

**Subtraction method and stability condition in extended random-phase approximation theories**

V. I. Tselyaev

*Nuclear Physics Department, V. A. Fock Institute of Physics, St. Petersburg State University, RU-198504 St. Petersburg, Russia*

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The extended random-phase approximation (RPA) theories are analyzed from the point of view of the problem of the stability of their solutions. Three kinds of such theories are considered: the second RPA and two versions of the quasiparticle-phonon coupling model within the time-blocking approximation: the model including  $1p1h$ ⊗phonon configurations and the two-phonon model. It is shown that stability is ensured by making use of the subtraction method proposed previously to solve the double counting problem in these theories. This enables one to generalize the famous Thouless theorem proved in the case of the RPA. These results are illustrated by an example of the schematic model.

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**I. INTRODUCTION**

One of the trends in modern nuclear structure theory is the calculations in a large model configuration space. On the one hand, this trend is caused by the requirement of the internal consistency of the theory. On the other hand, such calculations allow us in some cases to describe the nuclear structure effects which cannot be reproduced within the framework of the more simple models. However, the use of the large configuration space leads to problems of convergence and stability of the solutions obtained. It should be noted that, though the problems of convergence and stability are close to each other, they do not coincide. The convergence is understood in the usual mathematical sense, while stability, as applied to the description of the excited states, implies that all the calculated excitation energies should be real and positive.

The most widely used models, in which these problems can be resolved (or do not arise at all), are the Hartree-Fock (HF) approximation aimed at the description of the ground states and the random-phase approximation (RPA) within which the characteristics of the excited states can be calculated (see [1]). Usually, these models are referred to as the mean-field theories. In particular, the problem of stability is resolved in the HF based self-consistent RPA as was shown by Thouless in Refs. [2,3]. But these problems become actual and so far remain open in the models going beyond these approximations. The reasons for developing and using such extended models are well known (see, e.g., Ref. [4]). First of all, they are related to the fact that within the HF approximation and within the RPA one cannot describe the effects of the fragmentation of the nuclear states leading to the formation of the so-called spreading widths of the resonances.

There is a series of models within which these effects are included. One of them is the second RPA (SRPA, see [4–7]). The problems mentioned above arise in this model due to enlarging the configuration space which includes two-particles–two-holes ( $2p2h$ ) states in addition to the one-particle–one-hole ( $1p1h$ ) states incorporated in the RPA. In Refs. [8–11] it was obtained that calculations of giant resonances in  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ ,  $^{48}\text{Ca}$ , and  $^{90}\text{Zr}$  within the SRPA lead to very large (up to 10 MeV and more so) downward shifts of their centroids relative to the RPA values if the

size of the configuration space is sufficiently large. It was also found that some low-lying states in the SRPA become unstable, so the question arises as to whether the SRPA is applicable in the low-energy region (see [9]). In Refs. [12,13] the problem of the ultraviolet divergence appearing at the second order beyond the HF approximation was analyzed in the case of nuclear matter.

In the present paper we will consider in detail the problem of stability in the extended RPA (ERPA) theories. The problem of convergence will be only briefly touched upon. Note that the term ERPA is sometimes used with regard to the models taking into account the ground state correlations beyond the RPA (see, e.g., Refs. [14–16]). These effects are not analyzed here in detail, however they will be briefly discussed in Sec. VIII. The following models will be considered: the SRPA and two versions of the quasiparticle-phonon coupling model formulated within the Green function method on the basis of the time-blocking approximation (TBA): the model including  $1p1h$ ⊗phonon configurations [17–19] and the two-phonon model [20]. It will be shown that stability can be ensured by making use of the subtraction method [20]. This method was applied in the calculations of giant resonances within the quasiparticle TBA (QTBA) in [21–23] and within its relativistic generalization in [24–26] to eliminate double counting in these models. However, it was not analyzed previously in the context of the stability issue.

The paper is organized as follows. In Sec. II the problem of stability and the content of the Thouless theorem in the RPA framework are considered. In Sec. III the response function formalism is outlined within which the stability problem is revealed in more detail. The ERPA theories mentioned above are briefly described in Sec. IV. In Secs. V and VI the subtraction method and the stability condition in the ERPA are considered. The general results obtained in the previous sections are analyzed within the framework of the schematic model in Sec. VII. The conclusions are given in Sec. VIII.

**II. THOULESS THEOREM**

The Thouless theorem [2,3] determines the stability condition in the case of the self-consistent RPA. Let us briefly

recall the structure of the RPA equations and the content of this theorem because its generalization to the case of the ERPA theories can be carried out (see Sec. VI) using a simple analogy.

To build the RPA equations one needs the single-particle density matrix  $\rho_{12}$ , the single-particle Hamiltonian  $h_{12}$ , and the amplitude of the residual interaction  $V_{12,34}$ . Here and in the following the numerical indices (1, 2, 3, ...) stand for the sets of the quantum numbers of some single-particle basis. It is supposed that the following equalities are fulfilled:

$$\rho^2 = \rho, \quad [h, \rho] = 0. \quad (1)$$

Let us introduce the single-particle basis that diagonalizes operators  $h$  and  $\rho$ :

$$h_{12} = \varepsilon_1 \delta_{12}, \quad \rho_{12} = n_1 \delta_{12}, \quad (2)$$

where  $n_1$  is the occupation number. In what follows the indices  $p$  and  $h$  will be used to label the single-particle states of the particles ( $n_p = 0$ ) and holes ( $n_h = 1$ ) in this basis. The matrix

$$M_{12,34}^{\text{RPA}} = \delta_{13} \rho_{42} - \rho_{13} \delta_{42} \quad (3)$$

is the metric matrix in the RPA. The range of  $M^{\text{RPA}}$  forms the  $1p1h$  configuration space. The vectors  $z_{12}$  in this space have the components of  $z_{ph}$  and  $z_{hp}$  types. The RPA matrix  $\Omega_{12,34}^{\text{RPA}}$  acts in the  $1p1h$  space. In the general case it has the form

$$\Omega_{12,34}^{\text{RPA}} = h_{13} \delta_{42} - \delta_{13} h_{42} + \sum_{56} M_{12,56}^{\text{RPA}} V_{56,34}. \quad (4)$$

The RPA eigenvalue equation reads

$$\sum_{34} \Omega_{12,34}^{\text{RPA}} z_{34}^n = \omega_n z_{12}^n, \quad (5)$$

where  $\omega_n$  is the excitation energy,  $z_{12}^n$  is the transition amplitude. In the case of the self-consistent RPA, based on the energy density functional  $E[\rho]$ , the quantities  $h$  and  $V$  in Eq. (4) are linked by the equations

$$h_{12} = \frac{\delta E[\rho]}{\delta \rho_{21}}, \quad V_{12,34} = \frac{\delta^2 E[\rho]}{\delta \rho_{21} \delta \rho_{34}}. \quad (6)$$

Equation (1) plays the role of the equations of motion.

The Thouless theorem can be formulated in terms of the following general statement (see, e.g., Ref. [1]). Let a matrix  $A$  be representable in the form  $A = BC$  where the matrices  $B$  and  $C$  are Hermitian and  $C$  is positive semidefinite (i.e.,  $\langle z|C|z \rangle \geq 0$  for any complex vector  $|z \rangle$ ). Then all the eigenvalues of the matrix  $A$  are real. Indeed, consider the eigenvalue equation

$$A|x \rangle = a|x \rangle. \quad (7)$$

From the positive semidefiniteness of the Hermitian matrix  $C$  it follows that there exists Hermitian matrix  $C^{1/2}$  such that  $C = (C^{1/2})^2$ . Let us denote  $|y \rangle = C^{1/2}|x \rangle$ . If  $|y \rangle = 0$  then  $a = 0$ . If  $|y \rangle \neq 0$  then, by multiplying Eq. (7) with  $C^{1/2}$ , we obtain  $D|y \rangle = a|y \rangle$ , where  $D = C^{1/2} B C^{1/2}$ . The matrix  $D$  is Hermitian, consequently, the eigenvalue  $a$  is real.

Coming back to Eq. (5), let us define the RPA stability matrix

$$\mathfrak{G}^{\text{RPA}} = M^{\text{RPA}} \Omega^{\text{RPA}}. \quad (8)$$

Since  $(M^{\text{RPA}})^2 = 1$  in the  $1p1h$  space, Eq. (8) is equivalent to the equation

$$\Omega^{\text{RPA}} = M^{\text{RPA}} \mathfrak{G}^{\text{RPA}}. \quad (9)$$

Now we note that both the matrix  $M^{\text{RPA}}$  and the matrix  $\mathfrak{G}^{\text{RPA}}$  in Eq. (9) are Hermitian. Therefore, all eigenvalues  $\omega_n$  in Eq. (5) are real if the stability matrix  $\mathfrak{G}^{\text{RPA}}$  is positive semidefinite. This is the statement of the Thouless theorem. The positive semidefiniteness of the matrix  $\mathfrak{G}^{\text{RPA}}$  follows from the conditions of minimization of the energy density functional  $E[\rho]$  in the self-consistent theory (see [1,2]). Note that the matrix  $\mathfrak{G}^{\text{RPA}}$  is not positive definite because of the symmetry properties of  $E[\rho]$ .

Reality of the eigenvalues in Eq. (5) leads to the following symmetry property of the solutions of this equation. Let us introduce the permutation operator acting in the space of the pairs of the single-particle indices:  $\mathfrak{P}_{12,34} = \delta_{14} \delta_{23}$ . From the definitions (3), (4), and (6) it follows that  $\Omega^{\text{RPA}} = -\mathfrak{P} \Omega^{\text{RPA}*} \mathfrak{P}$ . This equality together with Eq. (5) and reality of  $\omega_n$  brings us to the equation

$$|z^{-n} \rangle = \mathfrak{P} |z^n \rangle^*, \quad (10)$$

where the eigenvectors  $|z^n \rangle$  and  $|z^{-n} \rangle$  correspond to the eigenvalues  $\omega_n$  and  $-\omega_n$ , respectively.

### III. RESPONSE FUNCTION FORMALISM

The other important consequences of the positive semidefiniteness of the stability matrix which will be used in the following in the context of the ERPA theories concern the properties of the response function  $R(\omega)$  defined in the RPA by the equation

$$R^{\text{RPA}}(\omega) = -(\omega - \Omega^{\text{RPA}})^{-1} M^{\text{RPA}}. \quad (11)$$

An overall sign in this formula is chosen in accordance with the usual definition of the response function in the Green function method (see Ref. [27]). The response function formalism is a conventional tool for the description of nuclear excitations. In the general case the distribution of the strength of transitions in the nucleus caused by some external field represented by the single-particle operator  $Q$  is determined by the (dynamic) polarizability  $\Pi(\omega)$  which is defined in terms of the response function as

$$\Pi(\omega) = -\langle Q | R(\omega) | Q \rangle. \quad (12)$$

The poles and residua of the function  $\Pi(\omega)$  coincide with the excitation energies and the transition probabilities [see Eq. (30) below].

Let us introduce an auxiliary matrix

$$\tilde{\mathfrak{G}}^{\text{RPA}} = \mathfrak{G}^{\text{RPA}} + \delta, \quad (13)$$

where  $\delta$  is a real positive number. If  $\mathfrak{G}^{\text{RPA}}$  is positive semidefinite, then the matrix  $\tilde{\mathfrak{G}}^{\text{RPA}}$  is positive definite and consequently there exists invertible Hermitian matrix  $\tilde{\mathfrak{G}}^{1/2}$  such that  $\tilde{\mathfrak{G}}^{\text{RPA}} = (\tilde{\mathfrak{G}}^{1/2})^2$ . Let us denote  $\tilde{\Omega}^{\text{RPA}} = M^{\text{RPA}} \tilde{\mathfrak{G}}^{\text{RPA}}$ ,

$$\tilde{R}^{\text{RPA}}(\omega) = -(\omega - \tilde{\Omega}^{\text{RPA}})^{-1} M^{\text{RPA}}. \quad (14)$$

Using the invertibility of the matrix  $\tilde{\mathfrak{S}}^{1/2}$  we obtain

$$\tilde{R}^{\text{RPA}}(\omega) = -(\tilde{\mathfrak{S}}^{1/2})^{-1}(\omega - \tilde{H}^{\text{RPA}})^{-1}\tilde{H}^{\text{RPA}}(\tilde{\mathfrak{S}}^{1/2})^{-1}, \quad (15)$$

where  $\tilde{H}^{\text{RPA}} = \tilde{\mathfrak{S}}^{1/2}M^{\text{RPA}}\tilde{\mathfrak{S}}^{1/2}$ . The matrices  $\tilde{\mathfrak{Q}}^{\text{RPA}}$  and  $\tilde{H}^{\text{RPA}}$  have the same set of the (nonzero) eigenvalues  $\{\tilde{\omega}_n\}$ . But, in contrast to  $\tilde{\mathfrak{Q}}^{\text{RPA}}$ , the matrix  $\tilde{H}^{\text{RPA}}$  is Hermitian.

Let  $\{|\tilde{y}^n\rangle\}$  be a complete set of the orthonormalized eigenvectors of the matrix  $\tilde{H}^{\text{RPA}}$ . Insertion of the sum  $\sum_n |\tilde{y}^n\rangle\langle\tilde{y}^n| = 1$  into Eq. (15) yields

$$\tilde{R}^{\text{RPA}}(\omega) = -\sum_n \frac{\text{sgn}(\tilde{\omega}_n)|\tilde{z}^n\rangle\langle\tilde{z}^n|}{\omega - \tilde{\omega}_n}, \quad (16)$$

where

$$\begin{aligned} |\tilde{z}^n\rangle &= \sqrt{|\tilde{\omega}_n|}(\tilde{\mathfrak{S}}^{1/2})^{-1}|\tilde{y}^n\rangle \\ &= \frac{\text{sgn}(\tilde{\omega}_n)}{\sqrt{|\tilde{\omega}_n|}}M^{\text{RPA}}\tilde{\mathfrak{S}}^{1/2}|\tilde{y}^n\rangle, \end{aligned} \quad (17)$$

$$\tilde{\mathfrak{Q}}^{\text{RPA}}|\tilde{z}^n\rangle = \tilde{\omega}_n|\tilde{z}^n\rangle, \quad (18)$$

$$\langle\tilde{z}^n|M^{\text{RPA}}|\tilde{z}^{n'}\rangle = \text{sgn}(\tilde{\omega}_n)\delta_{n,n'}. \quad (19)$$

Now, going to the limit  $\delta \rightarrow +0$ , we obtain

$$R^{\text{RPA}}(\omega) = R^{\text{RPA}(0)}(\omega) - \sum_n' \frac{\text{sgn}(\omega_n)a^n}{\omega - \omega_n}, \quad (20)$$

where

$$R^{\text{RPA}(0)}(\omega) = -\sum_{k=1}^2 \frac{a^{(0,k)}}{\omega^k}, \quad (21)$$

$$a^{(0,k)} = \lim_{\delta \rightarrow +0} \sum_n^{(0)} \text{sgn}(\tilde{\omega}_n)\tilde{\omega}_n^{k-1}|\tilde{z}^n\rangle\langle\tilde{z}^n|, \quad (22)$$

$$a^n = |z^n\rangle\langle z^n|. \quad (23)$$

Symbol  $\sum^{(0)}$  in Eq. (22) means the sum over all the states  $n$  for which  $\tilde{\omega}_n \rightarrow \pm 0$  at  $\delta \rightarrow +0$  (that is over the spurious states). Symbol  $\sum'$  in Eq. (20) means the sum over all the states  $n$  excluding the spurious states. Note that the sum over  $k$  in Eq. (21) is limited to the first two terms because, as follows from Eqs. (17) and (22),  $a^{(0,k)} = 0$  at  $k > 2$ .

The nonspurious eigenvectors  $|z^n\rangle$  satisfy Eq. (5) and are normalized by the condition

$$\langle z^n|M^{\text{RPA}}|z^{n'}\rangle = \text{sgn}(\omega_n)\delta_{n,n'} \quad (24)$$

following from Eq. (19). The matrices  $a^{(0,1)}$  and  $a^{(0,2)}$  are Hermitian and satisfy the equations

$$\Omega^{\text{RPA}}a^{(0,1)} = a^{(0,2)}, \quad \Omega^{\text{RPA}}a^{(0,2)} = 0, \quad (25)$$

$$a^{(0,1)}M^{\text{RPA}}a^{(0,k)} = a^{(0,k)}, \quad (26)$$

$$a^{(0,1)} = -\mathfrak{P}a^{(0,1)*}\mathfrak{P}, \quad (27)$$

$$a^{(0,2)} = \mathfrak{P}a^{(0,2)*}\mathfrak{P} \quad (27)$$

following from Eqs. (10), (18), (19), and (22). The closure relation

$$a^{(0,1)} + \sum_n' \text{sgn}(\omega_n)a^n = M^{\text{RPA}} \quad (28)$$

follows from Eqs. (11), (20), and (21).

Equation (23) implies that all the matrices  $a^n$  in the expansion (20) are Hermitian and positive semidefinite. In addition from Eqs. (10) and (23) we get

$$a^{-n} = \mathfrak{P}a^{n*}\mathfrak{P}. \quad (29)$$

These properties of the residua of the function  $R^{\text{RPA}}(\omega)$  coincide with the properties of the exact response function following from its spectral representation (see, e.g., Ref. [1]). Taking this into account and making use of Eq. (12) we obtain that

$$\Pi^{\text{RPA}}(\omega) = \sum_n' \frac{\text{sgn}(\omega_n)B_n(Q)}{\omega - \omega_n}, \quad (30)$$

where transition probabilities  $B_n(Q) = \langle Q|a^n|Q\rangle$  are real and non-negative and it is supposed that

$$\langle Q|a^{(0,k)}|Q\rangle = 0, \quad k = 1, 2. \quad (31)$$

From Eq. (29) we also obtain that  $B_{-n}(Q) = B_n(Q^\dagger)$ .

If the stability matrix does not possess the property of the positive semidefiniteness, the reality of the RPA eigenvalues  $\omega_n$  and the Hermiticity and the positive semidefiniteness of the matrices  $a^n$  are not guaranteed. In particular, this means that the eigenvectors with positive eigenvalues may have negative norms. As a consequence, the reality and the non-negativeness of the RPA transition probabilities  $B_n(Q)$  in Eq. (30) is also not guaranteed, and the strength function

$$S^{\text{RPA}}(E, \Delta) = -\frac{1}{\pi} \text{Im} \Pi^{\text{RPA}}(E + i\Delta) \quad (32)$$

may take negative values at  $E > 0$  and  $\Delta > 0$ . Note that the problem of the “negative transition probabilities” arising in this case can be treated as the problem of the “negative energies” since the function  $\Pi^{\text{RPA}}(\omega)$  will have positive residua at the poles  $\omega = \omega_n < 0$ .

#### IV. EXTENDED RPA

In the ERPA theories the eigenvalue equation (5) is usually replaced (see, e.g., [4]) by the equation with the energy-dependent matrix  $\Omega^{\text{ERPA}}(\omega)$ :

$$\sum_{34} \Omega_{12,34}^{\text{ERPA}}(\omega_\nu)z_{34}^\nu = \omega_\nu z_{12}^\nu, \quad (33)$$

where  $\Omega^{\text{ERPA}}(\omega)$  can be represented in the form

$$\Omega^{\text{ERPA}}(\omega) = \Omega^{\text{RPA}} + M^{\text{RPA}}W(\omega) \quad (34)$$

and it is supposed that Eqs. (33) and (34) are written in the  $1p1h$  subspace. The matrix  $W(\omega)$  is the interaction amplitude that includes contributions of complex ( $2p2h$ ) configurations. It has the following generic form:

$$W(\omega) = F(\omega - M^{\text{C}}\mathfrak{S}^{\text{C}})^{-1}M^{\text{C}}F^\dagger, \quad (35)$$

where  $\mathfrak{S}^{\text{C}}$ ,  $M^{\text{C}}$ , and  $F$  are the block matrices of the form

$$\mathfrak{S}^{\text{C}} = \begin{pmatrix} \mathfrak{S}^{\text{C}(+)} & 0 \\ 0 & \mathfrak{S}^{\text{C}(-)} \end{pmatrix}, \quad M^{\text{C}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (36)$$

$F = (F^{(+)}, F^{(-)})$ . The Hermitian matrices  $\mathfrak{S}^{\text{C}(\pm)}$ ,  $\mathfrak{S}^{\text{C}}$ , and  $M^{\text{C}}$  act in the subspace of complex configurations. The

matrices  $F$  and  $F^\dagger$  connect this subspace with the  $1p1h$  subspace. The matrices  $\mathfrak{S}^C$  and  $M^C$  play the role of the stability matrix and the metric matrix in the  $2p2h$  subspace, respectively. In addition, the following equalities are fulfilled:

$$\mathfrak{S}^{C(-)} = \mathfrak{S}^{C(+)*}, \quad F^{(-)} = \mathfrak{P} F^{(+)*}, \quad (37)$$

$$M^{\text{RPA}} F^{(\pm)} = \pm F^{(\pm)}. \quad (38)$$

Equation (37) leads to the symmetry property

$$\Omega^{\text{ERPA}}(\omega) = -\mathfrak{P} \Omega^{\text{ERPA}*}(-\omega^*) \mathfrak{P} \quad (39)$$

from which we obtain for the eigenvectors with the real eigenvalues in Eq. (33) the following relation

$$|z^{-\nu}\rangle = \mathfrak{P} |z^\nu\rangle^*, \quad (40)$$

where  $|z^{-\nu}\rangle$  is the eigenvector with the eigenvalue  $-\omega_\nu$ , as in the case of the RPA, see Eq. (10).

Using the complete sets of the eigenvectors of the matrices  $\mathfrak{S}^{C(\pm)}$  one can represent Eq. (35) in the more explicit form:

$$W_{12,34}(\omega) = \sum_{c, \sigma} \frac{\sigma F_{12}^{c(\sigma)} F_{34}^{c(\sigma)*}}{\omega - \sigma \Omega_c}, \quad (41)$$

where  $\sigma = \pm 1$ ,  $c$  is an index of the subspace of complex configurations,  $\Omega_c$  are the eigenvalues of the matrices  $\mathfrak{S}^{C(\pm)}$ . It is supposed that the matrices  $\mathfrak{S}^{C(\pm)}$  are positive definite and, consequently,  $\Omega_c > 0$ . Consider three models which can be formulated using Eq. (41) for the matrix  $W(\omega)$ . From Eqs. (37) and (38) it follows that  $F_{12}^{c(-)} = F_{21}^{c(+)*}$  and  $F_{ph}^{c(-)} = F_{hp}^{c(+)*} = 0$ . So only the quantities  $F_{ph}^{c(+)}$  and the energies  $\Omega_c$  should be specified.

(a) Second RPA in the so-called diagonal approximation [4,7–11]. In this case one can set  $c = \{p', p'', h', h''\}$ ,

$$\Omega_c = \varepsilon_{p'} + \varepsilon_{p''} - \varepsilon_{h'} - \varepsilon_{h''}, \quad (42)$$

$$F_{ph}^{c(+)} = \frac{1}{2} (\delta_{pp'} w_{h'h''} + \delta_{pp''} w_{h'h'} - \delta_{pp'} w_{h'h''} - \delta_{pp''} w_{h'h'} + \delta_{hh'} w_{p'h''} + \delta_{hh''} w_{p'h'} - \delta_{hh'} w_{p'h''} - \delta_{hh''} w_{p'h'}), \quad (43)$$

where  $w_{12,34} = -w_{21,34} = -w_{12,43}$  is an antisymmetrized amplitude of the two-particle interaction. In the first order we have  $V_{12,34} = w_{14,23}$ , however in the general case the amplitude of the residual interaction in Eq. (6) does not coincide with  $w$  and is not antisymmetric. Note that the full SRPA scheme is usually formulated by means of the equations similar to Eq. (35).

(b) TBA1: the quasiparticle-phonon coupling model within the TBA including  $1p1h \otimes$  phonon configurations [17–19] (without ground state correlations beyond the RPA included in [17–19]). In this case  $c = \{p', h', n\}$  where  $n$  is the phonon's index,

$$\Omega_c = \varepsilon_{p'} - \varepsilon_{h'} + \omega_n, \quad \omega_n > 0, \quad (44)$$

$$F_{ph}^{c(+)} = \delta_{pp'} g_{h'h}^n - \delta_{h'h} g_{pp'}^n, \quad (45)$$

$g_{12}^n$  is an amplitude of the quasiparticle-phonon interaction. In the self-consistent approach, these amplitudes (along with the phonon's energies  $\omega_n$ ) are determined by the positive frequency solutions of the RPA equations (5) and (24)

according to the formula

$$g_{12}^n = \sum_{34} V_{12,34} z_{34}^n. \quad (46)$$

Physical effects taken into account in the TBA1 and the general structure of the equations are the same as in the particle-vibration coupling model [28] and in the model of the coupling of  $1p1h$  configurations to the doorway states [29].

(c) TBA2: the quasiparticle-phonon coupling model within the TBA including two-phonon configurations [20]. This model is a straightforward generalization of the TBA1 by including additional correlations between particles and holes entering  $1p1h \otimes$  phonon configurations (but also without ground state correlations beyond the RPA and without pairing correlations included in [20]). Physically, this is similar, but not equivalent in details, to the first versions of the quasiparticle-phonon model [30]. Relativistic extension of the two-phonon model was developed in Ref. [26]. In the TBA2 we have  $c = \{n, n'\}$ , where  $n$  and  $n'$  are the phonon's indices,

$$\Omega_c = \omega_n + \omega_{n'}, \quad \omega_n > 0, \quad \omega_{n'} > 0, \quad (47)$$

$$F_{ph}^{c(+)} = \sum_{p''h''} (\delta_{pp''} g_{h''h}^n - \delta_{h''h} g_{pp''}^n) z_{p''h''}^{n'}. \quad (48)$$

The amplitudes  $g_{12}^n$ ,  $z_{12}^{n'}$  and the phonon's energies are determined by Eqs. (5), (24), and (46), as in the TBA1.

Obviously, the TBA2 reduces to the TBA1 in the case when the second phonon is noncollective, i.e., when  $\omega_{n'} = \varepsilon_{p'} - \varepsilon_{h'}$  in Eq. (47) and  $z_{p''h''}^{n'} = \delta_{p''p'} \delta_{h''h'}$  in Eq. (48). However, the connection between the TBA1 and the SRPA is not so simple because of the well-known problem of the second order contributions arising in the quasiparticle-phonon coupling model (see, e.g., Ref. [31]).

## V. SUBTRACTION METHOD

The starting point of the ERPA theories is the usual RPA. In many practically significant cases (except for the so-called *ab initio* approaches) the self-consistent RPA is based on the density functional theory (DFT, see, e.g., Refs. [32–34]) in which the energy density functional  $E[\rho]$  is constructed in such a way as to provide an optimal (exact in the limiting case) description of the nuclear ground state properties. Therefore,  $E[\rho]$  already effectively contains a part of the contributions of those complex configurations which are explicitly included in the ERPA. This part can be treated as the static contributions, in contrast to the dynamic ones which lead to the formation of the spreading widths of the resonances. To avoid double counting, these static contributions in the ERPA should be eliminated. A simple way to do this is to impose the condition:

$$\Omega^{\text{ERPA}}(0) = \Omega^{\text{RPA}}. \quad (49)$$

The reasons for this condition are as follows. Let  $Q$  be a local Hermitian single-particle operator representing some external field. Dynamic polarizability  $\Pi(\omega)$  corresponding to this field is defined by Eq. (12) in which the response function  $R(\omega)$  is defined by Eq. (11) in the RPA and by the equation

$$R^{\text{ERPA}}(\omega) = -(\omega - \Omega^{\text{ERPA}}(\omega))^{-1} M^{\text{RPA}} \quad (50)$$

in the ERPA. Consider an energy density functional

$$\mathcal{E}[\rho, \lambda] = E[\rho] + \lambda \text{Tr}(\rho Q), \quad (51)$$

where  $\lambda$  is a real parameter. According to the so-called dielectric theorem [35], we have

$$\Pi^{\text{RPA}}(0) = -2m_{-1}^{\text{RPA}} = \left( \frac{d}{d\lambda} \text{Tr}(\rho^{(\lambda)} Q) \right)_{\lambda=0}, \quad (52)$$

where  $\Pi^{\text{RPA}}(0)$  is the (static) polarizability calculated by making use of Eqs. (3), (4), (6), (11), and (12) in the self-consistent RPA based on the functional  $E[\rho]$ , the quantity  $m_{-1}^{\text{RPA}}$  is the inverse energy-weighted moment of the strength distribution in the RPA,  $\rho^{(\lambda)}$  is the equilibrium density matrix of the functional  $\mathcal{E}[\rho, \lambda]$ , and it is supposed that  $a^{(0,1)}|Q\rangle = 0$ . Assuming, in accordance with general principles of the DFT, that this theory gives in a sense an exact value of the quantity  $\text{Tr}(\rho^{(\lambda)} Q)$  at any  $\lambda$  near the point  $\lambda = 0$ , one can consider that  $\Pi^{\text{RPA}}(0) = -2m_{-1}$  where  $m_{-1}$  is the exact inverse energy-weighted moment of the strength distribution including contributions of all configurations. Then, the condition  $\Pi^{\text{ERPA}}(0) = \Pi^{\text{RPA}}(0)$  is natural and from this, using Eqs. (11), (12), and (50), we arrive at the condition (49). This condition will be fulfilled if we change the definition of the matrix  $\Omega^{\text{ERPA}}(\omega)$  taking instead of Eq. (34) the following ansatz:

$$\Omega^{\text{ERPA}}(\omega) = \Omega^{\text{RPA}} + M^{\text{RPA}} [W(\omega) - \kappa W(0)] \quad (53)$$

and setting  $\kappa = 1$ .

Thus, the method of eliminating the double counting consists in subtracting the static part  $W(0)$  from the interaction amplitude  $W(\omega)$  containing the contributions of complex configurations. This method was used in the calculations of giant resonances both within self-consistent [22–26] and within non-self-consistent [21] approaches. In the non-self-consistent models the problem of double counting arises because of the use of the phenomenologically fitted mean field and the residual interaction. In this case the subtraction method plays the same role as the so-called refinement procedure applied in Refs. [4,17–19].

## VI. STABILITY CONDITION IN THE EXTENDED RPA THEORIES

To analyze the properties of Eq. (33) with the matrix  $\Omega^{\text{ERPA}}(\omega)$  defined by Eqs. (53), (35), and (36) let us recast Eq. (33) in the extended space including  $1p1h$  and complex ( $2p2h$ ) configurations. Let us define the energy-independent matrix  $\widehat{\Omega}^{\text{ERPA}}$  in this space as the block matrix of the following form:

$$\widehat{\Omega}^{\text{ERPA}} = \begin{pmatrix} \Omega^{\text{RPA}(\kappa)} & M^{\text{RPA}} F \\ M^{\text{C}} F^\dagger & M^{\text{C}} \mathfrak{S}^{\text{C}} \end{pmatrix}, \quad (54)$$

where

$$\Omega^{\text{RPA}(\kappa)} = \Omega^{\text{RPA}} + \kappa M^{\text{RPA}} F (\mathfrak{S}^{\text{C}})^{-1} F^\dagger. \quad (55)$$

It is easy to verify that Eq. (33) is equivalent to the following linear eigenvalue equation:

$$\widehat{\Omega}^{\text{ERPA}} |Z^v\rangle = \omega_v |Z^v\rangle, \quad (56)$$

where

$$|Z^v\rangle = \begin{pmatrix} |z^v\rangle \\ |\zeta^v\rangle \end{pmatrix}. \quad (57)$$

The vector  $|z^v\rangle$  in Eq. (57) belongs to the  $1p1h$  subspace and coincides with the vector in Eq. (33). The vector  $|\zeta^v\rangle$  belongs to the subspace of complex configurations.

The matrix  $\widehat{\Omega}^{\text{ERPA}}$  can be represented in the form  $\widehat{\Omega}^{\text{ERPA}} = M^{\text{ERPA}} \mathfrak{S}^{\text{ERPA}}$  where

$$M^{\text{ERPA}} = \begin{pmatrix} M^{\text{RPA}} & 0 \\ 0 & M^{\text{C}} \end{pmatrix} \quad (58)$$

is the metric matrix,  $\mathfrak{S}^{\text{ERPA}}$  is the stability matrix in the ERPA which is defined in analogy to Eq. (8):

$$\mathfrak{S}^{\text{ERPA}} = M^{\text{ERPA}} \widehat{\Omega}^{\text{ERPA}}. \quad (59)$$

Using Eqs. (54), (55), (58), and (59) we obtain that for any complex vector  $|Z\rangle$ ,

$$|Z\rangle = \begin{pmatrix} |z\rangle \\ |\zeta\rangle \end{pmatrix}, \quad (60)$$

with arbitrary components  $|z\rangle$  and  $|\zeta\rangle$  the following equation is fulfilled:

$$\langle Z | \mathfrak{S}^{\text{ERPA}} | Z \rangle = \langle z | \mathfrak{S}^{\text{RPA}} | z \rangle + \langle \zeta' | \mathfrak{S}^{\text{C}} | \zeta' \rangle + (\kappa - 1) \langle \zeta'' | \mathfrak{S}^{\text{C}} | \zeta'' \rangle, \quad (61)$$

where

$$|\zeta'\rangle = |\zeta\rangle + |\zeta''\rangle, \quad |\zeta''\rangle = (\mathfrak{S}^{\text{C}})^{-1} F^\dagger |z\rangle. \quad (62)$$

From Eq. (61) it follows that the expectation value  $\langle Z | \mathfrak{S}^{\text{ERPA}} | Z \rangle \geq 0$  for all  $|Z\rangle$  if the RPA stability matrix  $\mathfrak{S}^{\text{RPA}}$  is positive semidefinite, the matrix  $\mathfrak{S}^{\text{C}}$  is positive definite, and  $\kappa \geq 1$ . That is, under these conditions, the matrix  $\mathfrak{S}^{\text{ERPA}}$  is positive semidefinite. Note that the positive definiteness of the matrix  $\mathfrak{S}^{\text{C}}$  is ensured in the models considered in Sec. IV and that Eqs. (37) and (38) are not used in the proof of this statement. Since the matrices  $M^{\text{ERPA}}$  and  $\mathfrak{S}^{\text{ERPA}}$  are Hermitian, in analogy to the case of the RPA (see Sec. II) we conclude that all eigenvalues  $\omega_v$  in Eqs. (33) and (56) are real if the subtraction method [ $\kappa = 1$  in Eq. (53)] is used. Without subtraction ( $\kappa = 0$ ) stability of the solutions of the ERPA equations is not guaranteed.

Let us introduce the ERPA response function in the extended space

$$\widehat{R}^{\text{ERPA}}(\omega) = -(\omega - \widehat{\Omega}^{\text{ERPA}})^{-1} M^{\text{ERPA}}. \quad (63)$$

The analysis of Sec. III is straightforwardly generalized to the case of the ERPA with subtraction. The orthonormalization condition for the nonspurious eigenvectors  $|Z^v\rangle$  of the matrix  $\widehat{\Omega}^{\text{ERPA}}$  in the extended space has the form

$$\langle Z^v | M^{\text{ERPA}} | Z^{v'} \rangle = \text{sgn}(\omega_v) \delta_{v, v'} \quad (64)$$

which is analogous to Eq. (24). In the  $1p1h$  subspace from this condition and from Eqs. (35), (54)–(58) we obtain

$$\langle z^v | M^{\text{RPA}} - W^{D(vv')} | z^{v'} \rangle = \text{sgn}(\omega_v) \delta_{v, v'}, \quad (65)$$

where

$$W^{D(vv')} = \frac{W(\omega_v) - W(\omega_{v'})}{\omega_v - \omega_{v'}}, \quad v \neq v', \quad (66)$$

$$W^{D(vv)} = \left( \frac{dW(\omega)}{d\omega} \right)_{\omega=\omega_v}. \quad (67)$$

From Eqs. (64) and (65) we see that, as in the RPA case, the eigenvectors with positive eigenvalues in the ERPA have positive norms.

Using the known properties of the block matrices one can readily show that  $\hat{R}_{12,34}^{\text{ERPA}}(\omega) = R_{12,34}^{\text{ERPA}}(\omega)$  where  $\hat{R}_{12,34}^{\text{ERPA}}(\omega)$  is the block of the matrix  $\hat{R}^{\text{ERPA}}(\omega)$  in the  $1p1h$  subspace and the matrix  $R^{\text{ERPA}}(\omega)$  is defined by Eq. (50). Then from the results obtained in Sec. III and from the positive semidefiniteness of the stability matrix  $\mathfrak{S}^{\text{ERPA}}$  at  $\kappa = 1$  it follows that in the case, when the subtraction method is used, the expansion of the type (20), where the matrices  $a^n$  are Hermitian and positive semidefinite, is valid for the response function  $R^{\text{ERPA}}(\omega)$ . Therefore, for the dynamic polarizability

$$\Pi^{\text{ERPA}}(\omega) = -\langle Q | R^{\text{ERPA}}(\omega) | Q \rangle \quad (68)$$

the expansion of the type (30) holds where the probabilities  $B_n$  are real and non-negative.

Though the problem of the convergence is not generally resolved within the framework of the subtraction method, one can see that its use at least improves the situation. This problem arises when the model configuration space is enlarged, i.e., when  $\Omega_c$  in Eq. (41) increases. Let us denote  $\bar{W}(\omega) = W(\omega) - W(0)$ . From Eq. (41) one obtains the following formal expansions:

$$W(\omega) = - \sum_{c, \sigma} \frac{|F^{c(\sigma)}\rangle\langle F^{c(\sigma)}|}{\Omega_c} \sum_{m=0}^{\infty} \left( \frac{\sigma\omega}{\Omega_c} \right)^m, \quad (69)$$

$$\bar{W}(\omega) = - \sum_{c, \sigma} \frac{|F^{c(\sigma)}\rangle\langle F^{c(\sigma)}|}{\Omega_c} \sum_{m=1}^{\infty} \left( \frac{\sigma\omega}{\Omega_c} \right)^m. \quad (70)$$

The convergence is determined by the rate of decrease of the terms in these expansions at  $\Omega_c \rightarrow \infty$ . The leading term in the expansion (69) is of order  $1/\Omega_c$ , while in the expansion (70) this term is of order  $1/\Omega_c^2$ . Thus, the use of the quantity  $\bar{W}(\omega)$  instead of  $W(\omega)$  in the subtraction method leads to the acceleration of the convergence.

## VII. THE CASE OF A SCHEMATIC MODEL

To illustrate the results of the previous sections consider a simple model in which the space of  $1p1h$  states is restricted to one particle-hole ( $ph$ ) pair with the single-particle energies  $\varepsilon_p$  and  $\varepsilon_h$  and with the matrix elements of the residual interaction  $V_{ph,ph} = V_{hp,hp}$  and  $V_{ph,hp} = V_{hp,ph}$  which are supposed to be real. The space of the complex configurations is also restricted to one state, so that index  $c$  in Eq. (41) takes only one value and we put:  $|F_{ph}^{c(+)}|^2 = |F_{hp}^{c(-)}|^2 = g^2$ ,  $F_{ph}^{c(-)} = F_{hp}^{c(+)} = 0$ .

Let us denote in accordance with usual notations of the RPA equations [1]:

$$A = \varepsilon_p - \varepsilon_h + V_{ph,ph}, \quad B = V_{ph,hp}. \quad (71)$$

Then we have

$$\Omega^{\text{RPA}} = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad \mathfrak{S}^{\text{RPA}} = \begin{pmatrix} A & B \\ B & A \end{pmatrix}, \quad (72)$$

$$M^{\text{RPA}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (73)$$

The eigenvalues of the matrix  $\Omega^{\text{RPA}}$  are  $\pm\omega_{\text{RPA}}$  where  $\omega_{\text{RPA}} = \sqrt{A^2 - B^2}$ . The eigenvalues of the matrix  $\mathfrak{S}^{\text{RPA}}$  are  $s_{\pm}^{\text{RPA}} = A \pm |B|$ . So, the RPA stability condition reads

$$A \geq |B|. \quad (74)$$

The ERPA matrix (53) in this model has the form

$$\Omega^{\text{ERPA}}(\omega) = \begin{pmatrix} A_\kappa + C(\omega) & B \\ -B & -A_\kappa - C(-\omega) \end{pmatrix}, \quad (75)$$

where

$$A_\kappa = A + \frac{\kappa g^2}{\Omega_c}, \quad C(\omega) = \frac{g^2}{\omega - \Omega_c}. \quad (76)$$

In what follows we suppose that Eq. (74) is fulfilled and that  $\Omega_c > \omega_{\text{RPA}}$ . This corresponds to the real conditions in the models described in Sec. IV.

Let us introduce the following dimensionless quantities:

$$\beta = B/A, \quad \gamma = g/\sqrt{A\Omega_c}, \quad \omega_c = \Omega_c/A, \quad (77)$$

$$\bar{s}_{\pm}^{\text{RPA}} = s_{\pm}^{\text{RPA}}/A = 1 \pm |\beta|. \quad (78)$$

Note that the parameter  $\gamma$  determines the strength of the coupling of the  $ph$  pair with complex configuration. Consider properties of the poles and residua of the ERPA response function defined by Eq. (50). Its poles coincide with roots of the secular equation

$$\det(\Omega^{\text{ERPA}}(\omega) - \omega) = 0 \quad (79)$$

which has four roots:  $\pm\omega_\tau$ , where  $\tau = \pm 1$ ,

$$\omega_\tau^2 = \frac{1}{2} (U_\kappa^2 + \tau D_\kappa^2), \quad (80)$$

$$U_\kappa^2 = A^2 [(1 + \kappa\gamma^2)^2 + \omega_c^2 - \beta^2 + 2\omega_c\gamma^2], \quad (81)$$

$$D_\kappa^4 = U_\kappa^4 + 4A^4\omega_c^2(\beta^2 - [1 + (\kappa - 1)\gamma^2]^2). \quad (82)$$

The values of  $\omega_\tau^2$  are always real because  $D_\kappa^4 \geq 0$  both at  $\kappa = 1$  and at  $\kappa = 0$ .

Substituting Eqs. (73) and (75) into Eq. (50), we obtain

$$R^{\text{ERPA}}(\omega) = - \sum_{\tau, \sigma} \frac{\sigma a_{\tau, \sigma}}{\omega - \sigma \omega_\tau}, \quad (83)$$

where  $\sigma = \pm 1$ ,

$$a_{\tau, \sigma} = \frac{\tau(\omega_\tau^2 - \Omega_c^2)}{2\omega_\tau D_\kappa^2} \begin{pmatrix} \tilde{A}_\kappa(-\sigma\omega_\tau) & -B \\ -B & \tilde{A}_\kappa(\sigma\omega_\tau) \end{pmatrix}, \quad (84)$$

$\tilde{A}_\kappa(\omega) = A_\kappa + C(\omega) - \omega$ . The residue matrices  $a_{\tau, \sigma}$  obey the condition

$$\text{Tr}([M^{\text{RPA}} - W^D(\sigma\omega_\tau)] a_{\tau, \sigma}) = \sigma, \quad (85)$$

where

$$W^D(\omega) = \frac{d}{d\omega} \begin{pmatrix} C(\omega) & 0 \\ 0 & C(-\omega) \end{pmatrix}. \quad (86)$$

In addition, we have  $\det(a_{\tau,\sigma}) = 0$ . So, the  $2 \times 2$  matrix  $a_{\tau,\sigma}$  has only one non-zero eigenvalue  $\alpha_\tau = \text{Tr}(a_{\tau,\sigma})$  which does not depend on  $\sigma$  and is determined by the formula

$$\alpha_\tau = \frac{\tau A[(1 + \kappa\gamma^2)(\omega_\tau^2 - \Omega_c^2) + \Omega_c^2\gamma^2]}{\omega_\tau D_\kappa^2}. \quad (87)$$

The product  $\alpha_\tau\omega_\tau$  is real for all  $\gamma$ ,  $\tau$ , and  $\kappa$ . However, at  $\kappa = 0$  and  $\tau = -1$  it changes sign at  $\gamma^2 = \gamma_0^2$  where  $\gamma_0^2 = 1 + \beta^2/(1 + \omega_c)^2$  and  $\bar{s}_-^{\text{RPA}} < \gamma_0^2 < \bar{s}_+^{\text{RPA}}$ .

In the limit  $\gamma^2 \rightarrow 0$  we have  $\omega_-^2 \rightarrow \omega_{\text{RPA}}^2$ ,  $\omega_+^2 \rightarrow \Omega_c^2$ ,  $\alpha_- \omega_- \rightarrow \alpha_{\text{RPA}} \omega_{\text{RPA}} = A$ ,  $\alpha_+ \omega_+ \rightarrow 0$  both for  $\kappa = 1$  and for  $\kappa = 0$ .

In the limit  $\gamma^2 \rightarrow \infty$  we obtain

$$\kappa = 1: \omega_-^2 \rightarrow 0, \omega_+^2 \rightarrow \infty, \alpha_- \omega_- \rightarrow 0, \alpha_+ \omega_+ \rightarrow \infty;$$

$$\kappa = 0: \omega_\pm^2 \rightarrow \infty, \alpha_\pm \omega_\pm \rightarrow \pm\infty.$$

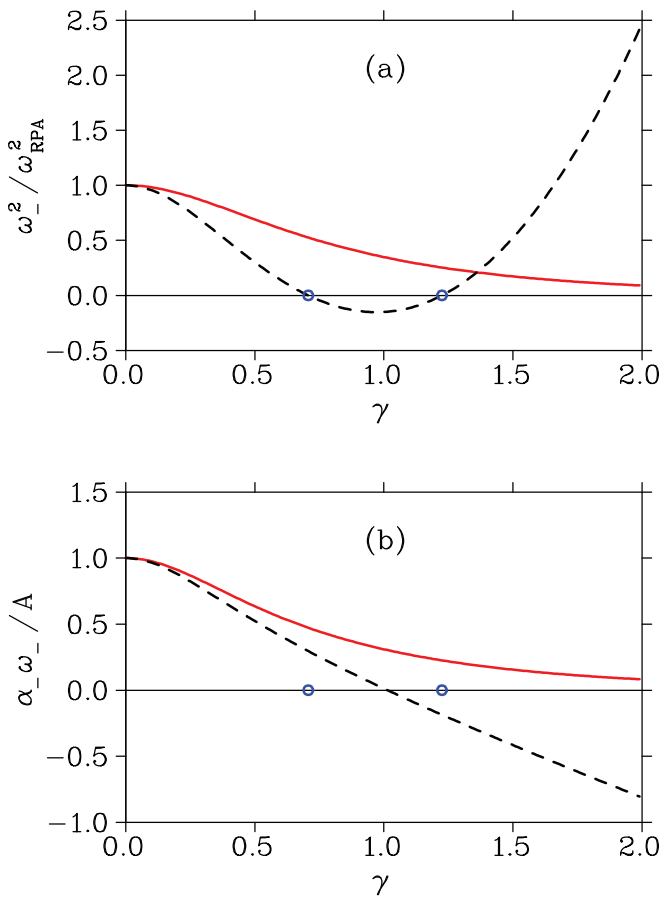


FIG. 1. (Color online) (a) Dependence of the squared ERPA eigenvalue  $\omega_-^2$  normalized to  $\omega_{\text{RPA}}^2$  on the parameter  $\gamma$  determining the strength of the coupling of the  $ph$  pair with complex configuration. The values of  $\omega_-^2$  are calculated by means of Eqs. (80)–(82) with  $\beta = 0.5$  and  $\omega_c = 2$ . Solid (red) line represents the ERPA results obtained with the use of subtraction method ( $\kappa = 1$ ). The dashed (black) line represents the results without subtraction ( $\kappa = 0$ ). The values of  $(\bar{s}_\pm^{\text{RPA}})^{1/2}$  are indicated by the blue circles on the  $\gamma$  axis. (b) The same dependence for the product  $\alpha_- \omega_-$  normalized to  $\alpha_{\text{RPA}} \omega_{\text{RPA}} = A$  (see text for details).

From Eqs. (80)–(82) and (87) it follows that at  $\kappa = 1$  all  $\omega_\tau$  and  $\alpha_\tau$  are real and all  $\alpha_\tau\omega_\tau > 0$ . In this case the normalization condition (65) is fulfilled due to Eq. (85). The matrices  $a_{\tau,\sigma}$  are Hermitian and positive semidefinite if we set  $\omega_\tau > 0$  (that is always possible if  $\omega_\tau$  are real).

At  $\kappa = 0$  we have

- (i) if  $\gamma^2 < \bar{s}_-^{\text{RPA}}$ , then  $\omega_\pm$  and  $\alpha_\pm$  are real and  $\alpha_\pm\omega_\pm > 0$ ;
- (ii) if  $\bar{s}_-^{\text{RPA}} < \gamma^2 < \bar{s}_+^{\text{RPA}}$ , then  $\omega_-$  and  $\alpha_-$  are imaginary,  $\omega_+$  and  $\alpha_+$  are real and  $\alpha_+\omega_+ > 0$ ;
- (iii) if  $\gamma^2 > \bar{s}_+^{\text{RPA}}$ , then  $\omega_\pm$  and  $\alpha_\pm$  are real,  $\alpha_+\omega_+ > 0$ , but  $\alpha_-\omega_- < 0$ ;
- (iv) if  $\gamma^2 = \bar{s}_\pm^{\text{RPA}}$ , then  $\omega_+$  and  $\alpha_+$  are real,  $\alpha_+\omega_+ > 0$ ,  $\omega_- = 0$ ,  $\alpha_-$  is indefinite.

These properties of the values  $\omega_\pm$  and  $\alpha_\pm$  do not depend on the value of the parameter  $\omega_c$  if  $\Omega_c > \omega_{\text{RPA}}$ .

Dependence of the values  $\omega_\pm^2$  and  $\alpha_\pm\omega_\pm$  on the parameter  $\gamma$  at  $\beta = 0.5$  and  $\omega_c = 2$  is shown in Figs. 1 and 2. Since  $|\beta| < 1$ , the RPA stability condition (74) is fulfilled. We see that in this case the ERPA solutions are also stable and the eigenvalues of the ERPA residue matrices are non-negative at all  $\gamma$  (and  $\omega_\pm > 0$ ) if the subtraction method is used. In the ERPA without subtraction the lowest eigenvalue  $\omega_-$  becomes imaginary in the finite region of the values of  $\gamma$  around the

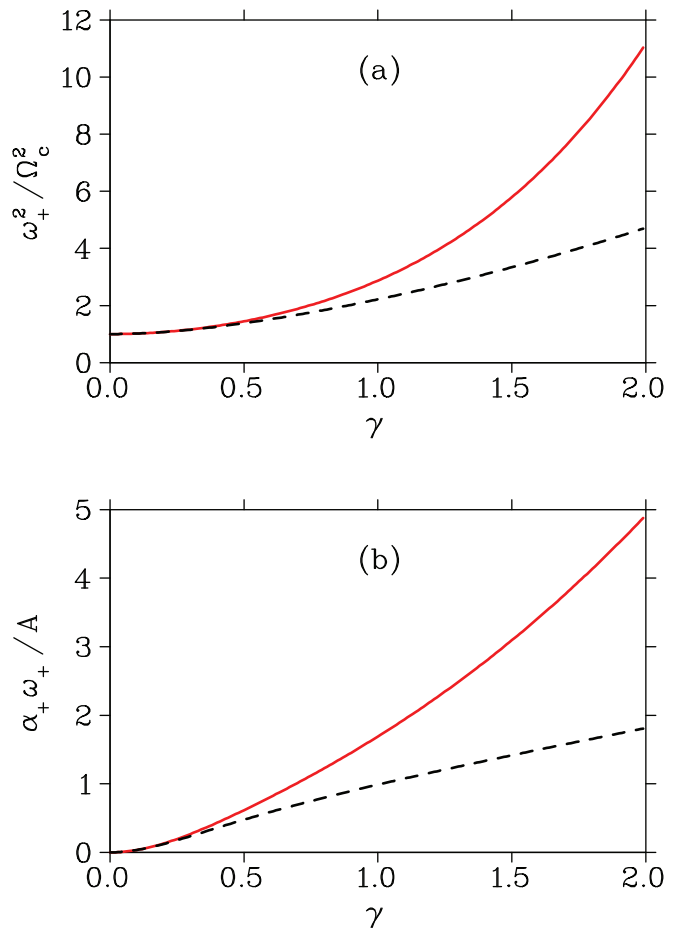


FIG. 2. (Color online) The same as Fig. 1 for  $\omega_+^2$  normalized to  $\Omega_c^2$  (a) and  $\alpha_+ \omega_+$  normalized to  $\alpha_{\text{RPA}} \omega_{\text{RPA}} = A$  (b).

point  $\gamma = 1$ . Outside of this region, the values of  $\omega_-$  at  $\kappa = 0$  are real, however at  $\gamma^2 > \gamma_0^2 = 1 + \beta^2/(1 + \omega_c)^2$  the product of  $\omega_-$  and the eigenvalue  $\alpha_-$  of the ERPA residue matrices  $a_{-, \pm}$  becomes negative. Using Eq. (85) we obtain that in this case the eigenvector with the positive eigenvalue  $\omega_-$  will have the negative norm. Therefore, the condition (65) is violated. In addition, in the region  $\gamma^2 > \bar{s}_+^{\text{RPA}}$ , where  $\alpha_- \omega_- < 0$ , the matrices  $a_{-, \pm}$ , though being Hermitian, become negative semidefinite at  $\omega_- > 0$  (positive semidefinite at  $\omega_- < 0$ ) that leads to the problem of the “negative transition probabilities” (or of the “negative energies”) as was explained in Sec. III.

From Eqs. (76) it follows that the subtraction effectively introduces additional repulsion into the matrix elements  $A_{ph,ph}$  and  $A_{hp,hp}$  of the matrix  $\Omega^{\text{RPA}}$ . As a result,  $\omega_-^2(\kappa = 1) > \omega_-^2(\kappa = 0)$  at least at  $\gamma^2 < \bar{s}_-^{\text{RPA}}$ . Nevertheless, as can be seen from Fig. 1,  $\omega_-^2 < \omega_{\text{RPA}}^2$  for all  $\gamma^2 > 0$  and  $\kappa = 1$  due to the attractive effect of the dynamic part of the interaction  $C(\omega)$  at  $\omega < \Omega_c$ .

### VIII. CONCLUSIONS AND DISCUSSION

In the paper the problem of stability of solutions in the extended RPA (ERPA) theories is considered. The extension of the RPA implies enlarging the configuration space by taking into account more complex configurations in addition to the  $1p1h$  states included in the RPA. The analysis of stability is based on the famous Thouless theorem proved in the case of the self-consistent RPA and on the response function formalism which enables one to study this problem in more detail. Two cases are considered: the ERPA with and without the subtraction method. This method was suggested previously to avoid double counting in the self-consistent ERPA approaches based on the density functional theory (DFT) with phenomenologically fitted energy density functionals. Justification of the subtraction method is provided by the dielectric theorem which associates the static polarizability calculated within the self-consistent RPA with the exact inverse energy-weighted moment of the strength distribution including contributions of all configurations. The subtraction method ensures the equality of the RPA and of the ERPA static polarizabilities and, consequently, equality of the respective inverse energy-weighted moments.

It is proved that the stability matrix in the ERPA theories with subtraction is positive semidefinite if the RPA stability matrix possesses this property. This ensures stability of solutions of the ERPA eigenvalue equations, positiveness of the norms of the eigenvectors with positive eigenvalues, and

non-negativeness of the respective transition probabilities. In the ERPA without subtraction these properties of the solutions are not guaranteed. In addition, it is shown that the subtraction method leads to the acceleration of the convergence in the ERPA though this problem is not generally resolved within the framework of this method.

The example of the schematic model is used to analyze dependence of the solutions of the ERPA equations on the effective parameter determining the strength of the coupling of a single particle-hole pair with a single complex configuration. It is demonstrated that, if the values of this parameter are sufficiently large, the ERPA without subtraction leads to the imaginary solutions of the respective eigenvalue equation and to the problem of the “negative transition probabilities” or of the “negative energies”. As in the general case, these problems do not arise when the subtraction method is applied.

Thus, in the ERPA theories based on the DFT principles the subtraction method plays a twofold role: it eliminates the double counting and resolves the stability problem. The situation is different in the ERPA which starts with the realistic nucleon-nucleon interaction (see Refs. [8,9]). Here, the problem of the double counting does not arise at least at the SRPA level, but the stability issue is actual. In this case the use of the subtraction method is not well justified. As was shown in a recent paper [16], another way to get stable ERPA solutions is to include the ground state correlations beyond the RPA. Note that within the (E)RPA+DFT approach this type of correlations is included implicitly on the mean-field level as follows from the dielectric theorem mentioned above. The role of the ground state correlations in the description of the nuclear excitations was discussed and investigated in a series of papers (see, e.g., [4,14–20,36] and references therein). In Ref. [16] it was found that taking into account these correlations in the ERPA increases the energies of the particle-hole pairs and, as a consequence, leads to the upward shift of the energies of the low-lying states. This direction of the energy shift is opposite to that obtained in the conventional SRPA, so resulting ERPA solution in the considered in Ref. [16] case of the first  $3^-$  state in the nucleus  $^{16}\text{O}$  appears to be stable. This indicates that the effects of the ground state correlations are an important part of the consistent theory but their more thorough study, in particular in connection with the stability problem, is needed.

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