ELIMINATION OF 0$^+$ SPURIOUS STATES IN THE QUASIPARTICLE TIME BLOCKING APPROXIMATION

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Abstract

The quasiparticle time blocking approximation (QTBA) is considered as a model for the description of excitations in open-shell nuclei. The QTBA is an extension of the quasiparticle random phase approximation that includes quasiparticle-phonon coupling. In the present version of the QTBA, the pairing correlations are included within the framework of the BCS approximation. Thus, in this model, the 0$^+$ spurious states appear, which are caused by the breaking of the symmetry related to the particle-number conservation. In this work, the method is described which solves the problem of the 0$^+$ spurious states in the QTBA with the help of the projection technique. The method is illustrated by calculations of 0$^+$ excitations in $^{120}$Sn nucleus.

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I. INTRODUCTION

Description of nuclear excitations within the models based on the mean-field approach faces the known difficulty of appearing the so-called spurious or ghost states (see, e.g., [1]). The spurious state arises because of the breaking of some symmetry. In particular, the breaking of the translation symmetry leads to the appearance of spurious $1^-$ states. In the fully self-consistent theory, for instance, in the self-consistent random phase approximation (RPA) or in the self-consistent quasiparticle RPA (QRPA), the broken symmetry is restored and the spurious states disappear [1–3]. The self-consistency means here a fulfillment of some constraints imposed on the mean-field operator and the amplitude of the residual interaction. However, it is difficult to achieve the full self-consistency in the models which go beyond the (Q)RPA framework by taking into account additional correlations. So, the problem of the spurious states becomes relevant again, even if it was solved on the (Q)RPA level. In this work, the quasiparticle time blocking approximation (QTBA, see Refs. [4, 5]) is considered. The QTBA is a model intended for the description of excitations in open-shell nuclei. The model is formulated in terms of the Green function method. Within the QTBA, the single-particle continuum, the pairing correlations, and the quasiparticle-phonon coupling (QPC) are included. In this sense, the QTBA is an extension of the QRPA. Note that all three components of the model mentioned above are necessary to describe the fragmentation and the width of the states in open-shell nuclei. In the present version of the QTBA, the pairing correlations are included within the framework of the Bardeen-Cooper-Schrieffer (BCS) approximation. Thus, in this model, the $0^+$ spurious states appear, which are caused by the breaking of the symmetry related to the particle-number conservation. In the QRPA, the $0^+$ spurious state is eliminated by taking into account the so-called dynamical pairing effects (particle-particle channel contributions, see Ref. [6]). However, in the QTBA, this is not sufficient because the spurious state is fragmented due to its coupling to the “two-quasiparticle⊗phonon” (2q⊗phonon) configurations. In this work, the method is described which solves the problem of the $0^+$ spurious states in the QTBA with the help of a combination of the so-called subtraction procedure (see [4, 5]) and the projection technique described below. The scheme proposed is illustrated by the calculations of $0^+$ excitations in $^{120}$Sn nucleus.
II. SYSTEM OF THE QTBA EQUATIONS AND ITS MODIFICATIONS

The basic equation, which has to be solved within the Green function method to calculate the physical observables related to the nuclear excitations, is the equation for the effective (renormalized) response function $R_{\text{eff}}(\omega)$. It has the same form both in the (Q)RPA and in the QTBA. In the symbolic notations it reads (in what follows we will use notations and definitions of Ref. [5]):

$$R_{\text{eff}}(\omega) = A(\omega) - A(\omega) \mathcal{F} R_{\text{eff}}(\omega)$$  \hspace{1cm} (1)

where $A(\omega)$ is a correlated propagator and $\mathcal{F}$ is an amplitude of the effective residual interaction. In the case of the QRPA, $A(\omega)$ reduces to the uncorrelated 2q propagator $\tilde{A}(\omega)$. In the general case including pairing correlations, the amplitude $\mathcal{F}$ can be represented as a sum of two terms

$$\mathcal{F} = \mathcal{F}^{(\text{ph})} + \mathcal{F}^{(\text{pp})}$$  \hspace{1cm} (2)

where the amplitude $\mathcal{F}^{(\text{ph})}$ represents interaction in the particle-hole (ph) channel and $\mathcal{F}^{(\text{pp})}$ includes contributions of the interaction both in the particle-particle (pp) and in the hole-hole (hh) channels (in the following for brevity we will use the unified term pp channel implying also the hh-channel contributions). The response function $R_{\text{eff}}(\omega)$ enables one to calculate the strength function $S(E)$ which determines the distribution of the transition strength caused by an external field $V^0$. These quantities are related by the following formulas:

$$S(E) = -\frac{1}{\pi} \text{Im} \Pi(E + i\Delta),$$  \hspace{1cm} (3)

$$\Pi(\omega) = -\frac{1}{2} \text{Tr} \left( (eV^0)^\dagger R_{\text{eff}}(\omega) (eV^0) \right),$$  \hspace{1cm} (4)

where $\Pi(\omega)$ is the nuclear polarizability, $E$ is an excitation energy, $\Delta$ is a smearing parameter, and $e$ is an effective charge operator.

One of the important questions arising in the QRPA and QTBA calculations is the question of completeness of the configuration space. The size of the basis in this space has an impact practically on all the calculated quantities. In particular, configurations with a particle in the continuum are responsible for the formation of the escape widths of the resonances. The well-known method to include these configurations on the RPA level is the use of the coordinate representation within the Green function formalism (see Ref. [7]). This method is used in the present approach as described in Ref. [5]. However, incorporation of the pp-channel contributions in the coordinate representation leads to considerable numerical difficulties. At the same time, the pp-channel contributions (dynamical pairing effects)
are very important in the calculations of $0^+$ excitations in the open-shell nuclei, primarily because of the problem of the $0^+$ spurious state. For this reason, in Ref. [8] a combined method was developed, which is a modification of the so-called $(r, \lambda)$ representation proposed in Ref. [9] for the QRPA problem. Within this method only the ph channel is treated in the coordinate space; the dynamical pairing effects are included in the discrete basis representation.

Consider the general case of the QTBA. By taking into account the decomposition (2) one can rewrite Eq. (1) in the form

$$R_{\text{eff}}(\omega) = A^{(\text{res+pp})}(\omega) - A^{(\text{res+pp})}(\omega) F^{(\text{ph})} R_{\text{eff}}(\omega)$$

(5)

where propagator $A^{(\text{res+pp})}(\omega)$ is a solution of the equation

$$A^{(\text{res+pp})}(\omega) = A(\omega) - A^{(\omega)} F^{(\text{pp})} A^{(\text{res+pp})}(\omega).$$

(6)

In the present work the version of the QTBA is used in which the ground state correlations caused by the QPC are neglected. In this case the correlated propagator $A(\omega)$ is defined by the equation

$$A(\omega) = \tilde{A}(\omega) - \tilde{A}(\omega) \Phi(\omega) A(\omega)$$

(7)

where $\tilde{A}(\omega)$ is the uncorrelated QRPA propagator,

$$\Phi(\omega) = \Phi^{(\text{res})}(\omega) - \Phi^{(\text{res})}(0),$$

(8)

and $\Phi^{(\text{res})}(\omega)$ is a resonant part of the interaction amplitude responsible for the QPC in the QTBA (see Refs. [4, 5] for details). Combining Eqs. (6) and (7) leads to the new equation for $A^{(\text{res+pp})}(\omega)$:

$$A^{(\text{res+pp})}(\omega) = \tilde{A}(\omega) - \tilde{A}(\omega) [\Phi(\omega) + F^{(\text{pp})}] A^{(\text{res+pp})}(\omega).$$

(9)

As a result we find that the pp-channel contributions can be included by modification of the equation for the correlated propagator, i.e. by replacing Eq. (7) by Eq. (9). The modification is reduced to the additional term $F^{(\text{pp})}$ added to the amplitude $\Phi(\omega)$.

Notice, however, that in practice Eq. (5) for $R_{\text{eff}}(\omega)$ is solved in the coordinate representation (to take into account the single-particle continuum), whereas Eq. (9) is solved in the restricted discrete basis representation. This fact greatly simplifies the problem as compared with the initial Eq. (1) in which both the ph-channel contribution and the pp-channel one are included in the coordinate representation. At the same time, the use of the restricted discrete basis representation for the pp channel is fully consistent with the BCS approximation in which the gap equation is solved in the same restricted basis. In more detail, this modification of the QTBA equations is described in Ref. [8].
III. THE METHOD OF ELIMINATING THE $0^+$ SPURIOUS STATE

The general scheme described above ensures that the energy of the $0^+$ spurious (ghost) state is equal to zero both in the QRPA and in the QTBA. Indeed, it is not difficult to show that Eq. (C1) of Ref. [5] for the transition amplitudes of the spherically symmetric nucleus in the QRPA has a non-zero solution at the energy $\omega_q = 0$ and at the total angular momentum and the parity $J_q^\pi = 0^+$ if the gap equation (A25) is fulfilled. The explicit form of this solution is

$$\rho^{0^+\text{(ghost)}}(12) = C \delta(12) \rho(1) \eta,$$  \hspace{1cm} (10)

where $C$ is an arbitrary constant,

$$\rho(1) = \eta \rho(1), \quad \rho(1) = \sqrt{2j_1 + 1}u(1)v(1), \quad \eta = \pm 1.$$  \hspace{1cm} (11)

Here and in the following it is supposed that the equations of the model are written in the representation of the single-quasiparticle basis functions in the doubled space $\tilde{\psi}_1$ which (according to the notations of Refs. [4, 5]) are labelled by the composite indices $1 = \{[1], m_1\}$ where $[1] = \{(1), \eta_1\}$, $(1) = \{\tau_1, n_1, l_1, j_1\}$, and $\eta_1 = \pm 1$ is the sign of the quasiparticle energy $E_1 = \eta_1 E(1)$. That is, the symbol “$(1)$” stands for the set of the single-particle quantum numbers excepting the projection of the total angular momentum $m_1$, $v^2(1)$ is the occupation probability, and $u(1) = \sqrt{1 - v^2(1)}$.

The existence of the solution (10) means that the response function $R^{\text{eff}}(\omega)$ as a solution of Eq. (5) in the QRPA has a pole at $\omega = 0$. The same is true for the QTBA since at $\omega = 0$ the QTBA equation (5) coincides with the QRPA one owing to the subtraction procedure determined by Eq. (8).

However, there still remains the following problem: in the QTBA the ghost state can be fragmented due to its coupling to the $2q \otimes$phonon configurations, despite the energy of the dominant ghost state is equal to zero. It can lead to the spurious states at low energies distorting respective strength functions. In particular, these fragmented spurious states will produce non-zero response to the particle-number operator which has to be exactly equal to zero in a correct theory (as, for instance, in the QRPA including pp channel that was proved by Migdal, see [6]).

To solve this problem, the following method is proposed. Let us recast Eq. (9) in the form

$$A^{\text{res+pp}}(\omega) = \tilde{A}^{\text{pp}}(\omega) - \tilde{A}^{\text{pp}}(\omega) \Phi(\omega) A^{\text{res+pp}}(\omega),$$  \hspace{1cm} (12)
where propagator \( \tilde{A}^{(pp)}(\omega) \) is a solution of the equation:

\[
\tilde{A}^{(pp)}(\omega) = \tilde{A}(\omega) - \tilde{A}(\omega) \mathcal{F}^{(pp)} \tilde{A}^{(pp)}(\omega),
\]

(13)

Consider the case \( J_q^\pi = 0^+ \) assuming diagonal approximation for the amplitude \( \mathcal{F}^{(pp)} \) (which is consistent with the gap equation in the BCS approximation, see Appendix C of Ref. [8]). In this case one can keep only diagonal parts of the matrix functions in Eq. (13). In the explicit form we have

\[
\tilde{A}^{(pp)}_{(1)\eta, (2)\eta'}(\omega) = \tilde{A}_{(1)\eta, (2)\eta'}(\omega) - \sum_{(3)\eta'', \eta'''} \tilde{A}_{(1)\eta, (3)\eta''}(\omega) \mathcal{F}_{(3)\eta'', (4)\eta'''}^{J=0(pp)} \tilde{A}^{(pp)}_{(4)\eta''', (2)\eta'}(\omega)
\]

(14)

where \( \tilde{A}_{(1)\eta, (2)\eta'}^{(pp)}(\omega) = \tilde{A}_{(11)\eta, (22)\eta'}^{(pp)}(\omega) \),

\[
\tilde{A}_{(1)\eta, (2)\eta'}(\omega) = -\frac{\eta \delta_{\eta, \eta'} \delta_{(12)}}{\omega - 2 \eta E_{(1)}},
\]

(15)

and \( \mathcal{F}_{(11)\eta, (22)\eta'}^{J=0(pp)} \) is defined by Eq. (C8) of Ref. [8].

The matrix function \( \tilde{A}^{(pp)}_{(1)\eta, (2)\eta'}(\omega) \) has two poles at \( \omega = 0 \) (first and second order ones) and can be represented in the form:

\[
\tilde{A}^{(pp)}(\omega) = \frac{a^{(2)}}{\omega^2} + \frac{a^{(1)}}{\omega} + \tilde{A}^{(pp) \text{reg}}(\omega),
\]

(16)

where function \( \tilde{A}^{(pp) \text{reg}}(\omega) \) is regular at \( \omega \to 0 \). From the symmetry properties of the matrix function \( \tilde{A}^{(pp)}_{(1)\eta, (2)\eta'}(\omega) \) it follows that the matrices \( a^{(2)} \) and \( a^{(1)} \) are real, symmetric:

\[
a^{(2)} = a^{(2)*} = a^{(2)T}, \quad a^{(1)} = a^{(1)*} = a^{(1)T},
\]

(17)

and possess properties:

\[
a^{(2)} = \hat{\eta} x a^{(2)} \hat{\eta} x, \quad a^{(1)} = -\hat{\eta} x a^{(1)} \hat{\eta} x,
\]

(18)

where

\[
\hat{\eta}^{(1)}_{(1)\eta, (2)\eta'} = \delta_{\eta, -\eta'} \delta_{(12)}.
\]

(19)

Further, by substituting (16) into Eq. (13) and putting the coefficients at the same powers of \( \omega \) to be equal to each other we obtain the following equations for the matrices \( a^{(2)} \) and \( a^{(1)} \):

\[
a^{(2)} = -\tilde{A}(0) \mathcal{F}^{(pp)} a^{(2)} = -a^{(2)} \mathcal{F}^{(pp)} \tilde{A}(0),
\]

(20)

\[
(1 + \tilde{A}(0) \mathcal{F}^{(pp)}) a^{(1)} = \tilde{A}(0) \hat{\eta} x a^{(2)},
\]

(21)
\[ a^{(2)} + a^{(2)} \hat{\eta}^z a^{(1)} = 0 , \]  

(22)

where

\[ \hat{\eta}^{(2)}_{\eta, (2)\eta'} = \eta \delta_{\eta, \eta'} \delta^{(12)} . \]  

(23)

Eqs. (13) and (16) uniquely determine the matrices \( a^{(2)} \) and \( a^{(1)} \). However, strictly speaking, from this it does not follow that a solution of Eqs. (20)–(22) constrained by the conditions (17) and (18) is unique. Nevertheless, we will find a particular solution of these equations assuming that it is a true answer. Calculations confirm the correctness of this assumption.

As follows from the above analysis (see Eqs. (10) and (11)), the solution of Eqs. (20) can be represented in the form:

\[ a^{(2)}_{(1)\eta, (2)\eta'} = a_0 \rho_{(1)\eta} \rho_{(2)\eta'} , \]  

(24)

where \( a_0 \) is a constant and \( \rho_{(1)\eta} \) is defined by Eqs. (11). In the symbolic notations we have

\[ a^{(2)} = a_0 |\rho\rangle \langle \rho| . \]  

(25)

Let us search for the matrix \( a^{(1)} \) in the form:

\[ a^{(1)} = \frac{a_0}{2} (|\rho\rangle \langle \xi| + |\xi\rangle \langle \rho| ) , \]  

(26)

or in the explicit form:

\[ a^{(1)}_{(1)\eta, (2)\eta'} = \frac{a_0}{2} (\rho_{(1)\eta} \xi_{(2)\eta'} + \xi_{(1)\eta} \rho_{(2)\eta'} ) . \]  

(27)

In addition, in agreement with Eqs. (11), (18), (19), and (27), we will assume that the quantity \( \xi_{(1)\eta} \) does not depend on \( \eta \), i. e.:

\[ \xi_{(1)\eta} = \xi_{(1)} . \]  

(28)

By substituting (25) and (26) into Eq. (21) we obtain:

\[ \xi_{(1)} = \sum_{(2)} (\Omega^{-1})_{(12)} \rho_{(2)} , \]  

(29)

where

\[ \Omega_{(12)} = \delta_{(12)} + \frac{\sqrt{(2j_1 + 1)(2j_2 + 1)}}{8\pi} (u^2_{(1)} - v^2_{(1)}) (u^2_{(2)} - v^2_{(2)}) \mathcal{F}^{\xi}_{(11,22)} . \]  

(30)

Here

\[ \mathcal{F}^{\xi}_{(12,34)} = \delta_{\tau_1, \tau_2} \delta_{\tau_3, \tau_4} \int_0^\infty dr r^2 R_{(1)}(r) R_{(2)}(r) R_{(3)}(r) R_{(4)}(r) \mathcal{F}^{\xi}(r) , \]  

(31)
$R_{(1)}(r)$ is the radial part of the single-particle wave function, the quantity $F_\xi(r)$ determines the effective residual interaction in the pp channel (see [5, 8]).

Substitution of Eqs. (25) and (26) into Eq. (22) yields:

$$a_0^{-1} = -\sum_{(1)} \rho_{(1)} \xi_{(1)}.$$  

(32)

Thus, the matrices $a^{(2)}$ and $a^{(1)}$ are completely determined.

Let us introduce the following matrices:

$$P = 1 + a^{(1)} \hat{\eta}^z, \quad P^\dagger = 1 + \hat{\eta}^z a^{(1)}.$$  

(33)

In the explicit form we have:

$$P_{(1)\eta, (2)\eta'} = \delta_{\eta, \eta'} \delta_{(12)} + \frac{a_0}{2} \left( \eta \rho_{(1)} \xi_{(2)} \eta' + \xi_{(1)} \rho_{(2)} \right),$$  

(34)

$$P^\dagger_{(1)\eta, (2)\eta'} = \delta_{\eta, \eta'} \delta_{(12)} + \frac{a_0}{2} \left( \rho_{(1)} \xi_{(2)} + \eta \xi_{(1)} \rho_{(2)} \right).$$  

(35)

In the general case of non-diagonal matrices these formulas acquire the form:

$$P_{(12)\eta, (34)\eta'} = \delta_{\eta, \eta'} \delta_{(13)} \delta_{(24)} + \delta_{(12)} \delta_{(34)} a^{(1)}_{(1)\eta, (3)\eta'} \eta'$$  

(36)

$$P^\dagger_{(12)\eta, (34)\eta'} = \delta_{\eta, \eta'} \delta_{(13)} \delta_{(24)} + \delta_{(12)} \delta_{(34)} \eta a^{(1)}_{(1)\eta, (3)\eta'}.$$  

(37)

It is easy to show that the following equalities are fulfilled:

$$PP = P, \quad P^\dagger P^\dagger = P^\dagger.$$  

(38)

Consequently, $P$ and $P^\dagger$ are the projection operators. In addition, we have:

$$P a^{(1,2)} = 0 = a^{(1,2)} P^\dagger.$$  

(39)

Eqs. (16) and (39) mean that one can use the operators $P$ and $P^\dagger$ to eliminate the coupling of complex (2q⊗phonon) configurations to the ghost state. From the above analysis it follows that the elimination can be achieved with the help of the replacement of the amplitude $\tilde{\Phi}(\omega)$ in formula (9) by the projected amplitude $\tilde{\Phi}^{\text{proj}}(\omega)$ defined as

$$\tilde{\Phi}^{\text{proj}}(\omega) = P^\dagger \tilde{\Phi}(\omega) P.$$  

(40)

In what follows this method will be referred to as the QTBA with $0^+$ projection.
IV. CALCULATIONS OF THE $0^+$ EXCITATIONS IN THE $^{120}$Sn NUCLEUS

As an illustration of the method described above consider results of calculations of the $0^+$ excitations in the semi-magic nucleus $^{120}$Sn. Calculational scheme is described in detail in Ref. [8]. It is based on the Hartree-Fock and BCS approximations and is fully self-consistent on the RPA level. The self-consistent mean field and the effective residual interaction (including the spin-orbital and the Coulomb contributions in both quantities) were derived from the Skyrme energy functional. In the present calculations, the T5 Skyrme force parametrization [10] was used. The single-particle continuum was included completely on the RPA level. The set of the phonons entering $2q\otimes$phonon configurations in the QTBA calculations included 29 collective modes with values of the spin $L$ in the interval $2 \leq L \leq 9$ and with natural parity $\pi = (-1)^L$. The smearing parameter $\Delta$ in Eq. (3) is equal to 200 keV in all the calculations.

![Graph](image)

**FIG. 1:** Strength function of the isoscalar giant monopole resonance in $^{120}$Sn calculated within the QRPA with (solid line) and without (dashed line) contributions of the pp channel.
According to this scheme, the following sorts of calculations were performed: (i) the QRPA and the QTBA calculations with and without taking into account contributions of the pp channel (they will be referred to as pp+ and pp− calculations, respectively); (ii) the QTBA calculations with and without 0+ projection (they will be referred to as proj+ and proj− calculations, respectively). In Figs. 1 and 2, the results of calculations of the isoscalar giant monopole resonance are shown. In Fig. 1, the results obtained within the QRPA (pp+) and the QRPA (pp−) are presented. Spurious 0+ excitations arise at low energies in the response calculated without contributions of the pp channel. These spurious excitations disappear when the pp-channel contributions are included. The same picture is obtained in the QTBA calculations. However, to eliminate spurious excitations in the QTBA it is insufficient to include the pp channel. Only the QTBA (pp+, proj+) that includes pp-channel contributions together with 0+ projection gives the 0+ response free

FIG. 2: Strength function of the isoscalar giant monopole resonance in $^{120}\text{Sn}$ calculated within the QTBA including contributions of the pp channel. The results with and without 0+ projection are represented by the solid line and the dashed line, respectively.
from the spurious states. In the calculations within QTBA (pp+, proj−) the fragmented ghost states remain in the low-energy region, though their strength is strongly suppressed as compared with calculations in which the pp-channel contributions are not included (see Fig. 2).

In Fig. 3, the 0+ response to the particle-number operator in $^{120}$Sn is shown. These results demonstrate that the QRPA (pp−) and the QTBA (pp+, proj−) produce non-zero response. In the calculations within the QRPA (pp+) and the QTBA (pp+, proj+) this response disappears within calculational accuracy as it should be.

FIG. 3: Strength function of the spurious excitations in $^{120}$Sn caused by the particle-number operator. The solid line represents calculation within the QTBA including contributions of the pp channel, but without 0+ projection. The dashed line represents calculation within the QRPA without contributions of the pp channel.
V. CONCLUSIONS

In this work, the projection method is formulated which solves the problem of the $0^+$ spurious states in the model intended for the description of excitations in open-shell nuclei with taking into account the single-particle continuum, the pairing correlations, and the quasiparticle-phonon coupling. The efficiency of the method is illustrated by the calculations of the $0^+$ excitations in the $^{120}$Sn nucleus within the self-consistent scheme based on the Skyrme-Hartree-Fock approximation.

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