Odd particle number random-phase approximation and extensions: Applications to particle and hole states around ^{16}O

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The hole-state random-phase approximation (hRPA) and the particle-state random-phase approximation (pRPA) for systems like odd A nuclei are discussed. These hRPA and pRPA are formulated based on the Hartree-Fock ground state. An extension of hRPA and pRPA based on a correlated ground state is given using time-dependent density-matrix theory. Applications to the single-particle states around ^{16}O are presented. It is shown that inclusion of ground-state correlation affects appreciably the results of hRPA and pRPA. The question of the coupling of the center-of-mass motion of the core to the particle (hole) is also discussed.

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I. INTRODUCTION

The one-particle states and one-hole states are basic excitation modes of a nucleus and other many-body systems. The experimental data on the properties of the single-particle states have been accumulated using nuclear reactions such as one-nucleon transfer and pickup and knock-out reactions [1], and it was found that there is a substantial depletion of the spectral strength of the single-particle states. Theoretical studies have shown that the strong short-range and tensor components of the nucleon-nucleon interaction are responsible for a part of the depletion [2] and a substantial part of the fragmentation of the single-particle strength is due to the coupling to low-lying collective modes [3,4]. The standard approach to study the single-particle properties may be the Green's function method. Various theoretical approaches have been proposed to implement the coupling to low-lying collective modes into the self-energy of the Green's function: the particle-phonon coupling model [3,5–7], the Tamm-Dancoff approximation (TDA) [8], and the more recent Faddeev random-phase approximation (FRPA) [9]. In the present paper we give a formulation of the hole-state RPA (hRPA) using the equation of motion approach (EoM) [10], which has often been used to derive the standard RPA, and discuss some aspects of hRPA such as the relation to the particle-state RPA (pRPA), which have not been clarified so far in the literature [8,11]. We also present an extension of odd A RPA (oRPA) based on a correlated ground state obtained from the time-dependent density-matrix theory (TDDM) [12–14]. The influence of the center-of-mass (c.m.) motion of the even core on the odd system is also discussed. The paper is organized as follows: the formulation of hRPA and its extension is given in Sec. II, some properties of the extended RPA are also discussed in Sec. II, the results obtained for the single-particle states around ^{16}O are presented in Sec. III, and Sec. IV is devoted to a discussion and the conclusion.

II. FORMULATION

Let us consider a nucleus consisting of A nucleons and assume that the total Hamiltonian H consists of the kinetic energy term and a two-body interaction. Let us assume that $|0\rangle$ is the ground state of the A nucleon system with A even and with energy E_0 and $|\mu\rangle$ an exact eigenstate of the Hamiltonian for the $A-1$ system with an eigenvalue E_μ ($H|\mu\rangle = E_\mu|\mu\rangle$).

A. Equations of motion for transition amplitudes

In direct reaction theories such as the the distorted wave impulse approximation and the distorted wave Born approximation the differential cross section for one nucleon transfer reactions is related to the spectral function $S_{\alpha\alpha'}(\omega)$,

$$S_{\alpha\alpha'}(\omega) = \sum_\mu \langle 0|a^+_{\alpha'}|\mu\rangle\langle\mu|a_\alpha|0\rangle\delta(\omega + E_\mu - E_0), \quad (1)$$

where a_α and a^+_α are the annihilation and creation operators of a nucleon in a single-particle state α, respectively. We consider the equations of motion for the transition amplitudes x^μ_α and $X^\mu_{\alpha\beta:\gamma}$ from the A nucleon system to the $A-1$ nucleon system. These amplitudes are defined by

$$x^\mu_\alpha = \langle 0|a^+_\alpha|\mu\rangle, \quad (2)$$
$$X^\mu_{\alpha\beta:\gamma} = \langle 0| : a^+_\alpha a^+_\beta a_\gamma : |\mu\rangle, \quad (3)$$

where :: implies

$$: a^+_\alpha a^+_\beta a_\gamma := a^+_\alpha a^+_\beta a_\gamma - (n_{\gamma\beta}a^+_\alpha - n_{\gamma\alpha}a^+_\beta). \quad (4)$$

Here, $n_{\alpha\alpha'}$ is the occupation matrix given by

$$n_{\alpha\alpha'} = \langle 0|a^+_{\alpha'}a_\alpha|0\rangle. \quad (5)$$

From the EoM relation,

$$\langle 0|[H, a^+_\alpha] = \langle 0|a^+_\alpha(E_0 - H), \quad (6)$$

we obtain the equation for x^μ_α,

$$\langle 0|[H, a^+_\alpha]|\mu\rangle = \omega_\mu\langle 0|a^+_\alpha|\mu\rangle = \omega_\mu x^\mu_\alpha, \quad (7)$$

where $\omega_\mu = E_0 - E_\mu$. The commutator on the left-hand side of the above equation includes terms with $a^+_\alpha a^+_\beta a_\gamma$. Therefore, x^μ_α couples to $X^\mu_{\alpha\beta:\gamma}$. In a way analogous to that used in deriving

Eq. (7), we obtain the equation for $X^{\mu}_{\alpha\beta:\gamma}$,

$$\langle 0|[H, :a^{+}_{\alpha}a^{+}_{\beta}a_{\gamma}:]|\mu\rangle = \omega_{\mu}\langle 0|:a^{+}_{\alpha}a^{+}_{\beta}a_{\gamma}:|\mu\rangle = \omega_{\mu}X^{\mu}_{\alpha\beta:\gamma}. \quad (8)$$

On the left-hand side of the above equation there appear expectation values of the terms consisting of three creation operators and two annihilation operators such as $\langle 0|a^{+}_{\lambda_1}a^{+}_{\lambda_2}a^{+}_{\lambda_3}a_{\lambda_4}a_{\lambda_5}|\mu\rangle$, which implies the coupling to a higher-level amplitude $\langle 0|:a^{+}_{\alpha}a^{+}_{\beta}a^{+}_{\gamma}a_{\beta'}a_{\alpha'}:|\mu\rangle$. To close the chain of the coupled equations, we factorize these terms using x^{μ}_{α} and $X^{\mu}_{\alpha\beta:\gamma}$ as

$$\langle 0|a^{+}_{\lambda_1}a^{+}_{\lambda_2}a^{+}_{\lambda_3}a_{\lambda_4}a_{\lambda_5}|\mu\rangle \approx \mathcal{A}S\big(n_{\lambda_4\lambda_3}X^{\mu}_{\lambda_1\lambda_2:\lambda_5} + C_{\lambda_5\lambda_4\lambda_2\lambda_3}x^{\mu}_{\lambda_1}\big), \quad (9)$$

where the correlation matrix $C_{\alpha\beta\alpha'\beta'}$ is defined by $C_{\alpha\beta\alpha'\beta'} = \langle 0|:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:|0\rangle$ and $\mathcal{A}S()$ means that the terms in the parentheses are properly antisymmetrized [12]. The obtained coupled equations are written as

$$(\epsilon_{\alpha}-\omega_{\mu})x^{\mu}_{\alpha} + \sum_{\lambda_1\lambda_2\lambda_3}\langle\lambda_1\lambda_2|v|\alpha\lambda_3\rangle X^{\mu}_{\lambda_1\lambda_2:\lambda_3} = 0, \quad (10)$$

$$\begin{aligned}(\epsilon_{\alpha}+\epsilon_{\beta}-\epsilon_{\gamma}-\omega_{\mu})X^{\mu}_{\alpha\beta:\gamma} &+ \sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \\ &\times\Big[\Big(\delta_{\lambda_3\alpha}\big((\delta_{\lambda_4\beta}-n_{\lambda_4\beta})n_{\gamma\lambda_2}-C_{\gamma\lambda_4\lambda_2\beta}\big) \\ &+\delta_{\lambda_3\beta}\big(n_{\lambda_4\alpha}n_{\gamma\lambda_2}+C_{\gamma\lambda_4\lambda_2\alpha}\big) \\ &+\delta_{\lambda_2\gamma}\Big(n_{\lambda_3\alpha}n_{\lambda_4\beta}+\frac{1}{2}C_{\lambda_3\lambda_4\alpha\beta}\Big)\Big)x^{\mu}_{\lambda_1} \\ &+\delta_{\lambda_3\alpha}n_{\gamma\lambda_1}X^{\mu}_{\lambda_2\beta:\lambda_4}+\delta_{\lambda_3\beta}n_{\gamma\lambda_2}X^{\mu}_{\lambda_1\alpha:\lambda_4} \\ &-\delta_{\lambda_1\gamma}\big(n_{\lambda_4\alpha}X^{\mu}_{\beta\lambda_2:\lambda_3}+n_{\lambda_3\beta}X^{\mu}_{\alpha\lambda_2:\lambda_4}\big) \\ &+\frac{1}{2}\big(\delta_{\lambda_3\alpha}\delta_{\lambda_4\beta}-\delta_{\lambda_3\alpha}n_{\lambda_4\beta}+\delta_{\lambda_3\beta}n_{\lambda_4\alpha}\big)X^{\mu}_{\lambda_1\lambda_2:\gamma}\Big] = 0, \end{aligned} \quad (11)$$

where the subscript A means that the corresponding matrix is antisymmetrized and the single-particle states are chosen as the eigenstates of the matrix,

$$\langle\alpha|t|\alpha'\rangle + \sum_{\lambda\lambda'}\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A n_{\lambda'\lambda}. \quad (12)$$

Here t is the kinetic energy operator. Equations (10) and (11) are written in matrix form:

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix} = \omega_{\mu}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix}. \quad (13)$$

The matrix elements of the above equation are given in Appendix A. The normalization of the amplitudes is given by

$$(\tilde{x}^{\mu *}\tilde{X}^{\mu *})\begin{pmatrix} x^{\mu'} \\ X^{\mu'} \end{pmatrix} = \delta_{\mu\mu'}, \quad (14)$$

where $\tilde{x}^{\mu *}_{\alpha\alpha'}$ and $\tilde{X}^{\mu *}_{\alpha\beta\alpha'\beta'}$ are the left eigenvector of Eq. (13). The occupation matrix and the correlation matrix, which enter Eq. (13) and which describe the ground-state correlations in the A nucleon system, can be determined in the framework of the time-dependent density matrix (TDDM) theory: the TDDM equations [12,14] consist of the coupled equations of motion for $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$,

$$i\hbar\dot{n}_{\alpha\alpha'} = \langle 0|[a^{+}_{\alpha'}a_{\alpha}, H]0\rangle, \quad (15)$$

$$i\hbar\dot{C}_{\alpha\beta\alpha'\beta'} = \langle 0|[:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:, H]|0\rangle. \quad (16)$$

The right-hand side of Eq. (16) contains the expectation values of three-body operators, which are approximated by the products of $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$ to close the coupled chain of the equations of motion. The ground state in TDDM is given as a stationary solution of the TDDM equations which satisfies $\dot{n}_{\alpha\alpha'} = 0$ and $\dot{C}_{\alpha\beta\alpha'\beta'} = 0$. The stationary solution can be obtained using the gradient method [15]. This method will be used in our numerical application given later.

In the Hartree-Fock approximation (HF), $n_{\alpha\alpha'} = \delta_{\alpha\alpha'}$ for hole states and $n_{\alpha\alpha'} = 0$ for particle states, and $C_{\alpha\beta\alpha'\beta'} = 0$. Keeping in Eq. (13) only the amplitudes $x^{\mu}_{\rm h}$ and $X^{\mu}_{\rm hh':p}$, where subscripts h and p are used to refer to occupied and unoccupied single-particle states, respectively, corresponds to the TDA equation of odd particle systems [16]. However, even within the HF ground state, Eq. (13) can have all components of $X^{\mu}_{\alpha\beta:\gamma}$; $X^{\mu}_{\rm hh':p}$, $X^{\mu}_{\rm pp':h}$, $X^{\mu}_{\rm hh':h''}$, $X^{\mu}_{\rm pp':p''}$, $X^{\mu}_{\rm hp:p'}$, and $X^{\mu}_{\rm hp:h'}$. Such equations have been proposed for the first time in Ref. [11] and they have been applied in Ref. [8]. This very much extended configuration space actually leads to some difficulties which have been discussed in Ref. [8]. We will take up this discussion again below.

In the following we discuss the relation of x^{μ}_{α} with $n_{\alpha\alpha}$. Using Eq. (10) for $x^{\mu}_{\alpha'}$ and $(\tilde{x}^{\mu}_{\alpha})^{*}$, we can eliminate ω_{μ} obtaining an equation for $\sum_{\mu}x^{\mu}_{\alpha'}(\tilde{x}^{\mu}_{\alpha})^{*}$,

$$\begin{aligned}(\epsilon_{\alpha}-\epsilon_{\alpha'})\sum_{\mu}x^{\mu}_{\alpha'}\big(\tilde{x}^{\mu}_{\alpha}\big)^{*} + \sum_{\lambda_1\lambda_2\lambda_3}\Big[\langle\alpha\lambda_3|v|\lambda_1\lambda_2\rangle\sum_{\mu}x^{\mu}_{\alpha'}\big(\tilde{\mathcal{X}}^{\mu}_{\lambda_1\lambda_2:\lambda_3}\big)^{*} \\ -\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle\sum_{\mu}X^{\mu}_{\lambda_1\lambda_2:\lambda_3}\big(\tilde{x}^{\mu}_{\alpha}\big)^{*}\Big] = 0, \end{aligned} \quad (17)$$

where $\tilde{\mathcal{X}}^{\mu}$ is the transition amplitude given by $\tilde{\mathcal{X}}^{\mu} = N_{22}\tilde{X}^{\mu}$ [17]. On the other hand the stationary condition $\dot{n}_{\alpha\alpha'} = 0$ for Eq. (15) gives [15]

$$\begin{aligned}(\epsilon_{\alpha}-\epsilon_{\alpha'})n_{\alpha\alpha'} + \sum_{\lambda_1\lambda_2\lambda_3}\big[&\langle\alpha\lambda_3|v|\lambda_1\lambda_2\rangle C_{\lambda_1\lambda_2\alpha'\lambda_3} \\ &-\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle C_{\alpha\lambda_3\lambda_1\lambda_2}\big] = 0. \end{aligned} \quad (18)$$

Equations (17) and (18) suggest that $\sum_{\mu}x^{\mu}_{\alpha'}(\tilde{x}^{\mu}_{\alpha})^{*}$ and $\sum_{\mu}X^{\mu}_{\alpha'\beta':\beta}(\tilde{x}^{\mu}_{\alpha})^{*}$ correspond to $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$, respectively, though the symmetry of $C_{\alpha\beta\alpha'\beta'}$ under the exchange of α and β is lost in $\sum_{\mu}X^{\mu}_{\alpha'\beta':\beta}(\tilde{x}^{\mu}_{\alpha})^{*}$. We will show below that $n_{\alpha\alpha} = \sum_{\mu}x^{\mu}_{\alpha}(\tilde{x}^{\mu}_{\alpha})^{*}$ approximately holds in the applications to ^{16}O.

The formulation based on Eqs. (7) and (8) is exact for an $A = 2$ system, which is given in Appendix B.

B. Equation of motion approach with excitation operator

Equation (13) lacks some effects such as self-energy contributions in the configuration $X^{\mu}_{\alpha\beta:\gamma}$, which should be included when a correlated ground state is used. To take

account of such effects, we present another formulation which is based on EoM [10]. Introducing the excitation operator q_μ^+,

$$q_\mu^+ = \sum_\alpha y_\alpha^\mu a_\alpha + \sum_{\alpha\beta\gamma} Y_{\alpha\beta:\gamma}^\mu : a_\gamma^+ a_\beta a_\alpha : \tag{19}$$

and assuming, as usual, $q_\mu^+|0\rangle = |\mu\rangle$ and $q_\mu|0\rangle = 0$ (for the existence of such a relation, see below), we obtain from Eqs. (7) and (8),

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix}, \tag{20}$$

where the matrices are defined as

$$A(\alpha : \alpha') = \langle 0|\{[H, a_\alpha^+], a_{\alpha'}\}|0\rangle, \tag{21}$$

$$B(\alpha\beta\gamma : \alpha') = \langle 0|\{[H, : a_\alpha^+ a_\beta^+ a_\gamma :], a_{\alpha'}\}|0\rangle, \tag{22}$$

$$C(\alpha : \alpha'\beta'\gamma') = \langle 0|\{[H, a_\alpha^+ :], : a_{\gamma'}^+ a_{\beta'} a_{\alpha'}\}|0\rangle, \tag{23}$$

$$D(\alpha\beta\gamma : \alpha'\beta'\gamma') = \langle 0|\{[H, : a_\alpha^+ a_\beta^+ a_\gamma :], : a_{\gamma'}^+ a_{\beta'} a_{\alpha'} :\}|0\rangle, \tag{24}$$

$$N_{11}(\alpha : \alpha') = \langle 0|\{a_\alpha^+, a_{\alpha'}\}|0\rangle = \delta_{\alpha\alpha'}, \tag{25}$$

$$N_{12}(\alpha : \alpha'\beta'\gamma') = \langle 0|\{a_\alpha^+, : a_{\gamma'}^+ a_{\beta'} a_{\alpha'} :\}|0\rangle = 0, \tag{26}$$

$$N_{21}(\alpha\beta\gamma : \alpha') = \langle 0|\{: a_\alpha^+ a_\beta^+ a_\gamma :, a_{\alpha'}\}|0\rangle = 0, \tag{27}$$

$$N_{22}(\alpha\beta\gamma : \alpha'\beta'\gamma') = \langle 0|\{: a_\alpha^+ a_\beta^+ a_\gamma, : a_{\gamma'}^+ a_{\beta'} a_{\alpha'} :\}|0\rangle. \tag{28}$$

Here $\{\}$ implies the anticommutator, $\{A, B\} = AB + BA$. The norm matrix N_{22} is given in Appendix A. The matrix elements in Eq. (20) can be expressed using those in Eq. (13) such as

$$A = a \times N_{11}, \tag{29}$$

$$B = b \times N_{11}, \tag{30}$$

$$C = c \times N_{22}. \tag{31}$$

The matrix D consists of the two types of terms, one expressed by $D_1 = d \times N_{22}$ and the other given by D_2, which originates from the terms with $: a_{\lambda_5}^+ a_{\lambda_4}^+ a_{\lambda_3}^+ a_{\lambda_2} a_{\lambda_1} :$ in $[H, : a_\alpha^+ a_\beta^+ a_\gamma :]$:

$$\begin{aligned}[H, : a_\alpha^+ a_\beta^+ a_\gamma :] &= \sum_{\alpha'} c(\alpha\beta\gamma : \lambda) a_{\alpha'}^+ + \sum_{\alpha'\beta'\gamma'} d(\alpha\beta\gamma : \alpha'\beta'\gamma') : a_{\alpha'}^+ a_{\beta'}^+ a_{\gamma'} : \\ &+ \sum_{\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5} e(\alpha\beta\gamma : \lambda_1\lambda_2\lambda_3\lambda_4\lambda_5) : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_3}^+ a_{\lambda_5} a_{\lambda_4} : .\end{aligned} \tag{32}$$

Using

$$\begin{aligned} &N_{32}(\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5 : \alpha\beta\gamma) \\ &= \langle 0|\{ : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_3}^+ a_{\lambda_5} a_{\lambda_4} :, : a_\gamma^+ a_\beta a_\alpha : \}|0\rangle, \end{aligned} \tag{33}$$

D_2 can be expressed as $e \times N_{32}$. These terms include, for example,

$$-\frac{1}{2}\delta_{\alpha\alpha'}\delta_{\beta\beta'} \sum_{\lambda_1\lambda_2\lambda_3} \langle\lambda_1\lambda_2|v|\gamma'\lambda_3\rangle_A C_{\gamma\lambda_3\lambda_1\lambda_2},$$

which is a self-energy contribution to the state γ. The self-energy contributions are schematically shown in Fig. 1.

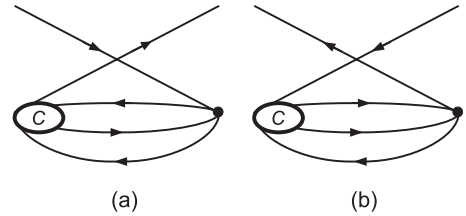


FIG. 1. (a) Self-energy contribution to a particle state and (b) to a hole state. The ellipses denote $C_{\alpha\beta\alpha'\beta'}$ and the dots the residual interaction.

The normalization of the amplitudes is given by

$$(y^{\mu*} Y^{\mu*}) \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \begin{pmatrix} y^{\mu'} \\ Y^{\mu'} \end{pmatrix} = \delta_{\mu\mu'}. \tag{34}$$

The closure relation is written as

$$\sum_\mu \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix} (y^{\mu*} Y^{\mu*}) \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} = I, \tag{35}$$

where I is the unit matrix. We refer to the formulation Eq. (20) as the extended odd-RPA (EoRPA).

In the following we discuss the relation between Eqs. (13) and (20). The transition amplitudes x_α^μ and $X_{\alpha\beta:\gamma}^\mu$ are given by y_α^μ and $Y_{\alpha\beta:\gamma}^\mu$ as

$$\begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix} = \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix}. \tag{36}$$

Inserting this expression into Eq. (13), we obtain

$$\begin{pmatrix} A & C \\ B & D_1 \end{pmatrix} \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \begin{pmatrix} y^\mu \\ Y^\mu \end{pmatrix}. \tag{37}$$

The difference between Eqs. (20) and (37) and thus between Eqs. (20) and (13) resides in the matrix D. Some effects of the ground-state correlations such as the self-energy contributions are missing in Eq. (37) and thus in Eq. (13) as mentioned above. The importance of these missing terms will be discussed below in the application section.

1. Symmetry properties

First we show that the Hamiltonian matrix of Eq. (20) is Hermitian. We use the operator identity,

$$\langle 0|\{[H, \hat{A}], \hat{B}\}|0\rangle + \langle 0|\{[H, \hat{B}], \hat{A}\}|0\rangle = \langle 0|[H, \{\hat{A}, \hat{B}\}]|0\rangle. \tag{38}$$

In Eq. (20), in the matrix A, the operators $\hat{A}$ and $\hat{B}$ are identified with a_α^+ and $a_{\alpha'}$, respectively. Because $\{\hat{A}, \hat{B}\}$ is unity, the right-hand side of Eq. (38) vanishes, which means $\langle 0|\{[H, \hat{A}], \hat{B}\}|0\rangle = -\langle 0|\{[H, \hat{B}], \hat{A}\}|0\rangle$ and

$$\begin{aligned} A(\alpha : \alpha')^* &= -\langle 0|\{[H, a_\alpha], a_{\alpha'}^+\}|0\rangle, \\ &= \langle 0|\{[H, a_{\alpha'}^+], a_\alpha\}|0\rangle = A(\alpha' : \alpha). \end{aligned} \tag{39}$$

In the case of the matrix B in Eq. (20) $\hat{A}$ is $: a_\alpha^+ a_\beta^+ a_\gamma :$ and $\hat{B}$ is $a_{\alpha'}$, and $\{\hat{A}, \hat{B}\}$ is reduced to a one-body operator. Due to the ground-state condition Eq. (15) the right-hand

side of Eq. (38) vanishes, which means $\langle 0|\{[H,\hat{A}],\hat{B}\}|0\rangle = -\langle 0|\{[H,\hat{B}],\hat{A}\}|0\rangle$ and

$$\begin{aligned} B(\alpha\beta\gamma:\alpha')^* &= -\langle 0|\{[H,:a^+_\gamma a_\beta a_\alpha:],a^+_{\alpha'}\}|0\rangle, \\ &= \langle 0|\{[H,a^+_{\alpha'}],:a^+_\gamma a_\beta a_\alpha:\}|0\rangle \\ &= C(\alpha':\alpha\beta\gamma). \end{aligned} \tag{40}$$

Similarly, for the matrix D in Eq. (20) $\hat{A}$ is $:a^+_\alpha a^+_\beta a_\gamma:$ and $\hat{B}$ is $:a^+_{\gamma'}a_{\beta'}a_{\alpha'}:$, and $\{\hat{A},\hat{B}\}$ is reduced to at most a two-body operator. Due to the ground-state conditions Eqs. (15) and (16) the right-hand side of Eq. (38) vanishes, which implies

$$D(\alpha\beta\gamma:\alpha'\beta'\gamma')^* = D(\alpha'\beta'\gamma':\alpha\beta\gamma). \tag{41}$$

Therefore, the Hamiltonian matrix in Eq. (20) is Hermitian. In the applications, shown below, we do not take all the matrix elements of $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$, which causes a violation of the Hermiticity of Eq. (20), though it will turn out to be small.

Next we discuss the relation between the formulations for a hole state and a particle state. We can obtain a formulation for a particle state using the excitation operator,

$$q^+_\mu = \sum_\alpha z^\mu_\alpha a^+_\alpha + \sum_{\alpha\beta\gamma} Z^\mu_{\alpha\beta:\gamma} :a^+_\alpha a^+_\beta a_\gamma:. \tag{42}$$

Because this operator is the conjugate of the hole-state excitation operator Eq. (19), it is easily shown that the formulation for a particle state is given as

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix}^t \begin{pmatrix} z^\mu \\ Z^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix}^t \begin{pmatrix} z^\mu \\ Z^\mu \end{pmatrix}, \tag{43}$$

where the superscript t means the transposition of the corresponding matrix and ω_μ is defined by $\omega_\mu = E_\mu - E_0$. Equation (43) implies that (z^μ, Z^μ) is the left-hand eigenvector of Eq. (20). Thus Eq. (20) gives simultaneously the particle states and the hole states. This is completely analogous to pp(hh)RPA (see Ref. [16]).

2. *Hartree-Fock approximation for the ground state*

If we make the usual approximation to take for the ground state $|0\rangle$ the HF one, N_{22} in Eq. (28) becomes

$$\begin{aligned} &N_{22}(\alpha\beta\gamma:\alpha'\beta'\gamma') \\ &= (\delta_{\alpha\alpha'}\delta_{\beta\beta'} - \delta_{\alpha\beta'}\delta_{\beta\alpha'})\delta_{\gamma'\gamma} \\ &\quad\times \left(n^0_{\gamma\gamma} + n^0_{\alpha\alpha}n^0_{\beta\beta} - n^0_{\gamma\gamma}n^0_{\alpha\alpha} - n^0_{\gamma\gamma}n^0_{\beta\beta}\right), \end{aligned} \tag{44}$$

where $n^0_{\alpha\alpha}$ is equal to 1 or 0. In HF, N_{22} is nonvanishing only for $Y^\mu_{\mathrm{pp':h}}$ and $Y^\mu_{\mathrm{hh':p}}$. These amplitudes $Y^\mu_{\mathrm{pp':h}}$ and $Y^\mu_{\mathrm{hh':p}}$ correspond to the backward amplitudes of y^μ_{h} and y^μ_{p}, respectively. Hereafter we refer to this formulation consisting of the four amplitudes, y^μ_{h}, y^μ_{p}, $Y^\mu_{\mathrm{pp':h}}$, and $Y^\mu_{\mathrm{hh':p}}$ as odd RPA (oRPA). For completeness, we give the full expression of oRPA,

$$\begin{aligned} &(\epsilon_\alpha - \omega_\mu)y^\mu_\alpha + \sum_{\mathrm{pp'h}}\langle \mathrm{pp'}|v|\alpha h\rangle \tilde{Y}^\mu_{\mathrm{pp':h}} + \sum_{\mathrm{hh'p}}\langle \mathrm{hh'}|v|\alpha p\rangle \tilde{Y}^\mu_{\mathrm{hh':p}} \\ &= 0, \end{aligned} \tag{45}$$

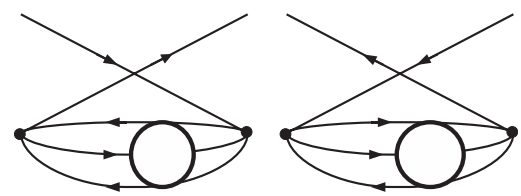
(a) (b)

FIG. 2. (a) Mass operator for a particle state described by $Y^\mu_{\mathrm{pp':h}}$ and (b) for a hole state described by $Y^\mu_{\mathrm{hh':p}}$. The circles mean the propagators given by $Y^\mu_{\mathrm{pp':h}}$ (a) and $Y^\mu_{\mathrm{hh':p}}$ (b), and the dots the residual interaction.

$$\begin{aligned} &(\epsilon_{\mathrm{p}} + \epsilon_{\mathrm{p'}} - \epsilon_{\mathrm{h}} - \omega_\mu)\tilde{Y}^\mu_{\mathrm{pp':h}} + \sum_\alpha \langle \alpha\mathrm{h}|v|\mathrm{pp'}\rangle_A y^\mu_\alpha \\ &\quad + \sum_{\mathrm{p_1p_2}}\langle \mathrm{p_1p_2}|v|\mathrm{pp'}\rangle \tilde{Y}^\mu_{\mathrm{p_1p_2:h}} + \sum_{p_1h_1}\Big[\langle \mathrm{hp_1}|v|\mathrm{ph_1}\rangle_A \tilde{Y}^\mu_{\mathrm{p_1p':h_1}} \\ &\quad + \langle \mathrm{hp_1}|v|\mathrm{p'h_1}\rangle_A \tilde{Y}^\mu_{\mathrm{pp_1:h_1}}\Big] = 0, \end{aligned} \tag{46}$$

$$\begin{aligned} &(\epsilon_{\mathrm{h}} + \epsilon_{\mathrm{h'}} - \epsilon_{\mathrm{p}} - \omega_\mu)\tilde{Y}^\mu_{\mathrm{hh':p}} + \sum_\alpha \langle \alpha\mathrm{p}|v|\mathrm{hh'}\rangle_A y^\mu_\alpha \\ &\quad - \sum_{\mathrm{h_1h_2}}\langle \mathrm{h_1h_2}|v|\mathrm{hh'}\rangle \tilde{Y}^\mu_{\mathrm{h_1h_2:p}} - \sum_{\mathrm{p_1h_1}}\Big[\langle \mathrm{ph_1}|v|\mathrm{hp_1}\rangle_A \tilde{Y}^\mu_{\mathrm{h_1h':p_1}} \\ &\quad + \langle \mathrm{ph_1}|v|\mathrm{h'p_1}\rangle_A \tilde{Y}^\mu_{\mathrm{hh_1:p_1}}\Big] = 0, \end{aligned} \tag{47}$$

where y^μ_α denotes y^μ_{h} and y^μ_{p}, and $\tilde{Y}^\mu_{\alpha\beta:\gamma}$ means $Y^\mu_{\alpha\beta:\gamma} - Y^\mu_{\beta\alpha:\gamma}$. The mass operators of the one-body Green's function derived from oRPA are schematically shown in Figs. 2 and 3 (see Appendix C). Becausee oRPA describes the hole states and particle states simultaneously, the single-particle strength can be spread over both positive and negative energy regions. We consider that the strength below the Fermi energy ϵ_F of the core nucleus belongs to the states in the $A-1$ system, while that above ϵ_F to the states in the $A+1$ system. The TDA hole-state equation is obtained by keeping only y^μ_{h} and $Y^\mu_{\mathrm{hh':p}}$: Because the coupling of y^μ_{h} to $Y^\mu_{\mathrm{hh':p}}$ is included in addition to the coupling to the backward amplitude $Y^\mu_{\mathrm{pp':h}}$, our oRPA actually corresponds to some sort of second RPA for even nucleon systems. One may think that in addition the amplitudes $Y^\mu_{\mathrm{hp:h'}}$ and $Y^\mu_{\mathrm{pp':p''}}$ should be included in oRPA because they, respectively, express the backward propagations of the particle-hole pair and the hole-hole pair in $Y^\mu_{\mathrm{hh':p}}$. However, these amplitudes cannot be included because the norm of these amplitudes is not defined in HF (the matrix elements N_{22} for $Y^\mu_{\mathrm{hp:h'}}$ and $Y^\mu_{\mathrm{pp':p''}}$ vanish in HF). As mentioned above, the formulation Eq. (13) allows us to implement all the $X^\mu_{\alpha\beta:\gamma}$ amplitudes including $X^\mu_{\mathrm{hp:h'}}$ and



(a) (b)

FIG. 3. (a) Mass operator for a particle state described by $Y^\mu_{\mathrm{hh':p}}$ and (b) for a hole state described by $Y^\mu_{\mathrm{pp':h}}$. The circles mean the propagators given by $Y^\mu_{\mathrm{hh':p}}$ (a) and $Y^\mu_{\mathrm{pp':h}}$ (b), and the dots the residual interaction.

$X^{\mu}_{\mathrm{pp}':\mathrm{p}''}$ because there is no restriction of the norm matrix. [If Eq. (37) is used instead of Eq. (13), $X^{\mu}_{\mathrm{hp:h}'}$ and $X^{\mu}_{\mathrm{pp}':\mathrm{p}''}$ are projected out, however.] The inclusion of all the amplitudes of $X^{\mu}_{\alpha\beta:\gamma}$ can give quite unphysical results because the sum of some unperturbed energies corresponding to $X^{\mu}_{\alpha\beta:\gamma}$ fall near ϵ_F, which makes it difficult to distinguish the hole states from the particle states (see also Ref. [8]). For these reasons we mainly present the results in EoRPA calculated using only the four amplitudes corresponding to y^{μ}_{h}, y^{μ}_{p}, $Y^{\mu}_{\mathrm{pp}':\mathrm{h}}$, and $Y^{\mu}_{\mathrm{hh}':\mathrm{p}}$ in oRPA, although the matrix elements of N_{22} are nonvanishing for all configurations due to the ground-state correlations and, therefore, all other $Y^{\mu}_{\alpha\beta:\gamma}$ could be included, in principle. We investigate the effect of inclusion of those other amplitudes in EoRPA in some limited cases.

3. The RPA ground-state wave function

The choice of the subspace spanned by the aforementioned four amplitudes $y^{\mu}_{\mathrm{h}}, y^{\mu}_{\mathrm{p}}, Y^{\mu}_{\mathrm{pp}':\mathrm{h}}, Y^{\mu}_{\mathrm{hh}':\mathrm{p}}$ may be given a different rationale. We consider the following two quasiparticle operators which consist only of the forward and backward amplitudes,

$$q^{+}_{\alpha} = \sum_{\mathrm{p}} y^{\alpha}_{\mathrm{p}} a^{+}_{\mathrm{p}} - \frac{1}{2}\sum_{\mathrm{hh}'\mathrm{p}} Y^{\alpha}_{\mathrm{hh}':\mathrm{p}} a^{+}_{\mathrm{h}} a^{+}_{\mathrm{h}'} a_{\mathrm{p}}, \tag{48}$$

$$q^{+}_{\rho} = \sum_{\mathrm{h}} y^{\rho}_{\mathrm{h}} a_{\mathrm{h}} - \frac{1}{2}\sum_{\mathrm{pp}'\mathrm{h}} Y^{\rho}_{\mathrm{pp}':\mathrm{h}} a^{+}_{\mathrm{h}} a_{\mathrm{p}} a_{\mathrm{p}'}, \tag{49}$$

and neglect the coupling of y^{α}_{p} to $Y^{\alpha}_{\mathrm{pp}':\mathrm{h}}$ and that of y^{ρ}_{h} to $Y^{\rho}_{\mathrm{hh}':\mathrm{p}}$. This oRPA scheme actually corresponds to the standard RPA for even nucleon systems. This can, for example, be seen in the following way. It can easily be shown that the operators q_{α} and q_{ρ} kill the following RPA vacuum, i.e., $q|Z\rangle = 0$ with

$$|Z\rangle = e^{\frac{1}{4}\sum z_{\mathrm{pp}'\mathrm{hh}'} a^{+}_{\mathrm{p}} a_{\mathrm{h}} a^{+}_{\mathrm{p}'} a_{\mathrm{h}'}} |\mathrm{HF}\rangle, \tag{50}$$

under the conditions,

$$\sum_{\mathrm{p}} y^{\alpha *}_{\mathrm{p}} z_{\mathrm{pp}'\mathrm{hh}'} = Y^{\alpha *}_{\mathrm{hh}':\mathrm{p}'}, \tag{51}$$

$$\sum_{h} y^{\rho *}_{h} z_{\mathrm{pp}'\mathrm{hh}'} = Y^{\rho *}_{\mathrm{pp}':\mathrm{h}'}, \tag{52}$$

where $|\mathrm{HF}\rangle$ is the HF ground state of an even A system.

These two quasiparticles [one for the particle addition (α) and one for the particle removal (ρ)] span, as seen, exactly the space of the four amplitudes discussed in Sec. II B2. However, the single equation for the four amplitudes is now split into two independent 2×2 equations corresponding to the two operators introduced in Eqs. (48) and (49), respectively. Using in these equations the HF ground state as in Sec. II B2, we see that we have one type of "forward" going amplitudes and one type of "backward going" amplitudes in analogy with what we know from standard ph-RPA for even systems with corresponding amplitudes X and Y. As a matter of fact, it recently was shown [18] that also for the standard ph-RPA a generalized operator can be found which annihilates the state Eq. (50). It is given by the following form:

$$Q_{\nu} = \sum_{\mathrm{ph}} \left[X^{\nu *}_{\mathrm{ph}} a^{+}_{\mathrm{h}} a_{\mathrm{p}} - Y^{\nu *}_{\mathrm{ph}} a^{+}_{\mathrm{p}} a_{\mathrm{h}} \right] + \frac{1}{2}\sum_{\mathrm{php}_1\mathrm{p}_2} \eta^{\nu}_{\mathrm{p}_1\mathrm{p}_2\mathrm{ph}} a^{+}_{\mathrm{p}_2} a_{\mathrm{p}_1} a^{+}_{\mathrm{p}} a_{\mathrm{h}} - \frac{1}{2}\sum_{\mathrm{phh}_1\mathrm{h}_2} \eta^{\nu}_{\mathrm{h}_1\mathrm{h}_2\mathrm{ph}} a^{+}_{\mathrm{h}_1} a_{\mathrm{h}_2} a^{+}_{\mathrm{p}} a_{\mathrm{h}}. \tag{53}$$

This destruction operator kills the vacuum Eq. (50), i.e., $Q|Z\rangle = 0$, under the conditions,

$$z_{\mathrm{php}'\mathrm{h}'} = \sum_{\nu} (X^{-1})^{\nu}_{\mathrm{ph}} Y^{\nu}_{\mathrm{p}'\mathrm{h}'}, \tag{54}$$

$$\eta^{\nu}_{\mathrm{p}_1\mathrm{p}_2\mathrm{ph}} = \frac{1}{2}\sum_{\mathrm{h}_1} X^{\nu}_{\mathrm{p}_1\mathrm{h}_1} z_{\mathrm{pp}_2\mathrm{hh}_1}, \tag{55}$$

$$\eta^{\nu}_{\mathrm{h}_1\mathrm{h}_2\mathrm{ph}} = \frac{1}{2}\sum_{\mathrm{p}_1} X^{\nu}_{\mathrm{p}_1\mathrm{h}_1} z_{\mathrm{pp}_1\mathrm{hh}_2}. \tag{56}$$

We see that there are additional terms to the standard ph-RPA operator which contain specific two-body terms. The corresponding terms in Q^{+}_{ν} can schematically be obtained in augmenting the addition operator Eq. (48) by a destructor a_{h} and the removal operator Eq. (49) by a creator a^{+}_{p}. The η terms are also small-amplitude (backward-going) terms which can be added to the standard RPA, evaluated with the HF state. They improve the results of the standard RPA [19]. We, therefore, see that complete consistency between the RPA in even and odd systems can be achieved.

It may be instructive to cast the above amplitude equations into Green's function language, which is given in Appendix C.

4. Spurious modes

First we discuss an RPA-like formulation that can bring the c.m. motion of an odd system at zero excitation energy. We consider for an $A+1$ system the ground state $|\Phi_0\rangle$ and an excited state $|\Phi_{\mu}\rangle$ with excitation energy ω_{μ}. Using the equation of motion,

$$\begin{aligned}\langle\Phi_0|[a^{+}_{\alpha'}a_{\alpha}, H]|\Phi_{\mu}\rangle &= \omega_{\mu}\langle\Phi_0|a^{+}_{\alpha'}a_{\alpha}|\Phi_{\mu}\rangle \\ &= \omega_{\mu} x^{\mu}_{\alpha\alpha'},\end{aligned} \tag{57}$$

and assuming $|\Phi_0\rangle = a^{+}_{p}|\mathrm{HF}\rangle$, we obtain the following equation:

$$\begin{aligned}\omega_{\mu} x^{\mu}_{\alpha\alpha'} &= (\epsilon_{\alpha} - \epsilon_{\alpha'}) x^{\mu}_{\alpha\alpha'} \\ &\quad - \left(n^{0}_{\alpha\alpha} - n^{0}_{\alpha'\alpha'}\right)\sum_{\lambda\lambda'} \langle\alpha\lambda'|v|\alpha'\lambda\rangle_{A} x^{\mu}_{\lambda\lambda'} \\ &\quad + \sum_{\lambda\lambda'}\left[\delta_{\alpha p}\langle p\lambda'|v|\alpha'\lambda\rangle_{A} - \delta_{\alpha' p}\langle\alpha\lambda'|v|p\lambda\rangle_{A}\right] x^{\mu}_{\lambda\lambda'} \\ &\quad + \sum_{\lambda}\left[\langle\alpha p|v|\lambda p\rangle_{A} x^{\mu}_{\lambda\alpha'} - \langle\lambda p|v|\alpha' p\rangle_{A} x^{\mu}_{\alpha\lambda}\right].\end{aligned} \tag{58}$$

The first two lines of the above equation have the same form as the standard RPA for an even A system, and the third and fourth terms are due to the additional nucleon in a particle state p. For the total momentum operator,

$$\boldsymbol{P} = \sum_{\alpha\alpha'} \langle\alpha'| - i\hbar\nabla|\alpha\rangle a^{+}_{\alpha'} a_{\alpha}, \tag{59}$$

which satisfies $[\boldsymbol{P}, H] = 0$, we evaluate $\omega_\mu \langle \Phi_0 | \boldsymbol{P} | \Phi_\mu \rangle$ as

$$\omega_\mu \langle \Phi_0 | \boldsymbol{P} | \Phi_\mu \rangle = \sum_{\alpha\alpha'} \langle \alpha' | -i\hbar\nabla | \alpha \rangle \omega_\mu x^\mu_{\alpha\alpha'}. \quad (60)$$

Using the right-hand side of Eq. (58) and the translational invariance of the interaction [20], we can show $\omega_\mu \langle \Phi_0 | \boldsymbol{P} | \Phi_\mu \rangle = 0$, which implies $\omega_\mu = 0$. Thus the excitation energy of the c.m. motion of an odd system given by Eq. (58) is zero from the ground state $|\Phi_0\rangle$ and ϵ_p from $|\mathrm{HF}\rangle$. To obtain this conclusion, however, we need to include all components of $x^\mu_{\alpha\alpha'}$ because of the last two terms on the right-hand side of Eq. (58).

Now we discuss the c.m. of a core nucleus in odd A nuclei whose treatment is of particular relevance. In the standard particle vibration coupling model [3,5] the spurious mode is simply discarded, first, for the translational mode, on physical grounds but also because the RPA amplitudes of a zero mode cannot be normalized. On the other hand, e.g., in the case of rotations, it would be very important to find a way to include the rotational mode, because it is a physical state. To learn something about the coupling of single-particle motion and recoil of the core nucleus, we first show that $\omega_\mu \langle \mu | \boldsymbol{P} a_\alpha | 0 \rangle = \epsilon_\alpha \langle \mu | a_\alpha | 0 \rangle$ holds in the mean-field approximation. Using the complex conjugate of Eq. (8), we evaluate $\omega_\mu \langle \mu | \boldsymbol{P} a_\alpha | 0 \rangle$ such that

$$\begin{aligned} \omega_\mu \langle \mu | \boldsymbol{P} a_\alpha | 0 \rangle &= \langle \mu | [\boldsymbol{P} a_\alpha, H] | 0 \rangle \\ &= \langle \mu | [\boldsymbol{P}, H] a_\alpha | 0 \rangle + \langle \mu | \boldsymbol{P} [a_\alpha, H] | 0 \rangle \\ &= \langle \mu | \boldsymbol{P} [a_\alpha, H] | 0 \rangle, \end{aligned} \quad (61)$$

where we use $[\boldsymbol{P}, H] = 0$. If we use the mean-field approximation for $[a_\alpha, H]$, that is, $[a_\alpha, H] = \epsilon_\alpha a_\alpha$, then we obtain $\omega_\mu \langle \mu | \boldsymbol{P} a_\alpha | 0 \rangle = \epsilon_\alpha \langle \mu | a_\alpha | 0 \rangle$, which means that the strength $|\langle \mu | \boldsymbol{P} a_\alpha | 0 \rangle|^2$ is concentrated at the state with $\omega_\mu = \epsilon_\alpha$. In the general case the mean-field approximation is not valid as Eq. (10) indicates. In the realistic applications of our oRPA or EoRPA approaches shown below, we will, therefore, see that a large portion of the strength is distributed to an energy region lower than ϵ_α, which can be interpreted as a recoil effect of the core nucleus.

In the past, the question of the spurious modes appeared essentially in the particle-vibration coupling model [5] which is derived from the Green's function method factorizing in the mass operator the 2p-1h (2h-1p) propagator into an ph-RPA propagator and a HF single-particle propagator. In the spectral representation of the RPA propagator the spurious mode is then discarded because of the zero energy mode and the ensuing diverging amplitudes. On the other hand, if one could solve the 2p-1h (2h-1p) propagator in the mass operator exactly (e.g., in a model) or with a consistent higher order theory, surely no problem with a spurious motion of the core nucleus would be present. From our analysis above, it appears that the mass operator should be calculated with 2h-1p (2p-1h) TDA amplitudes. It could very well be that this approach gives more realistic results than the particle vibration coupling model where the spurious mode is discarded. That is what our derivation seems to indicate.

In any case, e.g., in the case of rotations, it would be necessary to include this mode, because it is physical. One could push the argument even further and assume that, because, e.g., the rotation is very collective, the factorization of the 2h-1p (2p-1h) TDA into a ph-TDA + plus a hole (particle) is a good approximation (the neglected terms coming only from exchange). Because of its strong collectivity, eventually all the other couplings to intrinsic ph modes could be neglected. Actually analogous questions would arise in cold fermionic atom systems where one could ask the question what happens to an odd fermion which is coupled to the so-called Kohn mode, i.e., a coherent c.m. motion of the underlying even system, in the external harmonic container. Because the mass of the core can be very large, e.g., with a million atoms, the factorization can become quite valid and also the ph-TDA for the Kohn mode will become very collective. It could be interesting to investigate this question in more detail theoretically and experimentally because the treatment of Goldstone modes in single-particle mass operators is, to the best of our knowledge, an unsolved problem.

III. APPLICATIONS TO ^{16}O

A. Calculational details

In this paper, we make a first schematic application of our theory to proton hole states in ^{15}N and proton particle states in ^{17}F. We do not consider the corresponding neutron states because there are less experimental data. We consider the $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$, $2s_{1/2}$, $1d_{3/2}$, $2p_{3/2}$, $2p_{1/2}$, $1f_{7/2}$, and $1f_{5/2}$ states for both protons and neutrons. The continuum states are discretized by confining the single-particle wave functions in a sphere of radius 12 fm. We use a simplified residual interaction which consists only of the t_0 and t_3 terms of the Skyrme III force. Its strength is reduced by 20% to put the spurious c.m. motion of ^{16}O at approximately zero energy in the standard RPA. For the ground-state calculation of ^{16}O in TDDM, we only use the bound single-particle states, the $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$, and $2s_{1/2}$ states, and consider only the two-particle–two-hole-type correlations in $C_{\alpha\beta\alpha'\beta'}$. We also neglect the off-diagonal elements of $n_{\alpha\alpha'}$ between the $1s_{1/2}$ and $2s_{1/2}$ states. The y^μ_p amplitudes for the proton $2s_{1/2}$, $2p_{1/2}$, and $2p_{1/2}$ states are neglected because their contributions are negligible.

B. Ground state

The occupation probabilities calculated in TDDM are shown in Table I. The largest deviation from the HF values ($n^0_{\alpha\alpha} = 1$ or 0) is about 10%, which means that the ground

TABLE I. Single-particle energies ϵ_α and occupation probabilities $n_{\alpha\alpha}$ calculated in TDDM. The single-particle energies in HF are given in parentheses.

Orbit	ϵ_α (MeV)		$n_{\alpha\alpha}$	
	Proton	Neutron	Proton	Neutron
$1s_{1/2}$	−32.5 (−32.1)	−36.2 (−35.9)	0.98	0.98
$1p_{3/2}$	−18.3 (−18.2)	−21.8 (−21.8)	0.93	0.93
$1p_{1/2}$	−12.3 (−12.0)	−15.8 (−15.6)	0.91	0.91
$1d_{5/2}$	−3.8 (−3.8)	−7.1 (−7.2)	0.08	0.08
$2s_{1/2}$	1.2 (1.5)	−1.5 (−1.2)	0.02	0.02

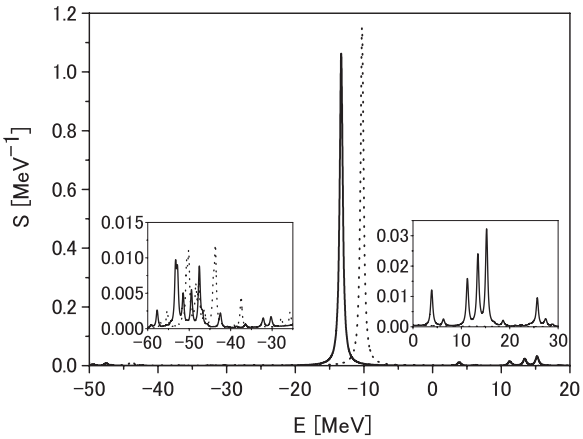


FIG. 4. Spectral function of the proton $1p_{1/2}$ state in ^{15}N calculated in EoRPA (solid line). The dotted line shows the result in TDA. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV. The strength distribution in the positive energy region is due to the coupling to the backward amplitude $Y^{\mu}_{\mathrm{pp'{:}h}}$ and indicates the states in ^{17}F. The small strength distributions in the positive and negative energy regions are shown in the insets.

state of ^{16}O is a strongly correlated state. A recent shell-model calculation by Utsuno and Chiba [21] also gives a similar result for the ground state of ^{16}O. The correlation energy E_c in the ground state, which is defined by $E_c = \sum_{\alpha\beta\alpha'\beta'}\langle\alpha\beta|v|\alpha'\beta'\rangle C_{\alpha'\beta'\alpha\beta}/2$, is -19.6 MeV. A large portion of the correlation energy is compensated by the increase in the mean-field energy due to the fractional occupation of the single-particle states. The resulting energy gain due to the ground-state correlations, which is given by the total energy difference between HF and TDDM, is with 5.2 MeV relatively small. Such kind of scenario is similar to the one well known from BCS theory [16].

C. Spectral functions

In Figs. 4 and 5 the spectral functions of the proton $1p_{1/2}$ and $1p_{3/2}$ hole states in ^{15}N calculated in EoRPA [Eq. (20)] (solid line) are shown, respectively, and compared with the results in TDA (dotted line). Because the results in oRPA are similar to the EoRPA results, they are not shown. As already mentioned, in the EoRPA calculations we consider only the same $Y^{\mu}_{\alpha\beta:\gamma}$ amplitudes as those used in oRPA. To facilitate a comparison of various calculations, we smooth the distributions using an artificial width $\Gamma = 0.5$ MeV. As shown in Table I the HF energies of the proton $1p_{1/2}$ and $1p_{3/2}$ states are -12.0 MeV and -18.2 MeV, respectively. In TDA the main peak is shifted upwards from the HF position due to the coupling to the configurations $Y^{\mu}_{\mathrm{hh'{:}p}}$ whose unperturbed energies are distributed below -40 MeV. In EoRPA (and oRPA) the main peak is slightly shifted downwards from the HF position due to the coupling to both $Y^{\mu}_{\mathrm{hh'{:}p}}$ and the backward amplitudes $Y^{\mu}_{\mathrm{pp'{:}h}}$ whose unperturbed energies are located above 0 MeV (see Figs. 4 and 5). The strength distribution in the positive energy region corresponds to the states in ^{17}F. The strengths of the main peak of the proton $1p_{1/2}$ state calculated in EoRPA, oRPA, and TDA are 0.88, 0.82, and 0.95, respectively. When the forward amplitude $Y^{\mu}_{\mathrm{hh'{:}p}}$ is neglected in oRPA, the main peak is further shifted down to -14.9 MeV and has strength 0.89. This indicates that the coupling to the backward amplitudes $Y^{\mu}_{\mathrm{pp'{:}h}}$ plays an important role in depleting the single-particle strength. The effects of the ground-state correlations included in EoRPA play a role in slightly reducing the correlations in oRPA due to fractional occupation of the single-particle states. The sum of the strength of the proton $1p_{1/2}$ state distributed in the negative energy region is 0.91 in EoRPA, which corresponds to $n_{\alpha\alpha} = 0.91$ in TDDM, (see Table I). Thus the relation $n_{\alpha\alpha} = \sum_{\mu}|\langle\mu|a_{\alpha}|0\rangle|^2$ holds to a good approximation. The single-particle strengths of the main peak of the proton $1p_{3/2}$ state calculated in EoRPA, RPA, and TDA are 0.88, 0.82, and 0.93, respectively. The sum of the occupation probabilities of the proton $1p_{3/2}$ state distributed in the negative energy region is 0.93 in EoRPA, which corresponds to $n_{\alpha\alpha} = 0.93$ in TDDM. Summing the whole spectral weights in negative and positive energy regions gives, of course, the sum rule value of one.

The results for the proton $1s_{1/2}$ state are shown in Fig. 6. The HF energy of the proton $1s_{1/2}$ hole state is -32.1 MeV. The strength is fragmented due to the coupling to the configurations $Y^{\mu}_{\mathrm{hh'{:}p}}$: The unperturbed energy of the configuration $(1p_{1/2})^{-1}(1p_{3/2})^{-1}1d_{5/2}$ is about -26 MeV. Because the

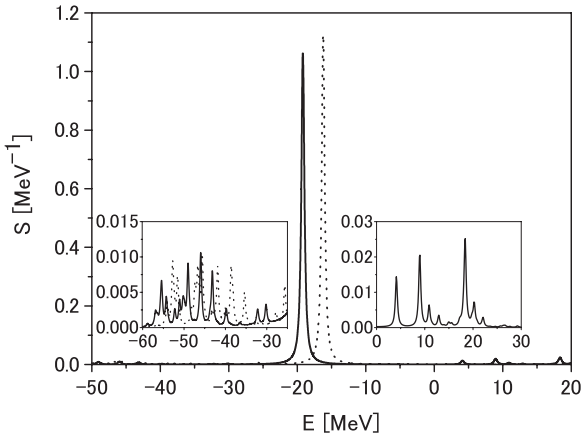


FIG. 5. Same as Fig. 4 but for the proton $1p_{3/2}$ state.

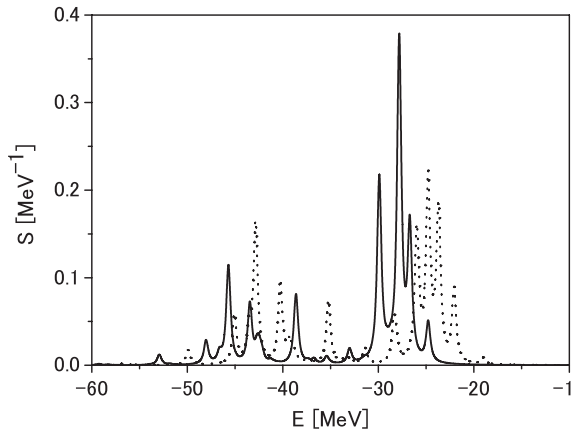


FIG. 6. Same as Fig. 4 but for the proton $1s_{1/2}$ state.

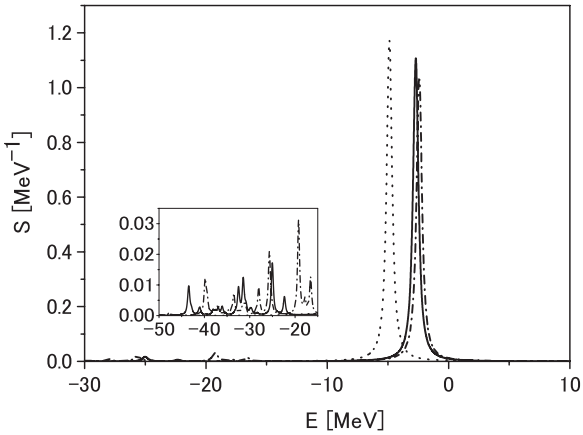


FIG. 7. Same as Fig. 4 but for the proton $1d_{5/2}$ state in ^{17}F. The dot-dashed line shows the result in oRPA. The strength distribution below -15 MeV is due to the coupling to the backward amplitude $Y^{\mu}_{\mathrm{hh'}:\mathrm{p}}$ and shows the states in ^{15}N.

backward configurations $Y^{\mu}_{\mathrm{pp'}:\mathrm{h}}$ are energetically well separated, there is no significant difference between the TDA and oRPA results. Therefore, the oRPA result is not shown in Fig. 6. Comparing with the results obtained from Eq. (37), we found that the D_2 term in the matrix D, which is given by $e \times N_{32}$ and describes the self-energy contributions to the one-particle–two-hole configurations, play a role in shifting the strength to lower energy region. The summed occupation probability of the proton $1s_{1/2}$ state distributed in the negative energy region is 0.98 in EoRPA, which corresponds to $n_{\alpha\alpha} = 0.98$ in TDDM.

The spectral function of the proton $1d_{5/2}$ state in ^{17}F is shown in Fig. 7. The HF energy of the $1d_{5/2}$ state is -3.8 MeV. The main peak is shifted downwards from the HF position in TDA due to the coupling to $Y^{\mu}_{\mathrm{pp'}:\mathrm{h}}$, while, on the contrary, it is shifted upward in oRPA due to the additional coupling to the backward amplitudes $Y^{\mu}_{\mathrm{hh'}:\mathrm{p}}$. The ground-state correlations included in EoRPA play a role in slightly reducing correlations in oRPA. The states located below the single-particle energy of the proton $1p_{1/2}$ state correspond to the states in ^{15}N. The summed occupation probability of the proton $1d_{5/2}$ state distributed below the proton $1p_{1/2}$ state is 0.06 in EoRPA, while the corresponding value for $n_{\alpha\alpha}$ in TDDM is 0.08.

D. Comparison with experiment

The spectroscopic factors [defined by $(2j+1)\times$transition strength] calculated in EoRPA for the proton $1p_{1/2}$ and $1p_{3/2}$ states are compared with experiment [22] (red bars) in Fig. 8. The main peak of the proton $1p_{1/2}$ state is considered as the ground state of ^{15}N and the hole-state energy is measured from this threshold in the following. The results in EoRPA are reasonable though they overestimate the experimental data and cannot reproduce the strength distribution around -10 MeV. This is a common feature of TDA- and RPA-type calculations [8,9]. Studies on the effect of short-range correlations have predicted a strength reduction of about 10% in ^{16}O [23–25]. The spectroscopic factors for the proton $1s_{1/2}$ and $2s_{1/2}$ states calculated in oRPA is compared with experiment [22] (red bars) in Fig. 9. The EoRPA results are also compared with

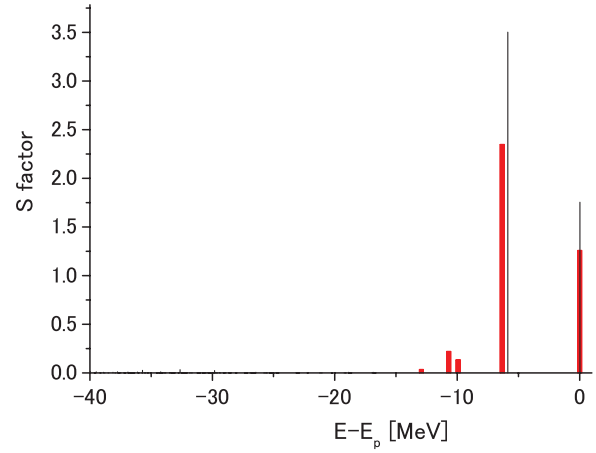


FIG. 8. (Color online) Spectroscopic factors for the proton $1p_{1/2}$ and $1p_{3/2}$ states calculated in EoRPA are compared with experiment [22] (red bars).

experiment (red bars) in Fig. 10. Because the inclusion of ground-state correlations causes a downward shift of the strength, the agreement with the data becomes somewhat worse in EoRPA. The strong fragmentation below -15 MeV cannot be reproduced in these oRPA and EoRPA calculations. Probably higher configurations are needed. The spectroscopic factors for the proton $1d_{5/2}$ and $1d_{3/2}$ states calculated in oRPA are compared with experiment [22] (red bars) in Fig. 11. The EoRPA results are also compared with experiment in Fig. 12. Due to a downward shift of the strength, the agreement with the data is worsened in EoRPA. We point out that there is a similar situation in the first 3^- state in ^{16}O. The effects of the ground-state correlations can be included into the standard RPA using $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$ as in SCRPA [26]. The first 3^- state of ^{16}O calculated in this modified RPA scheme comes about 5 MeV higher than the result in the standard RPA. This is the same situation as the EoRPA results shown above. We found that inclusion of the coupling of the particle-hole amplitude to higher two-particle–two-hole amplitudes brings down the first 3^- state to the right position [27]. Therefore, more elaborate

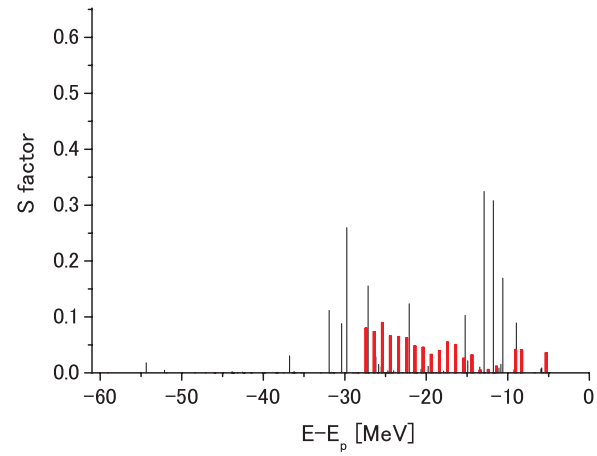


FIG. 9. (Color online) Spectroscopic factors for the proton $1s_{1/2}$ and $2s_{1/2}$ states calculated in oRPA are compared with experiment [22] (red bars).

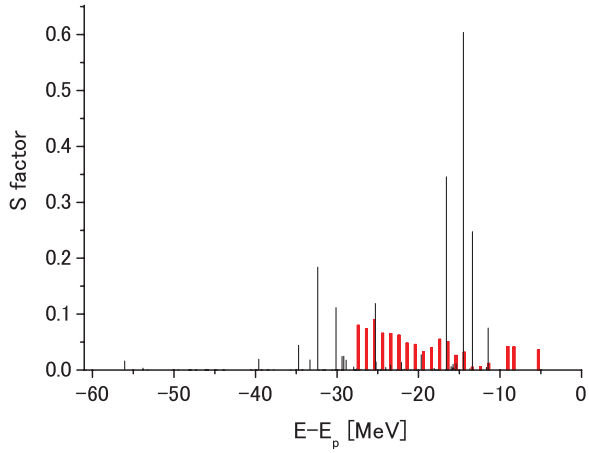


FIG. 10. (Color online) Same as Fig. 9 but for EoRPA.

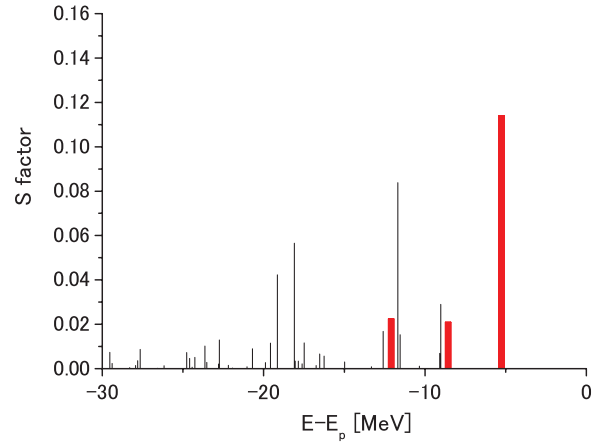


FIG. 12. (Color online) Same as Fig. 11 but for EoRPA.

calculations using a larger number of the $Y^{\mu}_{\alpha\beta:\gamma}$ amplitudes and also the higher amplitudes $Y^{\mu}_{\alpha\beta\gamma:\lambda\lambda'}$ could shift the strength upward and bring a better agreement with the data. Globally, one may say that the agreement of spectroscopic factors with experiment is only marginally satisfactory indicating the need for inclusion of higher configurations.

E. Effects of other amplitudes

We investigate the effects of inclusion of the amplitude $Y^{\mu}_{\mathrm{hp:h'}}$ in EoRPA, which describes backward scattering of a particle-hole pair in $Y^{\mu}_{\mathrm{hh':p}}$. We use for $Y^{\mu}_{\mathrm{hp:h'}}$ the same truncated single-particle space as that used in the ground-state calculation because it is important to include the self-energy contribution to all single-particle states in $Y^{\mu}_{\mathrm{hp:h'}}$. To reduce the dimension size, we neglect the amplitude $Y^{\mu}_{\mathrm{pp':h}}$. The obtained result for the proton $1p_{1/2}$ state is shown in Fig. 13 and compared with the result (red bars) of the calculation based on Eq. (13) where the ground state is assumed to be the HF ground state and only the amplitudes $X^{\mu}_{\mathrm{hp:h'}}$ and $X^{\mu}_{\mathrm{hh':p}}$ are included. As shown in Fig. 13, the inclusion of $X^{\mu}_{\mathrm{hp:h'}}$ gives quite unphysical results: The main peak is fragmented and some states have negative strength. The reason for the fragmentation of the main peak is that unperturbed energies of some $X^{\mu}_{\mathrm{hp:h'}}$ fall near the energy of the proton $1p_{1/2}$ state. For example, the unperturbed energy of the configuration $(1s_{1/2})^{-1}2s_{1/2}(1p_{3/2})^{-1}$ that couples to the proton $1p_{1/2}$ state is -12.4 MeV, which is close to the energy of this state ($\epsilon_{\alpha} = -12.0$ MeV). These unphysical properties are not seen in the EoRPA result. We consider that this is due both to the self-energy insertion to the configurations $Y^{\mu}_{\mathrm{hp:h'}}$ and to their small normalization N_{22}. The energy of the configuration $Y^{\mu}_{\mathrm{hp:h'}}$ is significantly shifted by the amount determined by the self-energy and the normalization. This shift probably plays a role in reducing the coupling to the single-hole state. We performed a similar EoRPA calculation for the proton $1s_{1/2}$ state (see Fig. 14) and the obtained result (solid line) is compared with the EoRPA result without $Y^{\mu}_{\mathrm{hp:h'}}$ (dotted line). The coupling to $Y^{\mu}_{\mathrm{hp:h'}}$ plays a role in shifting some strength upward, which improves the agreement with the experiment. However, we found that the inclusion of other amplitudes such

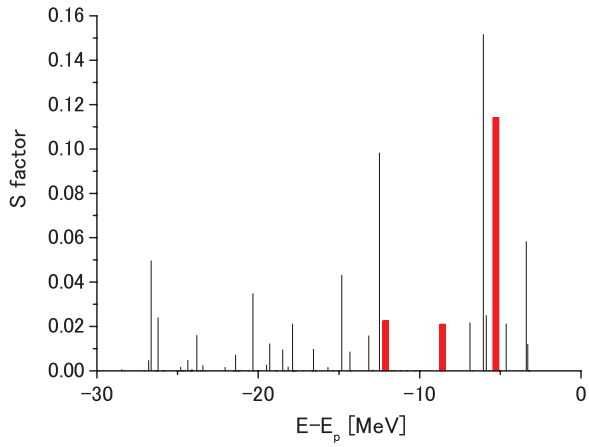


FIG. 11. (Color online) Spectroscopic factors for the proton $1d_{5/2}$ and $1d_{3/2}$ states calculated in oRPA are compared with experiment [22] (red bars).

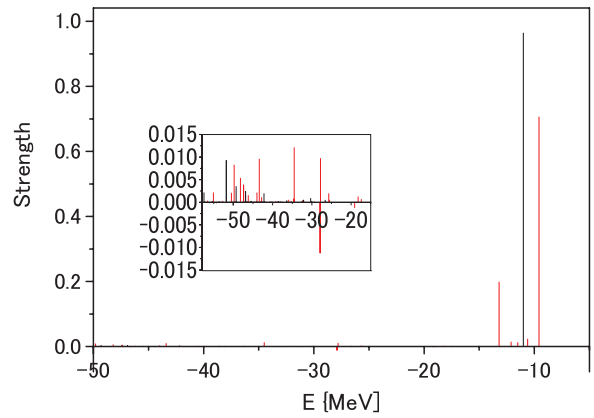


FIG. 13. (Color online) Strength distribution of the proton $1p_{1/2}$ state calculated in EoRPA including the amplitude $Y^{\mu}_{\mathrm{hp:h'}}$. The red bars show the result of the calculation based on Eq. (13) where only the amplitudes $X^{\mu}_{\mathrm{hp:h'}}$ and $X^{\mu}_{\mathrm{hh':p}}$ are included under the assumption of the HF ground state. Small strengths in the low-energy region are shown in the inset.

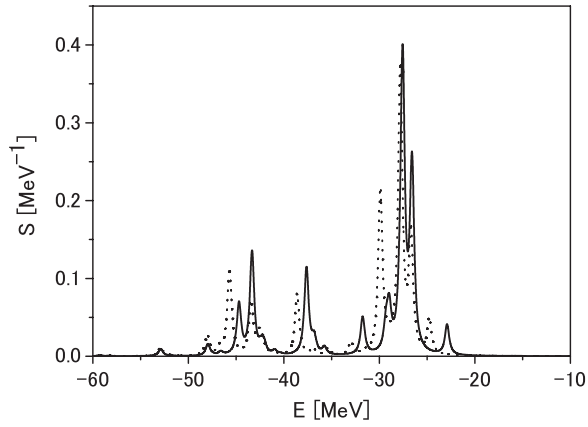


FIG. 14. Strength distribution of the proton $1s_{1/2}$ state calculated in EoRPA with (solid line) and without (dotted line) $Y^{\mu}_{\mathrm{hp:h'}}$.

as $Y^{\mu}_{\mathrm{hh':h''}}$ and $Y^{\mu}_{\mathrm{hp:p'}}$ brings unphysical fragmentation of the strength of the $1p_{1/2}$ state as seen in Fig. 13. Therefore, it requires further investigation whether the amplitudes of $Y^{\mu}_{\alpha\beta:\gamma}$ with small normalizations should be included or not in EoRPA.

F. Center-of-mass motion of ^{16}O

Finally we discuss the coupling of a hole state to the c.m. motion of the core nucleus ^{16}O using oRPA. The strength distribution of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ among the states which couple to the proton $1s_{1/2}$ state is shown in Fig. 15, where the proton $1p_{1/2}$ and $1p_{3/2}$ states are taken for α. The upper part of Fig. 15 shows the strength of the proton $1s_{1/2}$ state (the same as Fig. 9) and the lower part $-|\langle\mu|P_z a_\alpha|0\rangle|^2$ for $\alpha = 1p_{1/2}$ (red bars) and $1p_{3/2}$ (green bars). The strength $|\langle\mu|P_z a_\alpha|0\rangle|^2$ for $\alpha = 1p_{1/2}$ is concentrated in a single state and the coupling of the proton $1s_{1/2}$ state to this state is negligible. Therefore, this state may be interpreted as a spurious mode consisting of a pure c.m. motion of ^{16}O and the proton $1p_{1/2}$ state, though it is located about 7 MeV below the single-particle energy of the proton $1p_{1/2}$ state (−12.0 MeV). This energy shift from the single-particle energy is related to the fact that the TDA calculation for the c.m. motion of ^{16}O gives the excitation energy of 7.7 MeV. This fact may look perturbing, because we know that the spurious mode of the core comes at zero energy in the standard RPA. As already mentioned above, it is not guaranteed in an odd system that the c.m. motion of the core comes at zero energy, and the coupling of the spurious mode to the physical spectrum is very week, so that the position of the spurious mode is not so perturbing. We also performed a TDA calculation for the c.m. motion of ^{208}Pb using the single-particle states and the residual interaction which put the spurious mode at zero energy in RPA and found that it comes at 4.7 MeV. This suggests that the c.m. of very heavy systems could come close to zero excitation energy even in TDA. The strength $|\langle\mu|P_z a_\alpha|0\rangle|^2$ for $\alpha = 1p_{3/2}$ is somewhat fragmented. Because the dominant components of the c.m. motion of the core consists of the transitions from the $1p_{3/2}$ to $1d_{5/2}$ states, the large fragmentation of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ for $\alpha = 1p_{3/2}$ is explained by the coupling to the configurations with different coupling schemes of angular momenta: In the case of $\alpha = 1p_{3/2}$, $Y^{\mu}_{\alpha\mathrm{h:p}}$ consisting of the particle-hole pairs $(1p_{3/2})^{-1}1d_{5/2}$ with angular momentum $L = 1\hbar$ can couple not only to $Y^{\mu}_{\alpha\mathrm{h:p}}$ which has the same particle-hole pairs with $L = 2\hbar$ but also to $Y^{\mu}_{\alpha\mathrm{h:p}}$ consisting of the particle-hole pairs $(1p_{1/2})^{-1}1d_{5/2}$ with $L = 2\hbar$. In the case of $\alpha = 1p_{1/2}$ the particle-hole pairs $(1p_{3/2})^{-1}1d_{5/2}$ in $Y^{\mu}_{\alpha\mathrm{h:p}}$ can have only $L = 1\hbar$ and does not couple to nearby configurations. The exchange effect may also play a role in weakening the coherence of the c.m. motion of ^{16}O for $\alpha = 1p_{3/2}$: We tried an oRPA calculation for $\alpha = 1p_{3/2}$ where all exchange terms are neglected and observed the appearance of such a coherent state as that observed for $\alpha = 1p_{1/2}$. Thus, in the case of the proton $1s_{1/2}$ state and $\alpha = 1p_{3/2}$ the c.m. motion of the core nucleus is embedded in the physical states of the $A-1$ nucleus and cannot be neglected. The distributions of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ among the states which couple to the proton $1p_{1/2}$ and $1p_{3/2}$ states are shown in Figs. 16 and 17, respectively, where α is the proton $1s_{1/2}$ state. In the case of the proton $1p_{1/2}$ state the strength $|\langle\mu|P_z a_\alpha|0\rangle|^2$ is concentrated in a single state and the coupling of the proton $1p_{1/2}$ state to

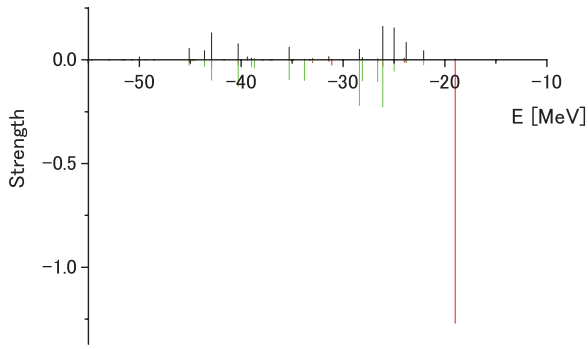


FIG. 15. (Color online) Strength distribution of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ in the states which couple to the proton $1s_{1/2}$ state. The upper part shows the strength of the proton $1s_{1/2}$ state and the lower part $-|\langle\mu|P_z a_\alpha|0\rangle|^2$ (in arbitrary units) for $\alpha =$ the proton $1p_{1/2}$ state (red bars) and the proton $1p_{3/2}$ state (green bars). The strength $|\langle\mu|P_z a_\alpha|0\rangle|^2$ for $\alpha = 1p_{3/2}$ is fragmented due to the coupling to the configurations which have the particle-hole pairs with angular momentum $L = 2\hbar$.

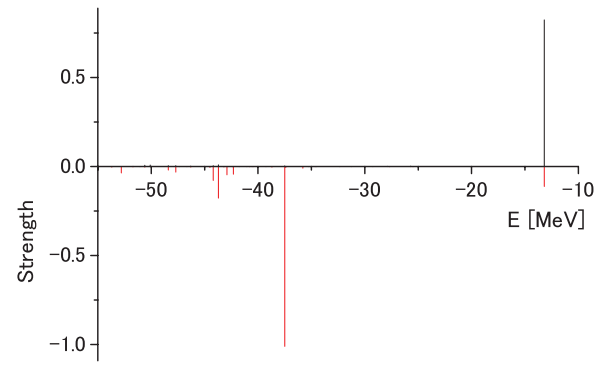


FIG. 16. (Color online) Strength distribution of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ in the states which couple to the proton $1p_{1/2}$ state. The upper part shows the strength of the proton $1p_{1/2}$ state and the lower part $-|\langle\mu|P_z a_\alpha|0\rangle|^2$ (in arbitrary units) for $\alpha =$ the proton $1s_{1/2}$ state (red bars).

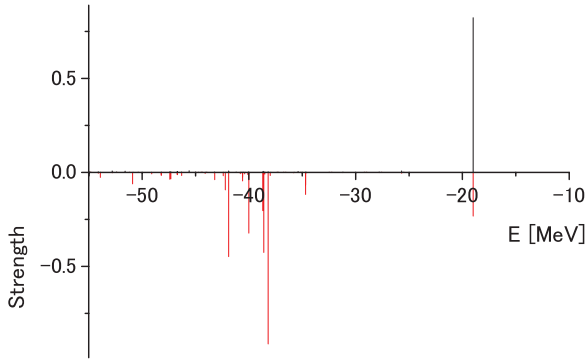


FIG. 17. (Color online) Same as Fig. 16 but for the proton $1p_{3/2}$ state.

this state is negligible. As in the case of the proton $1s_{1/2}$ state this state may be interpreted as a spurious mode consisting of the c.m. motion of ^{16}O and the proton $1s_{1/2}$ state, though it is located about 5 MeV below the single-particle energy of the proton $1s_{1/2}$ state (−32.1 MeV). The fragmentation of $|\langle\mu|P_z a_\alpha|0\rangle|^2$ for the proton $1p_{3/2}$ state is larger than that for the proton $1p_{1/2}$ state. This is explained by the coupling to the configurations with different angular momentum couplings: In the case of the $1p_{3/2}$ state the particle-hole pairs $(1p_{3/2})^{-1}1d_{5/2}$ in $Y^{\mu}_{\alpha\mathrm{h:p}}$ can carry angular momentum $L = 1\hbar$ and $2\hbar$, whereas the pairs cannot have $L = 2\hbar$ in the case of the $1p_{1/2}$ state.

IV. SUMMARY

In this paper, we took up the old subject of the RPA approach to odd particle systems. Those equations based on the usual equation of motion method (EoM) encountered in the past some difficulties [8]. This gave raise to the so-called Faddeev-RPA (FRPA) approach [9]. However, whenever the RPA breaks down, so does FRPA. We located some of the difficulties of the old odd particle RPA (oRPA) and proposed some cure, limiting the configuration space to the normalizable subspace. We showed that p-RPA and h-RPA equations give identical results which is very similar to the property of pp(hh)RPA for even system [16]. We also discussed the influence of the c.m. motion of the core on the odd particle (p or h). No difficulty with a breakdown seems to arise. It turns out that the recoil of the core influences the spectrum. This aspect may be most important for rotational states in deformed nuclei where the so-called spurious modes are, in fact, physical states. We also showed how to include ground-state correlations explicitly in EoRPA, similar to what is done in TDDM, on top of the oRPA equations. We made a first schematic application, using a simplified Skyrme force, to the hole and particle states around ^{16}O. We compared Tamm Dancoff, oRPA, and EoRPA solutions. It was shown that in some cases all three approaches give very similar results but that in others the influence of extra RPA correlations was significant. The comparison with experiment is sufficiently encouraging to develop this kind of RPA approach further. In fact, the spirit of oRPA is quite close to second RPA. We encountered problems for the odd systems, e.g., that the spectrum becomes too much shifted downwards. Such open problems may be a subject for the future. In addition, the connection between a common RPA vacuum in the even and odd systems, as proposed recently [18], may be an interesting further line of research.

APPENDIX A: MATRIX ELEMENTS

The matrix elements of Eq. (13) are given below:

$$a(\alpha:\alpha') = \epsilon_\alpha \delta_{\alpha\alpha'}, \tag{A1}$$

$$\begin{aligned} b(\alpha\beta\gamma:\alpha') = {} & \sum_\lambda \langle\alpha'\lambda|v|\alpha\beta\rangle_A n_{\gamma\lambda} \\ & - \sum_{\lambda\lambda'}\Big[\langle\alpha'\lambda'|v|\alpha\lambda\rangle_A (n_{\lambda\beta}n_{\gamma\lambda'} + C_{\gamma\lambda\lambda'\beta}) \\ & + \langle\alpha'\lambda'|v|\lambda\beta\rangle_A (n_{\lambda\alpha}n_{\gamma\lambda'} + C_{\gamma\lambda\lambda'\alpha}) \\ & - \langle\alpha'\gamma|v|\lambda\lambda'\rangle_A \left(n_{\lambda\alpha}n_{\lambda'\beta} + \frac{1}{2}C_{\lambda\lambda'\alpha\beta}\right)\Big], \end{aligned} \tag{A2}$$

$$c(\alpha:\alpha'\beta'\gamma') = \langle\alpha'\beta'|v|\alpha\gamma'\rangle, \tag{A3}$$

$$\begin{aligned} & d(\alpha\beta\gamma:\alpha'\beta'\gamma') \\ & = (\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma)\delta_{\alpha\alpha'}\delta_{\beta\beta'}\delta_{\gamma\gamma'} + \frac{1}{2}\langle\alpha'\beta'|v|\alpha\beta\rangle_A \delta_{\gamma\gamma'} \\ & \quad + \sum_\lambda\Big[\langle\lambda\alpha'|v|\alpha\gamma'\rangle_A n_{\gamma\lambda}\delta_{\beta\beta'} - \langle\lambda\alpha'|v|\beta\gamma'\rangle_A n_{\gamma\lambda}\delta_{\alpha\beta'} \\ & \quad + \langle\gamma\beta'|v|\lambda\gamma'\rangle_A n_{\lambda\alpha}\delta_{\beta\alpha'} - \langle\gamma\beta'|v|\lambda\gamma'\rangle_A n_{\lambda\beta}\delta_{\alpha\alpha'} \\ & \quad - \frac{1}{2}\delta_{\gamma\gamma'}(\langle\alpha'\beta'|v|\alpha\lambda\rangle_A n_{\lambda\beta} + \langle\alpha'\beta'|v|\lambda\beta\rangle_A n_{\lambda\alpha})\Big]. \end{aligned} \tag{A4}$$

The norm matrix N_{22} is given as

$$\begin{aligned} & N_{22}(\alpha\beta\gamma:\alpha'\beta'\gamma') \\ & = (\delta_{\alpha\alpha'}\delta_{\beta\beta'} - \delta_{\alpha\beta'}\delta_{\beta\alpha'})n_{\gamma'\gamma} \\ & \quad + \delta_{\gamma\gamma'}(n_{\alpha\alpha'}n_{\beta\beta'} - n_{\alpha\beta'}n_{\beta\alpha'} + C_{\alpha\beta\alpha'\beta'}) \\ & \quad - \delta_{\alpha\alpha'}(n_{\gamma'\gamma}n_{\beta\beta'} + C_{\gamma'\beta\gamma\beta'}) - \delta_{\beta\beta'}(n_{\gamma'\gamma}n_{\alpha\alpha'} + C_{\gamma'\alpha\gamma\alpha'}) \\ & \quad + \delta_{\alpha\beta'}(n_{\gamma'\gamma}n_{\beta\alpha'} + C_{\gamma'\beta\gamma\alpha'}) + \delta_{\beta\alpha'}(n_{\gamma'\gamma}n_{\alpha\beta'} + C_{\gamma'\alpha\gamma\beta'}). \end{aligned} \tag{A5}$$

APPENDIX B: THE $A = 2$ CASE

We show that our formulation is exact for an $A = 2$ system. In the case of an $A = 2$ system, TDDM gives the coupled equations of motion for $n_{\alpha\alpha'}$ and the two-body density matrix $\rho_{\alpha\beta\alpha'\beta'}$, which are defined as

$$n_{\alpha\alpha'}(t) = \langle\Phi(t)|a^+_{\alpha'}a_\alpha|\Phi(t)\rangle, \tag{B1}$$

$$\rho_{\alpha\beta\alpha'\beta'}(t) = \langle\Phi(t)|a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha|\Phi(t)\rangle, \tag{B2}$$

where $|\Phi(t)\rangle$ is the time-dependent total wave function $|\Phi(t)\rangle = \exp[-iHt]|\Phi(t=0)\rangle$. The equations in TDDM are

written as [28]

$$i\hbar\dot{n}_{\alpha\alpha'} = \sum_{\lambda}(\langle\alpha|t|\lambda\rangle n_{\lambda\alpha'} - \langle\lambda|t|\alpha'\rangle n_{\alpha\lambda}) + \sum_{\lambda_1\lambda_2\lambda_3}[\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle\rho_{\lambda_2\lambda_3\alpha'\lambda_1} - \rho_{\alpha\lambda_1\lambda_2\lambda_3}\langle\lambda_2\lambda_3|v|\alpha'\lambda_1\rangle], \quad \text{(B3)}$$

$$i\hbar\dot{\rho}_{\alpha\beta\alpha'\beta'} = \sum_{\lambda}(\langle\alpha|t|\lambda\rangle\rho_{\lambda\beta\alpha'\beta'} + \langle\beta|t|\lambda\rangle\rho_{\alpha\lambda\alpha'\beta'} - \langle\lambda|t|\alpha'\rangle\rho_{\alpha\beta\lambda\beta'} - \langle\lambda|t|\beta'\rangle\rho_{\alpha\beta\alpha'\lambda}) + \sum_{\lambda_1\lambda_2}[\langle\alpha\beta|v|\lambda_1\lambda_2\rangle\rho_{\lambda_1\lambda_2\alpha'\beta'} - \langle\lambda_1\lambda_2|v|\alpha'\beta'\rangle\rho_{\alpha\beta\lambda_1\lambda_2}]. \quad \text{(B4)}$$

Here the single-particle states are arbitrary. Because there are no higher-level reduced density matrices in an $A = 2$ system, these two equations are exact. When the two-body density matrix in Eq. (B3) is approximated by antisymmetrized products of the occupation matrices, Eq. (B3) is equivalent to the equation in the time-dependent HF theory. The ground state is given as a stationary solution of these equations.

The equation for the transition amplitude x^{μ}_{α} is

$$\sum_{\lambda}(\langle\lambda|t|\alpha\rangle - \delta_{\alpha\lambda}\omega_{\mu})x^{\mu}_{\lambda} + \sum_{\lambda_1\lambda_2\lambda_3}\langle\lambda_1\lambda_2|v|\alpha\lambda_3\rangle\tilde{X}^{\mu}_{\lambda_1\lambda_2:\lambda_3} = 0, \quad \text{(B5)}$$

where $\tilde{X}^{\mu}_{\alpha\beta:\gamma} = \langle 0|a^{+}_{\alpha}a^{+}_{\beta}a_{\gamma}|\mu\rangle$. The equation for $\tilde{X}^{\mu}_{\alpha\beta:\gamma}$ is given as

$$\sum_{\lambda}\left((\langle\lambda|t|\alpha\rangle - \delta_{\alpha\lambda}\omega_{\mu})\tilde{X}^{\mu}_{\lambda\beta:\gamma} + \langle\lambda|t|\beta\rangle\tilde{X}^{\mu}_{\alpha\lambda:\gamma} - \langle\gamma|t|\lambda\rangle\tilde{X}^{\mu}_{\alpha\beta:\lambda}\right) + \sum_{\lambda_1\lambda_2}\langle\lambda_1\lambda_2|v|\alpha\beta\rangle\tilde{X}^{\mu}_{\lambda_1\lambda_2:\gamma} = 0. \quad \text{(B6)}$$

Because there are no higher-level transition amplitudes in an $A = 2$ system, these two equations are also exact. From Eq. (B5) we obtain

$$\frac{1}{2}\sum_{\mu\alpha\alpha'}(\langle\alpha'|t|\alpha\rangle + \delta_{\alpha\alpha'}\omega_{\mu})x^{\mu}_{\alpha'}\left(x^{\mu}_{\alpha}\right)^{*} = \sum_{\alpha\alpha'}\langle\alpha'|t|\alpha\rangle n_{\alpha\alpha'} + \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle\rho_{\lambda_3\lambda_4\lambda_1\lambda_2} = \langle 0|H|0\rangle, \quad \text{(B7)}$$

where $n_{\alpha\alpha'}$ and $\rho_{\alpha\beta\alpha'\beta'}$ are exactly given by

$$n_{\alpha\alpha'} = \sum_{\mu}x^{\mu}_{\alpha'}\left(x^{\mu}_{\alpha}\right)^{*}, \quad \text{(B8)}$$

$$\rho_{\alpha\beta\alpha'\beta'} = \sum_{\mu}\tilde{X}^{\mu}_{\alpha'\beta':\beta}\left(x^{\mu}_{\alpha}\right)^{*}. \quad \text{(B9)}$$

Equation (B7) corresponds to the relation between the total ground-state energy and the single-particle Green's function [29].

APPENDIX C: GREEN'S FUNCTION DESCRIPTION

The equations for the amplitudes in Eqs. (48) and (49) are cast into Green's function language. For this we write down a Dyson equation,

$$G^{\omega}_{kk'} = G^{0}_{k}\delta_{kk'} + G^{0}_{k}\sum_{k_1}M^{\omega}_{kk_1}G^{\omega}_{k_1k'}, \quad \text{(C1)}$$

where

$$G^{0}_{k} = \frac{1 - n^{(0)}_{k}}{\omega - \varepsilon_k + i\eta} + \frac{n^{(0)}_{k}}{\omega - \varepsilon_k - i\eta} \quad \text{(C2)}$$

is the free or HF Green's function with the occupation numbers $n^{(0)}_{k}$ equal to 0 or 1. The mass operator is given by

$$M_{kk'} = \sum_{\alpha\mathrm{hh}'p_1p_2p'_1p'_2}\langle kh|v|p_1p_2\rangle\frac{Y^{\rho}_{p_1p_2:h}Y^{\rho *}_{p'_1p'_2:h'}}{\omega - \Omega^{N+1}_{\rho} + i\eta} \times \langle p'_1p'_2|v|h'k'\rangle + \sum_{\rho\mathrm{pp}'\mathrm{h}_1\mathrm{h}_2\mathrm{h}'_1\mathrm{h}'_2}\langle kp|v|h_1h_2\rangle\frac{Y^{\alpha}_{\mathrm{h}_1\mathrm{h}_2:p}Y^{\alpha *}_{\mathrm{h}'_1\mathrm{h}'_2:p'}}{\omega - \Omega^{N-1}_{\alpha} - i\eta} \times \langle \mathrm{h}'_1\mathrm{h}'_2|v|p'k'\rangle, \quad \text{(C3)}$$

where $Y^{\alpha,\rho}$ and $\Omega_{\alpha,\rho}$ are the TDA 2p-1h and 2h-1p amplitudes and eigenvalues, respectively, obtained from the corresponding TDA equations [16]. In the case where we strictly work with oRPA corresponding to the ground state Eq. (50), the coupled system of particle and hole propagation in the above Dyson equation decouples into two separate Dyson equations, one for the particles [with the α part of the mass operator corresponding to Fig. 3(a)] and one for the holes [with the ρ part of the mass operator corresponding to Fig. 3(b)]. It may certainly be appealing to work with an approach which is based on a ground-state wave function.

Going beyond the use of an HF ground state, we can do as in this work considering EoRPA as described above. However, there is also the possibility to mix even and odd RPA's. For example it has turned out that self-consistent RPA (SCRPA) based on the vacuum Eq. (50) gives very good results [18]. For instance, it also solves the two-particle case exactly. One thus could use SCRPA to calculate the correlation functions appearing in an extended oRPA. To use the ansätze Eqs. (48) and (49) directly seems difficult because they correspond to a nonlinear transformation among the fermion operators.

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