^\dagger(\tau \tau', JM) - Y_{(\tau \tau', J)} \tilde{A}(\tau \tau', JM) \right]. \quad (2)
\]

where \(X_{(\tau \tau', J)}, Y_{(\tau \tau', J)}\) denotes free variational amplitudes, which are calculated by solving the RQRPA equations; \(A^\dagger(\tau \tau', JM)\) and \(A(\tau \tau', JM)\) (\(\tau\) and \(\tau'\) denote single-particle quantum numbers including isospin projection) are the two quasi-particle creation and annihilation operators:

\[
A^\dagger(\tau \tau', JM) = \begin{bmatrix} a^\dagger_\tau \alpha^\dagger_{\tau'} \end{bmatrix}_{JM} \equiv \sum_{m_r, m'_r} C^J_{m_r m'_r j, j, m_r} a^\dagger_{\tau m_r} a^\dagger_{\tau' m'_r}. \quad (3)
\]

The quasiparticle creation and annihilation operators \(a^\dagger_{\tau m_r}\) and \(a_{\tau m_r}\) are defined by the Bogoliubov transformation

\[
\begin{pmatrix}
a^\dagger_{\tau m_r} \\
a_{\tau m_r}
\end{pmatrix} = \begin{pmatrix} u_\tau & v_\tau \\ -v_\tau & u_\tau \end{pmatrix} \begin{pmatrix} c^\dagger_{\tau m_r} \\
\tilde{c}_{\tau m_r}
\end{pmatrix}, \quad (4)
\]

\(3\)
where \( c_{\tau m}^+ \) (\( c_{\tau m} \)) denotes the particle creation (annihilation) operator. The tilde symbol indicates the time-reversal operation, e.g. \( \tilde{a}_{\tau m} = (-1)^{j_\tau - m_\tau} a_{\tau - m_\tau} \).

However it turns out, that the most appropriate way is to analyze the phonon structure in terms of the particle creation and annihilation operators (instead of the quasiparticle ones). Let us first mention two quite general conditions which should be kept in mind while constructing the phonon operator. Namely, because the phonon operator is assumed to create a nuclear state of \( A \) nucleons acting on the \( 0^+ \) ground state of the initial nucleus (also of \( A \) nucleons), the operator has to

1) have good angular momentum \( J \) and the projection \( M \) (it has been taken into account in Eqs. (2),(3));

2) commute with the total particle number operator \( \hat{A} = \hat{N} + \hat{Z} = \sum \tau_m c_{\tau m}^+ c_{\tau m} \). Neutral excitations can be further distinguished from the charge-exchange ones using their commutativity with \( \hat{N} - \hat{Z} \).

The first rule tells us that the simplest building blocks for the phonon operator are \( \left[ c_{\tau}^+ \bar{c}_{\tau'} \right]_{JM}, \left[ c_{\tau}^+ c_{\tau'} \right]_{JM} \) together with their hermitian conjugates. Applying the second rule leads to a further restriction of the phonon operator structure:

\[
Q_{JM}^\dagger = \sum_{\tau' \tau} \left[ x_{(\tau' \tau, J)} C^\dagger(\tau \tau', JM) - y_{(\tau' \tau, J)} \tilde{C}(\tau \tau', JM) \right].
\] (5)

with \( C^\dagger(\tau \tau', JM) = \left[ c_{\tau}^+ \bar{c}_{\tau'} \right]_{JM} \) and \( \tilde{C}(\tau \tau', JM) = (-)^{J-M} C(\tau \tau', J - M) \). For the neutral excitations \( \tau \) and \( \tau' \) have the same isospin projections, whereas for the charge-exchange ones - opposite. Therefore, in terms of the original particle creation and annihilation operators \( Q \) consists of scattering terms only. Going now into the quasiparticle representation, one gets:

\[
C^\dagger(\tau \tau', JM) = u_{\tau} v_{\tau} A^\dagger(\tau \tau', JM) + u_{\tau} v_{\tau} A(\tau \tau', JM) + u_{\tau} v_{\tau} B^\dagger(\tau \tau', JM) - v_{\tau} v_{\tau} \tilde{B}(\tau \tau', JM) = u_{\tau} v_{\tau} A^\dagger(\tau \tau', JM) + v_{\tau} u_{\tau} \tilde{A}(\tau \tau', JM).
\] (6)

with the following definitions: \( B^\dagger(\tau \tau', JM) = \left[ a_{\tau}^+ \bar{a}_{\tau'} \right]_{JM} \) for the quasiparticle scattering term and \( A^\dagger = A^\dagger + (u_{\tau} v_{\tau} B^\dagger - u_{\tau} v_{\tau} \tilde{B})/(v_{\tau}^2 - v_{\tau'}^2) \) for the bifermionic operator \( \tilde{A}^\dagger \).

Now we are able to rewrite (4) in the form which is similar to (2):

\[
Q_{JM}^\dagger = \sum_{\tau' \tau} \left[ X_{(\tau' \tau, J)} \tilde{A}^\dagger(\tau \tau', JM) - Y_{(\tau' \tau, J)} \tilde{A}(\tau \tau', JM) \right],
\] (7)

where \( X = u_{\tau} v_{\tau} x - v_{\tau} u_{\tau} y \), \( Y = u_{\tau} v_{\tau} y - v_{\tau} u_{\tau} x \). Thus, instead of \( A^\dagger, A \), bifermionic operators \( \tilde{A}^\dagger, \tilde{A} \) are now the basic terms in which the RQRPA should be formulated. The key point is that the latter automatically contain the quasiparticle scattering terms which, however, are not associated with any additional degrees of freedom. That means that there are no spurious low-lying solutions in the present theoretical scheme.

From this point we can follow the usual way to formulate the RQRPA [3] substituting everywhere \( A \) by \( \tilde{A} \). The forward- and backward- going free variational amplitudes \( X \) and \( Y \) satisfy the equation:
\[
\begin{pmatrix}
A & B \\
B & A
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}
= \mathcal{E}_{\text{QRPA}}
\begin{pmatrix}
U & 0 \\
0 & -U
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix},
\]
where
\[
\begin{align*}
A &= \langle 0^+_\text{RPA} | [\hat{A}, [H_F, \hat{A}^\dagger]] | 0^+_\text{RPA} \rangle, \\
B &= -\langle 0^+_\text{RPA} | [\hat{A}, [H_F, \hat{A}]] | 0^+_\text{RPA} \rangle,
\end{align*}
\]
\(H_F\) is the nuclear Hamiltonian and the renormalization matrix \(U_{\tau\tau'}\) is
\[
U_{\tau\tau'} = \langle 0^+_\text{RPA} | \left[\hat{A}(\tau', JM), \hat{A}^\dagger(\sigma', J'M)\right] | 0^+_\text{RPA} \rangle = \delta_{\tau\sigma}\delta_{\tau\sigma'}D_{\tau\tau'},
\]
\[
D_{\tau\tau'} = 1 + \left((u_{\tau\sigma}^2 - v_{\tau\sigma}^2)N_{\tau}\gamma - (u_{v\tau\sigma}^2 - v_{v\tau\sigma}^2)N_{\tau}\gamma\right)/\left(v_{\tau\sigma}^2 - v_{\tau\sigma}^2\right)
\]
Here, the exact (fermionic) expressions of the commutators are taken into account and
\[
N_{\tau} = \hat{j}_{\tau}^{-2}\langle 0^+_\text{RPA} | \sum_{m\sigma} a_{\tau m\sigma}^\dagger a_{\tau m\sigma} | 0^+_\text{RPA} \rangle = -\hat{j}_{\tau}^{-1}\langle 0^+_\text{RPA} | B(\tau, 00) | 0^+_\text{RPA} \rangle
\]
gives the relative quasiparticle occupation number for the level \(\tau\) in the RQRPA vacuum (\(\hat{j} \equiv \sqrt{2j + 1}\)). The method to calculate these occupation numbers can be found elsewhere [9]. It is useful to introduce the notation:
\[
\bar{X} = U^{1/2}X, \quad \bar{Y} = U^{1/2}Y,
\]
\[
\bar{A} = U^{-1/2}AU^{-1/2}, \quad \bar{B} = U^{-1/2}BU^{-1/2}.
\]
Then the amplitudes \(\bar{X}\) and \(\bar{Y}\) satisfy the equation of usual QRPA:
\[
\begin{pmatrix}
\bar{A} & \bar{B} \\
\bar{B} & \bar{A}
\end{pmatrix}
\begin{pmatrix}
\bar{X} \\
\bar{Y}
\end{pmatrix}
= \mathcal{E}_{\text{QRPA}}
\begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\begin{pmatrix}
\bar{X} \\
\bar{Y}
\end{pmatrix},
\]
Solving the FR-QRPA equations, one gets the fully renormalized amplitudes \(\bar{X}, \bar{Y}\) with the usual normalization and closure relation, which will be used below to prove the fulfillment of the ISR:
\[
\sum_{\tau\tau'} \bar{X}_{(\tau\tau', J)}^m \bar{Y}_{(\tau\tau', J)}^k - \delta_{km} = 0,
\]
\[
\sum_m \bar{X}_{(\tau\tau', J)}^m \bar{Y}_{(\tau\tau', J)}^m - \delta_{\tau\tau_1} = 0,
\]
\[
\sum_m \bar{X}_{(\tau\tau', J)}^m \bar{Y}_{(\tau\tau', J)}^m = 0.
\]
Here, \(m\) and \(k\) mark different roots of the QRPA equations for a given \(J^z\).

Now we are ready to prove the fulfillment of the ISR within the FR-QRPA. Let restrict ourselves to the charge-exchange pn-FR-QRPA and write down the definition for the ISR:
\[
\text{ISR} = \sum_m \langle JM, m | \beta_{JM}^2 | 0^+_\text{RPA} \rangle^2 - \sum_{m'} \langle J - M, m' | \beta_{JM} | 0^+_\text{RPA} \rangle^2.
\]
Here, we would like to consider the Fermi and Gamow-Teller transitions simultaneously by defining:

$$\beta_{JM}^\dagger = \sum_{pm,mp,mn} \langle pm || q_{JM} || nm \rangle c_p^\dagger c_n = -\hat{J}^{-1} \sum_{pm} \langle p || q_J || n \rangle C^\dagger (pn, JM),$$

where $q_{00} = 1$ (Fermi transitions) and $q_{1\mu} = \sigma_\mu$ (Gamow-Teller transitions) and one has for both cases $ISR = N - Z$ (in the latter case - just because of the only fixed angular momentum projection). One can use Eqs. (6), (7) to get:

$$\langle JM, m || \beta_{JM}^\dagger || 0^+_\text{RPA} \rangle = -\hat{J}^{-1} \sum_{pm} \langle p || q_J || n \rangle \left( u_p v_n \hat{X}^m_{(pn, J)} + v_p u_n \hat{Y}^m_{(pn, J)} \right) \sqrt{D_{pn}},$$

$$\langle J - M, m || \beta_{JM} || 0^+_\text{RPA} \rangle = -(J - M)^{J - 1} \sum_{pm} \langle n || q_J || p \rangle \left( u_p v_n \hat{Y}^m_{(pn, J)} + v_p u_n \hat{X}^m_{(pn, J)} \right) \sqrt{D_{pn}}.$$

Substituting (18) into (16) and making use of the closure conditions (15), one ends up with

$$ISR = \hat{J}^{-2} \sum_{pm} \langle p || q_J || n \rangle^2 (v_n^2 - v_p^2) D_{pn}.$$

Within the usual QBA one has $D_{pn} = 1$ and

$$ISR = \hat{J}^{-2} \left( \sum_{np} \langle p || q_J || n \rangle^2 v_n^2 - \sum_{np} \langle p || q_J || n \rangle^2 v_p^2 \right) = N - Z,$$

making use of $\sum_n \langle p || q_J || n \rangle^2 = \hat{J}^2 j_n^2$, $\sum_n \langle p || q_J || n \rangle^2 = \hat{J}^2 j_p^2$ and of the equations for the BCS chemical potentials $\lambda_n, \lambda_p$

$$\langle 0^+_\text{HFB} || \hat{N} || 0^+_\text{HFB} \rangle = \sum_n \hat{j}_n^2 v_n^2 = N, \quad \langle 0^+_\text{HFB} || \hat{Z} || 0^+_\text{HFB} \rangle = \sum_p \hat{j}_p^2 v_p^2 = Z.$$  (21)

This corresponds to the fulfillment of the ISR for the usual QRPA.

In the case of the FR-QRPA with $D_{pn}$ determined by Eq. (10) one has

$$ISR = \sum_n \hat{j}_n^2 \left( v_n^2 + (u_n^2 - v_n^2) N_n \right) - \sum_p \hat{j}_p^2 \left( v_p^2 + (u_p^2 - v_p^2) N_p \right) = N - Z$$

(22)

because of the modified FR-QRPA equations for the chemical potentials:

$$\langle 0^+_\text{RPA} || \hat{N} || 0^+_\text{RPA} \rangle = \sum_n \hat{j}_n^2 \left( v_n^2 + (u_n^2 - v_n^2) N_n \right) = N,$$

$$\langle 0^+_\text{RPA} || \hat{Z} || 0^+_\text{RPA} \rangle = \sum_p \hat{j}_p^2 \left( v_p^2 + (u_p^2 - v_p^2) N_p \right) = Z.$$  (23)

In conclusion, we have reformulated the RQRPA into Fully-Renormalized QRPA (FR-QRPA) for even-even nuclei using restrictions imposed by the commutativity of the phonon creation operator with the total particle number operator. The FR-QRPA is free from the spurious low-energy solutions. We have also shown analytically that the Ikeda sum rule is fulfilled within the FR-QRPA.
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