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On the Random Phase Approximation Based on the Thermo Field Dynamics Formalism

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A comparative study of the random phase approximation is reported in the case of the following three approaches based on the thermo field dynamics formalism: (A) the Tanabe approach, (B) the Hatsuda approach and (C) the approach developed by the present authors. The basic viewpoint is to formulate the random phase approximation by picking up the quadratic terms with respect to bosons in the boson expansion theory for the thermo field dynamics formalism. It is concluded that the approach (C) appears to be superior to the other two approaches.

§ 1. Introduction

The study of phenomena occurring in highly exicited nuclear states, in the framework provided by the nuclear many-body theory, has received the attention of many authors. Such phenomena are expected to be interpreted in the language of the theory of thermal equilibrium with a temperature $T \neq 0$. In response to the situation mentioned above, three papers have appeared along an idea of constructing the random phase approximation (RPA) in the frame of the thermo field dynamics formalism:[1] (A) the Tanabe approach,[2] (B) the Hatsuda approach[3] and (C) the approach developed by the present authors.[4] The thermo field dynamic formalism is regarded as useful for describing mixed states such as the states of thermal equilibrium with $T \neq 0$. In this formalism, as a technique for the trace calculation, the fermion space in which the system is described is enlarged from the original one. With the use of the solution of the Schrödinger equation given in the enlarged space, statistical ensemble average of any physical quantity is automatically reduced to quantum mechanical calculation of the expectation value.

In the above three papers, the RPA methods were formulated on the basis of the thermo field dynamics formalism. In the present paper, we will call the RPA formulated in the frame of the thermo field dynamics formalism the TFRPA. Further, we will use the notations the TFRPA (A), (B) and (C) for the TFRPA based on the approach (A), (B) and (C), respectively. Since in the above three papers the starting ideas are different from each other, the resultant equations are also different from each other. In (A), the starting Hamiltonian for the Schrödinger equation in the enlarged space is expressed only in terms of the variables in the original space. The TFRPA (A) equation called the extended TRPA (ETRPA) equation in the original paper of (A) is different from that of the RPA for $T \neq 0$ which is not based on the thermo field dynamics formalism and called the TRPA equation in (A).[5] However, from the careful investigation of the detailed formulation of (A), we notice that the approach (A) seems to contain unclear aspects which should be reexamined concerning the position of the thermal equilibrium and the interpretation of the single-particle excitation energies. In contrast to the above case, the approach (B) starts from the Hamiltonian expressed in terms of the whole variables in the enlarged space. However, the formulation shown in (B) is not so concrete and the detailed form of the TFRPA (B) equation is not given. Therefore, physical meaning of the results such as the frequencies obtained in the TFRPA (B) equation is unclear. In (C), the starting Hamiltonian is essentially the same as that in (A). However, some of the variables in the enlarged space do not have any counterparts in the original space. Therefore, quantities which relate to these variables should be constrained. Under these constraints, the equation of the collective submanifold is given and in the small amplitude limit, the TFRPA (C) is formulated. However, it starts from a single collective degree of freedom. Therefore, for example, the maximum number of the degrees of freedom in the enlarged space, which is independent of the constraints, cannot be given. This fact shows that the approach (C) is, in its present form, unpowerful for describing the couplings among various modes. Anyhow, the above three approaches contain some unclear points which should be reexamined.

The aim of this paper is to clarify the unclear points contained in the approaches (A), (B) and (C). For this aim, we start from the Hamiltonian of the separable type interaction, with the aid of which the TFRPA equation can be given in a concrete form. First of all, we define fermion annihilation and creation operators, $(\hat{a}_i, \hat{a}_i^*)$ and $(\hat{b}_i, \hat{b}_i^*)$ which play the same role as that of the particle and hole operators, respectively, in the static Hartree-Fock theory. Fermion operators $(\hat{c}_i, \hat{c}_i^*)$ which are defined in the original space can be expressed in the form $\hat{c}_i = u_i\hat{a}_i + v_i\hat{b}_i^*$, $\hat{c}_i^* = u_i\hat{a}_i^* + v_i\hat{b}_i$. Here, the coefficients u_i and v_i are defined by $u_i = \sqrt{1-n_i}$ and $v_i = \sqrt{n_i}$ $(0 \leq n_i \leq 1)$. The quantity n_i denotes the occupation probability of the state i at the equilibrium point. Further, additional fermion operators $(\tilde{d}_i, \tilde{d}_i^*)$, which compose the enlarged space with the fermions $(\hat{c}_i, \hat{c}_i^*)$, are given in the form $\tilde{d}_i = -v_i\hat{a}_i^* + u_i\hat{b}_i$, $\tilde{d}_i^* = -v_i\hat{a}_i + u_i\hat{b}_i^*$. Then, the bi-linear forms of these fermion operators are given by the forms $\hat{c}_i^*\hat{c}_j = n_i\delta_{ij} + \hat{F}_{ij}$ and $\tilde{d}_j^*\tilde{d}_i = n_i\delta_{ij} + \tilde{G}_{ij}$. Here, $\hat{F}_{ij}$ and $\tilde{G}_{ij}$ are expressed in terms of linear combinations for $\hat{a}_i^*\hat{b}_j^*$, $\hat{b}_i\hat{a}_j$, $\hat{a}_i^*\hat{a}_j$ and $\hat{b}_j^*\hat{b}_i$. These operators can be transcribed in the boson space, i.e., we can get the boson expansion theory for mixed states. Further, its classical limit can be obtained by replacing the boson operators by the classical canonical variables. This classical limit is, in its formalism, nothing but the TDHF theory parametrized in terms of the canonical variables.[6] Then, we can express any one body physical quantity as a function of $\hat{c}_i^*\hat{c}_j$ in terms of the equilibrium value plus the fluctuation. Of course, the fluctuation is expressed in terms of $\hat{F}_{ij}$ and it starts from the linear terms for the bosons or their classical counterpart. If we rewrite the starting Hamiltonian in the frame of the above fermion bi-linear forms, the Hamiltonian can be expressed by the boson operators or classical canonical variables. Then, picking up the terms up to the quadratic order for the bosons, we can get the approximate Hamiltonian which leads us to the TFRPA. Through the diagonalization of the Hamiltonian, the eigenvalue equation is obtained. In this paper, we will investigate the Hamiltonians for the TFRPA and the eigenvalue equations in the approaches (A), (B) and (C). Through this investigation, the unclear points in the three approaches can be clarified.

After giving the Hamiltonian and some basic formulae in § 2, the TFRPA Hamiltonians in the approaches (A) and (B) are given in § 3. Especially, the TFRPA (B) equation is investigated in detail. In § 4, the TFRPA equation is presented on the basis of the approach (C). A general one body physical operator is expressed in terms of the variables which are free from the constraints. Finally, in § 5, the results based on the approachs (B) and (C) are given and several concluding remarks, for example, such as that the result given in (C) coincides with that given by the present authors (J. P. and C. F.),[7] are mentioned.

§ 2. Preliminaries

In this section, we will give the preparation for the later discussion. With the aim of illustrating our idea in a concrete form, we describe a system, the Hamiltonian of which consists of kinetic energy and two-body interaction of the separable type:

$$\hat{H}=\sum_{ij} t_{ij}\hat{c}_i^* \hat{c}_j-\chi/2\cdot[\sum_{ij} q_{ij}\hat{c}_i^* \hat{c}_j]^2\,, \tag{2·1}$$

$$t_{ij}=t_{ji}\,, \qquad q_{ij}=q_{ji}\,. \tag{2·1a}$$

Here, the single-particle states are denoted by in terms of the Latin subscripts i, j, k and l. The operators $\hat{c}_i$ and $\hat{c}_i^*$ stand for the fermion annihilation and creation operator in the state i, respectively. Since we are concerned with the interaction of the separable type, the exchange matrix elements for the interaction will be neglected. Associated with the operators $\hat{c}_i$ and $\hat{c}_i^*$, we introduce another type of fermion operators $\hat{d}_i$ and $\hat{d}_i^*$, which are independent of $\hat{c}_i$ and $\hat{c}_i^*$. Further, the following Hamiltonian is defined:

$$\tilde{H}=\sum_{ij} t_{ij}\hat{d}_j^* \hat{d}_i-\chi/2\cdot[\sum_{ij} q_{ij}\hat{d}_j^* \hat{d}_i]^2\,. \tag{2·2}$$

In the approaches (A)[2] and (C)[4], the following Schrödinger equation is adopted:

$$i\partial_t|m(t)\rangle\!\rangle=\hat{H}|m(t)\rangle\!\rangle\,. \tag{2·3}$$

Here, $|m(t)\rangle\!\rangle$ denotes a mixed state. The approach (B)[3] starts in the Schrödinger equation

$$i\partial_t|m(t)\rangle\!\rangle=\hat{K}|m(t)\rangle\!\rangle\,, \qquad \hat{K}=\hat{H}-\tilde{H}\,. \tag{2·4}$$

Following the thermo field dynamics formalism, let us introduce fermion operators $(\hat{a}_i, \hat{a}_i^*)$ and $(\hat{b}_i, \hat{b}_i^*)$ in the following forms:

$$\hat{c}_i=+u_i\hat{a}_i+v_i\hat{b}_i^*\,, \qquad \hat{c}_i^*=+u_i\hat{a}_i^*+v_i\hat{b}_i\,, \tag{2·5}$$

$$\hat{d}_i=-v_i\hat{a}_i^*+u_i\hat{b}_i\,, \qquad \hat{d}_i^*=-v_i\hat{a}_i+u_i\hat{b}_i^*\,. \tag{2·6}$$

Here, u_i and v_i are given by

$$u_i=\sqrt{1-n_i}\,, \qquad v_i=\sqrt{n_i}\,. \qquad (u_i^2+v_i^2=1) \tag{2·7}$$

The quantity n_i means the occupation probability of the state i in the vacuum $|0\rangle\!\rangle$ for the fermions $\hat{a}_i$ and $\hat{b}_i$ ($\hat{a}_i|0\rangle\!\rangle=\hat{b}_i|0\rangle\!\rangle=0$). With the use of ($\hat{a}_i$, $\hat{a}_i^*$) and ($\hat{b}_i$, $\hat{b}_i^*$), the operators $\hat{c}_i^*\hat{c}_j$ and $\hat{d}_j^*\hat{d}_i$ can be expressed as

$$\hat{c}_i^*\hat{c}_j=n_i\delta_{ij}+\hat{F}_{ij}\,, \tag{2·8}$$

$$\hat{F}_{ij}=+u_iv_j\hat{a}_i^*\hat{b}_j^*+v_iu_j\hat{b}_i\hat{a}_j+u_iu_j\hat{a}_i^*\hat{a}_j-v_iv_j\hat{b}_j^*\hat{b}_i\,, \tag{2·8a}$$

$$\hat{d}_j^*\hat{d}_i=n_i\delta_{ij}+\tilde{G}_{ij}\,, \tag{2·9}$$

$$\tilde{G}_{ij}=+v_iu_j\hat{a}_i^*\hat{b}_j^*+u_iv_j\hat{b}_i\hat{a}_j+u_iu_j\hat{b}_j^*\hat{b}_i-v_iv_j\hat{a}_i^*\hat{a}_j\,. \tag{2·9a}$$

The expectation value of $\hat{c}_i^*\hat{c}_j$ for the vacuum $|0\rangle\!\rangle$ is $n_i\delta_{ij}$. Then, the term $\hat{F}_{ij}$ denotes the fluctuation around the value n_i and the aim of the TFRPA is to determine the fluctuation at the lowest order. If the mixed state $|m(t)\rangle\!\rangle$ obeys the Schrödinger equation (2·3), the expectation value of $\tilde{G}_{ij}$ should not depend on the time. Therefore, we can set up

$$\langle\!\langle m(t)|\tilde{G}_{ij}|m(t)\rangle\!\rangle(=\boldsymbol{G}_{ij})=0\,. \tag{2·10}$$

The above relation (2·10) appears only in the approach (C) and it plays a role of a constraint for the fluctuation around n_i.

With the aid of the relations (2·8) and (2·9), we rewrite the Hamiltonians (2·1) and (2·2) as follows:

$$\tilde{H}=E_0+\sum_i\varepsilon_i\hat{F}_{ii}-\chi/2\cdot[\sum_{ij}q_{ij}\hat{F}_{ij}]^2\,, \tag{2·11}$$

$$\tilde{H}=E_0+\sum_i\varepsilon_i\tilde{G}_{ii}-\chi/2\cdot[\sum_{ij}q_{ij}\tilde{G}_{ij}]^2\,. \tag{2·12}$$

Here, E_0 and ε_i denote, respectively,

$$E_0=\sum_k t_{kk}n_k-\chi/2\cdot[\sum_k q_{kk}n_k]^2\,, \tag{2·13}$$

$$\varepsilon_i\delta_{ij}=t_{ij}-\chi q_{ij}[\sum_k q_{kk}n_k]\,. \tag{2·14}$$

We assumed that the quantity $t_{ij}-\chi q_{ij}[\sum_k q_{kk}n_k]$ is diagonal for i and j and obeys the following relation:

$$\varepsilon_i>\varepsilon_j \quad \text{if} \quad n_i<n_j\,. \tag{2·15}$$

The quantity ε_i corresponds the single-particle energy of the state i in the conventional Hartree-Fock theory

As is well known in the boson expansion theory, the fermion pairs $\hat{a}_i^*\hat{b}_j^*$, $\hat{b}_i\hat{a}_j$, $\hat{a}_i^*\hat{a}_j$ and $\hat{b}_j^*\hat{b}_i$ can be expressed in terms of the boson operators $\hat{C}_{ij}$ and $\hat{C}_{ji}^*$ in the following forms:

$$a_i^*\hat{b}_j^*=\sum_k\hat{C}_{jk}^*(\sqrt{1-\hat{C}^\dagger\hat{C}})_{ik}=\hat{C}_{ji}^*-\cdots\,,$$

$$\hat{b}_i\hat{a}_j=\sum_k(\sqrt{1-\hat{C}^*\hat{C}^T})_{ki}\hat{C}_{kj}=\hat{C}_{ij}-\cdots\,,$$

$$\hat{a}_i{}^* \hat{a}_j = \sum_k \hat{C}^*_{ki} \hat{C}_{kj} , \qquad \hat{b}_j{}^* \hat{b}_i = \sum_k \hat{C}^*_{jk} \hat{C}_{ik} . \tag{2·16}$$

Here, $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$ satisfy the commutation relations

$$[\hat{C}_{ij}, \hat{C}^*_{lk}] = \delta_{jk}\delta_{il} ,$$

$$[\hat{C}_{ij}, \hat{C}_{kl}] = [\hat{C}^*_{ji}, \hat{C}^*_{lk}] = 0 . \tag{2·17}$$

Under the above preliminary consideration, we will analyze the TFRPA based on the approaches (A) and (B) in the next section.

§ 3. The TFRPA equations in the approaches (A) and (B)

In this section, we will give the TFRPA in the approaches (A) and (B). Let us start from the approach (A).[2] In this case, the Hamiltonian is of the form given in Eq. (2·11). Substituting the forms (2·16) into Eq. (2·11), together with Eq. (2·8a), we have

$$\hat{H} = E_0 + \hat{H}_Q + \hat{H}_L , \tag{3·1}$$

$$\hat{H}_Q = \sum_{ij} (\varepsilon_j u_j{}^2 - \varepsilon_i v_i{}^2) \hat{C}^*_{ij} \hat{C}_{ij} - \chi/2 \cdot [\sum_{ij} q_{ij} (u_i v_j \hat{C}^*_{ji} + v_i u_j \hat{C}_{ij})]^2 , \tag{3·1a}$$

$$\hat{H}_L = \sum_i \varepsilon_i u_i v_i (\hat{C}^*_{ii} + \hat{C}_{ii}) . \tag{3·1b}$$

The expansion is stopped at the quadratic terms for the bosons $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$. Although we do not show explicitly, the diagonalization of the Hamiltonian $(E_0 + \hat{H}_Q)$ gives us the TFRPA (A) equation (the ETRPA equation). However, the existence of the term $\hat{H}_L$ should not be forgotten and, in this case, the total Hamiltonian $\hat{H}$ must be diagonalized.

Since the term $\hat{H}_L$, which is linear for the bosons, exists, we have to diagonalize the Hamiltonian (3·1) by choosing appropriate values of γ_{ij} and γ^*_{ji} in the following relations:

$$\hat{C}_{ij} = \gamma_{ij} + \hat{C}'_{ij} , \quad \hat{C}^*_{ji} = \gamma^*_{ji} + \hat{C}'^*_{ji} . \tag{3·2}$$

Therefore, in the present case, the expansion in Eq. (2·16) should be performed for $\hat{C}'_{ij}$ and $\hat{C}'^*_{ji}$ and, in this expansion, the linear terms for $\hat{C}'_{ij}$ and $\hat{C}'^*_{ji}$ appear also from the terms, the powers of which are higher than the linear for $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$. Therefore, it may be clear that the diagonalization of the Hamiltonian (3·1) cannot give us reliable result for the approximate diagonalization of the original Hamiltonian. Further, we start the formulation by expecting that the state $|0\rangle\rangle$ plays a role of the thermal equilibrium and the fluctuations around this point are described by the bosons $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$. However, if the relation (3·2) is necessary, the equilibrium is displaced from the state $|0\rangle\rangle$. This fact contradicts to the starting expectation. It should be recalled that, in the standard understanding, the RPA describes the fluctuations around the equilibrium in the lowest order and, then, the Hamiltonian should be quadratic for the fluctuations. In addition to the above fact, the term contained in the Hamiltonian (3·1), $(\varepsilon_j u_j{}^2 - \varepsilon_i v_i{}^2)$, may be of an unnatural form. If ε_i corresponds to the single-particle energy in the conventional Hatree-Fock theory, the single-particle excitation energy from the state i to j must be of the form $(\varepsilon_j - \varepsilon_i)$. The effect of n_i, $n_j \neq 0$ or 1 influences only to the probability of the excitation such as from the state i to j. From the above-mentioned few points, we have to conclude that the TFRPA (A) disagrees with the standard understanding and form of the RPA.

Next, let us investigate the approach (B).[3] As was mentioned in § 1, the TFRPA (B) equation has not been formulated in a concrete form in the original paper. Then, we will give the derivation in detail. In this case, as the Hamiltonian, the form $\hat{K}(=\hat{H}-\tilde{H})$ is adopted. The Hamiltonian $\tilde{H}$ can be expanded for $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$ in the following form:

$$\tilde{H}=E_0+\tilde{H}_Q+\tilde{H}_L\,, \tag{3·3}$$

$$\tilde{H}_Q=-\sum_{ij}(\varepsilon_j v_j^2-\varepsilon_i u_i^2)\hat{C}^*_{ij}\hat{C}_{ij}-\chi/2\cdot[\sum_{ij}q_{ij}(v_i u_j \hat{C}^*_{ji}+u_i v_j \hat{C}_{ij})]^2\,, \tag{3·3a}$$

$$\tilde{H}_L=\sum_i \varepsilon_i u_i v_i(\hat{C}^*_{ii}+\hat{C}_{ii})\,. \tag{3·3b}$$

Then, the Hamiltonian $\hat{K}$ can be expressed as

$$\hat{K}=\sum_{ij}(\varepsilon_j-\varepsilon_i)\hat{C}^*_{ij}\hat{C}_{ij}-\chi/2\cdot[\sum_{ij}q_{ij}(u_i v_j \hat{C}^*_{ji}+v_i u_j \hat{C}_{ij})]^2$$
$$+\chi/2\cdot[\sum_{ij}q_{ij}(v_i u_j \hat{C}^*_{ji}+u_i v_j \hat{C}_{ij})]^2\,. \tag{3·4}$$

We can see that the Hamiltonian $\hat{K}$ does not contain any linear term for $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$ and is of the standard form for the RPA.

Let us diagonalize the Hamiltonian (3·4). For this aim, we introduce the following operators:

$$\hat{X}_{ij}=u_i v_j \hat{C}^*_{ji}+v_i u_j \hat{C}_{ij}\,,$$
$$\hat{Y}_{ij}=v_i u_j \hat{C}^*_{ji}+u_i v_j \hat{C}_{ij}\,. \qquad (\text{for } n_i \neq n_j) \tag{3·5}$$

The above operators satisfy the relations

$$\hat{X}^*_{ij}=\hat{X}_{ji}\,,\quad [\hat{X}_{ij},\hat{X}_{kl}]=\delta_{jk}\delta_{il}(n_i-n_j)\,, \tag{3·6a}$$

$$\hat{Y}^*_{ij}=\hat{Y}_{ji}\,,\quad [\hat{Y}_{ij},\hat{Y}_{kl}]=\delta_{jk}\delta_{il}(n_j-n_i)\,, \tag{3·6b}$$

$$[\hat{X}_{ij},\hat{Y}_{kl}]=0\,,$$
$$[\hat{X}_{ij},\hat{C}_{kl}]=[\hat{Y}_{ij},\hat{C}_{kl}]=0\,. \quad (\text{for } n_k=n_l) \tag{3·6c}$$

For $n_i \neq n_j$, the inverse of the relation (3·5) is given by

$$\hat{C}_{ij}=(v_i u_j \hat{X}_{ij}-u_i v_j \hat{Y}_{ij})/(n_i-n_j)\,. \tag{3·7}$$

With the use of the operators defined above, the Hamiltonian $\hat{K}$ can be expressed as

$$\hat{K}=\hat{K}_X-\hat{K}_Y+\hat{K}_Z\,, \tag{3·8}$$

$$\hat{K}_X=\sum_{ij}{}'(\varepsilon_j-\varepsilon_i)/2(n_i-n_j)\cdot\hat{X}_{ji}\hat{X}_{ij}-\chi/2\cdot[\sum_{ij}{}' q_{ij}\hat{X}_{ij}]^2\,, \tag{3·8a}$$

$$\hat{K}_Y=\sum_{ij}{}'(\varepsilon_j-\varepsilon_i)/2(n_i-n_j)\cdot\hat{Y}_{ji}\hat{Y}_{ij}-\chi/2\cdot[\sum_{ij}{}'q_{ij}\hat{Y}_{ij}]^2\,, \tag{3·8b}$$

$$\hat{K}_Z=\sum_{ij}{}''(\varepsilon_j-\varepsilon_i)\cdot\hat{C}^*_{ij}\hat{C}_{ij}-\chi\cdot[\sum_{ij}{}'q_{ij}(\hat{X}_{ji}-\hat{Y}_{ij})]\cdot[\sum_{ij}{}''q_{ij}u_iv_i(\hat{C}^*_{ji}-\hat{C}_{ij})]\,. \tag{3·8c}$$

The symbols Σ'_{ij} and Σ''_{ij} denote the summations for $n_i\neq n_j$ and $n_i=n_j$, respectively. The commutation relations for $\hat{X}_{ij}$ and $\hat{Y}_{ij}$, further, $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$ $(n_i=n_j)$ for the Hamiltonian $\hat{K}$ are given in the following:

$$[\hat{K},\hat{X}_{ij}]=(\varepsilon_i-\varepsilon_j)\hat{X}_{ij}-\chi q_{ij}(n_j-n_i)\sum_{kl}{}'q_{kl}\hat{X}_{kl}$$
$$-\chi q_{ij}(n_j-n_i)\sum_{kl}{}''q_{kl}u_kv_k(\hat{C}^*_{lk}+\hat{C}_{kl})\,, \tag{3·9a}$$

$$[\hat{K},\hat{Y}_{ij}]=(\varepsilon_i-\varepsilon_j)\hat{Y}_{ij}-\chi q_{ij}(n_j-n_i)\sum_{kl}{}'q_{kl}\hat{Y}_{kl}$$
$$-\chi q_{ij}(n_j-n_i)\sum_{kl}{}''q_{kl}u_kv_k(\hat{C}^*_{lk}+\hat{C}_{kl})\,, \tag{3·9b}$$

$$[\hat{K},\hat{C}_{ij}]=(\varepsilon_i-\varepsilon_j)\hat{C}_{ij}+\chi q_{ij}u_iv_i\sum_{kl}{}'q_{kl}(\hat{X}_{kl}-\hat{Y}_{kl})\,, \tag{3·10a}$$

$$[\hat{K},\hat{C}^*_{ji}]=(\varepsilon_i-\varepsilon_j)\hat{C}^*_{ji}-\chi q_{ij}u_iv_i\sum_{kl}{}'q_{kl}(\hat{X}_{kl}-\hat{Y}_{kl})\,. \tag{3·10b}$$

With the use of the above commutation relations, we search for the operator $\hat{B}^*$ which satisfies the relation

$$[\hat{K},\hat{B}^*]=\omega\hat{B}^*\,,\qquad[\hat{B},\hat{B}^*]=1\,, \tag{3·11}$$

$$\hat{B}^*=\sum_{ij}{}'(U_{ij}\hat{X}_{ij}+V_{ij}\hat{Y}_{ij})+\sum_{ij}{}''(\Psi_{ij}\hat{C}^*_{ji}+\Phi_{ij}\hat{C}_{ij})\,. \tag{3·12}$$

The above relations give us the following eigenvalue equations:

$$(\varepsilon_i-\varepsilon_j)U_{ij}-\chi q_{ij}\sum_{kl}{}'q_{kl}(n_l-n_k)U_{kl}-\chi q_{ij}\sum_{kl}{}''q_{kl}u_kv_k[\Psi_{kl}-\Phi_{kl}]=\omega U_{ij}\,, \tag{3·13a}$$

$$(\varepsilon_i-\varepsilon_j)V_{ij}-\chi q_{ij}\sum_{kl}{}'q_{kl}(n_l-n_k)V_{kl}+\chi q_{ij}\sum_{kl}{}''q_{kl}u_kv_k[\Psi_{kl}-\Phi_{kl}]=\omega V_{ij}\,, \tag{3·13b}$$

$$(\varepsilon_i-\varepsilon_j)\Psi_{ij}-\chi q_{ij}u_iv_i\sum_{kl}{}'q_{kl}(n_l-n_k)[U_{kl}+V_{kl}]=\omega\Psi_{ij}\,, \tag{3·14a}$$

$$(\varepsilon_i-\varepsilon_j)\Phi_{ij}-\chi q_{ij}u_iv_i\sum_{kl}{}'q_{kl}(n_l-n_k)[U_{kl}+V_{kl}]=\omega\Phi_{ij}\,. \tag{3·14b}$$

The addition and the subtraction of Eqs. (3·13) and (3·14) give us

$$(\varepsilon_i-\varepsilon_j)[U_{ij}+V_{ij}]-\chi q_{ij}\sum_{kl}{}'q_{kl}(n_l-n_k)[U_{kl}+V_{kl}]=\omega[U_{ij}+V_{ij}]\,, \tag{3·15a}$$

$$(\varepsilon_i-\varepsilon_j)[U_{ij}-V_{ij}]-\chi q_{ij}\sum_{kl}{}'q_{kl}(n_l-n_k)[U_{kl}-V_{kl}]$$
$$-2\chi q_{ij}\sum_{kl}{}''q_{kl}u_kv_k[\Psi_{kl}-\Phi_{kl}]=\omega[U_{ij}-V_{ij}]\,, \tag{3·15b}$$

$$(\varepsilon_i-\varepsilon_j)[\Psi_{ij}+\Phi_{ij}]-2\chi q_{ij}u_iv_i\sum_{kl}{}'q_{kl}(n_l-n_k)[U_{kl}+V_{kl}]=\omega[\Psi_{ij}+\Phi_{ij}]\,, \tag{3·16a}$$

$$(\varepsilon_i-\varepsilon_j)[\Psi_{ij}-\Phi_{ij}]=\omega[\Psi_{ij}-\Phi_{ij}]\,. \tag{3·16b}$$

Let us search for solutions of Eqs. (3·15) and (3·16). By eliminating $[U_{ij}+V_{ij}]$ in

Eq. (3·15a), possible solutions of Eq. (3·15a) are obtained by solving the following equations:

$$\chi F(\omega)=1\,, \tag{3·17}$$

$$F(\omega)=\sum_{ij}{}' \frac{q_{ij}^2(n_j-n_i)(\varepsilon_i-\varepsilon_j)}{(\varepsilon_i-\varepsilon_j)^2-\omega^2}\,. \tag{3·18}$$

Since $F(\omega)$ is a function of ω^2, the solutions of Eq. (3·17) are labeled by

$$\omega=\pm\omega_n\,. \qquad (\omega_n>0\,,\quad n=1,2,\cdots) \tag{3·19}$$

In order to stress the connection with the eigenvalues $\pm\omega_n$, U_{ij}, V_{ij}, Ψ_{ij} and Φ_{ij} are denoted as $U_{ij}^{(\pm n)}$, $V_{ij}^{(\pm n)}$, $\Psi_{ij}^{(\pm n)}$ and $\Phi_{ij}^{(\pm n)}$, respectively. Equation (3·16b) gives us

$$(\varepsilon_i-\varepsilon_j)[\Psi_{ij}^{(\pm n)}-\Phi_{ij}^{(\pm n)}]=\pm\omega_n[\Psi_{ij}^{(\pm n)}-\Phi_{ij}^{(\pm n)}]\,. \tag{3·20}$$

We investigate the case $\pm\omega_n\neq\varepsilon_i-\varepsilon_j$ $(n_i=n_j)$. In this case, Eq. (3·20) gives us

$$\Psi_{ij}^{(\pm n)}-\Phi_{ij}^{(\pm n)}=0\,. \tag{3·21}$$

Rewriting Eq. (3·15a) and substituting the result (3·21) into Eqs. (3·15a) and (3·15b), we obtain the following equations:

$$(\varepsilon_i-\varepsilon_j)[U_{ij}^{(\pm n)}+V_{ij}^{(\pm n)}]-\chi q_{ij}\sum_{kl}{}' q_{kl}(n_l-n_k)[U_{kl}^{(\pm n)}+V_{kl}^{(\pm n)}]$$
$$=\pm\omega_n[U_{ij}^{(\pm n)}+V_{ij}^{(\pm n)}]\,, \tag{3·22a}$$

$$(\varepsilon_i-\varepsilon_j)[U_{ij}^{(\pm n)}-V_{ij}^{(\pm n)}]-\chi q_{ij}\sum_{kl}{}' q_{kl}(n_l-n_k)[U_{kl}^{(\pm n)}-V_{kl}^{(\pm n)}]$$
$$=\pm\omega_n[U_{ij}^{(\pm n)}-V_{ij}^{(\pm n)}]\,. \tag{3·22b}$$

In the above equations, generally, we can put

$$V_{ij}^{(+n)}=U_{ij}^{(-n)}=0\,. \tag{3·23}$$

For determining $U_{ij}^{(+n)}$ and $V_{ij}^{(-n)}$, we set up an eigenvalue equation

$$(\varepsilon_i-\varepsilon_j)W_{ij}-\chi q_{ij}\sum_{kl}{}' q_{kl}(n_l-n_k)W_{kl}=\omega W_{ij}\,. \qquad (\text{for } n_i\neq n_j) \tag{3·24}$$

The eigenvalues of Eq. (3·24) are given by solving Eq. (3·17), that is, $\omega=\pm\omega_n$. Then, $W_{ij}^{(\pm n)}$ which correspond to $\pm\omega_n$, are determined in the form

$$W_{ij}^{(\pm n)}=N^{(\pm n)}q_{ij}/(\varepsilon_i-\varepsilon_j\mp\omega_n)\,. \tag{3·25}$$

Here, $N^{(\pm n)}$ are normalization constants. Making positive and negative n-th eigenvalues of the above equation correspond to $\pm\omega_n$, we put

$$U_{ij}^{(+n)}=W_{ij}^{(+n)}\,, \qquad V_{ij}^{(-n)}=W_{ij}^{(-n)}\,. \tag{3·26}$$

Substituting the above result into Eq. (3·16a) and using Eq. (3·21), we have

$$\Psi_{ij}^{(\pm n)}=\Phi_{ij}^{(\pm n)}=N^{(\pm n)}q_{ij}u_i v_i/(\varepsilon_i-\varepsilon_j\mp\omega_n)\,. \tag{3·27}$$

Thus, the following forms for the operators $\hat{B}^*$ are obtained:

$$\hat{B}^*_{+n}=N^{(+n)}[\sum_{ij}{}' q_{ij}\hat{X}_{ij}/(\varepsilon_i-\varepsilon_j-\omega_n)+\sum_{ij}{}'' q_{ij}u_iv_i(\hat{C}^*_{ji}+\hat{C}_{ij})/(\varepsilon_i-\varepsilon_j-\omega_n)]\,, \quad (3\cdot28a)$$

$$\hat{B}^*_{-n}=N^{(-n)}[\sum_{ij}{}' q_{ij}\hat{Y}_{ij}/(\varepsilon_i-\varepsilon_j+\omega_n)+\sum_{ij}{}'' q_{ij}u_iv_i(\hat{C}^*_{ji}+\hat{C}_{ij})/(\varepsilon_i-\varepsilon_j+\omega_n)]\,. \quad (3\cdot28b)$$

The normalization constants are determined by setting up the relation $[\hat{B}_{\pm n}, \hat{B}^*_{\pm n}]=1$:

$$N^{(\pm n)}=[\sum_{ij}{}' q^2_{ij}(n_j-n_i)/(\varepsilon_i-\varepsilon_j\mp\omega_n)^2]^{-1/2}\,. \quad (3\cdot29)$$

Equations (3·15) and (3·16) have another type of solutions. We investigate the following case: If $\varepsilon_i-\varepsilon_j=\varepsilon_a-\varepsilon_b$ ($n_i\neq n_j$, $n_a=n_b$), the single-particle states i and j coincide with a and b, respectively, i.e., $i=a$ and $j=b$. Then, Eq. (3·16b) has the following solutions:

$$\omega=\varepsilon_a-\varepsilon_b\,, \quad (3\cdot30)$$

$$\Psi^{(ab)}_{ij}-\Phi^{(ab)}_{ij}=0\,, \qquad (\text{for} \quad (ij)\neq(ab)) \quad (3\cdot31a)$$

$$\Psi^{(ab)}_{ij}-\Phi^{(ab)}_{ij}\neq0\,. \qquad (\text{for} \quad (ij)=(ab)) \quad (3\cdot31b)$$

For discriminating the eigenvalues and the eigenvectors, we used the notation (ab), for example, as are shown in $\Psi^{(ab)}_{ij}$ and $\Phi^{(ab)}_{ij}$. Since $\pm\omega_n\neq\varepsilon_a-\varepsilon_b$, Eq. (3·15a) gives us

$$U^{(ab)}_{ij}+V^{(ab)}_{ij}=0\,. \quad (3\cdot32)$$

Substituting Eq. (3·32) into Eq. (3·16a), we have

$$(\varepsilon_i-\varepsilon_j)[\Psi^{(ab)}_{ij}+\Phi^{(ab)}_{ij}]=(\varepsilon_a-\varepsilon_b)[\Psi^{(ab)}_{ij}+\Phi^{(ab)}_{ij}]\,. \quad (3\cdot33)$$

Solutions of Eq. (3·33) are as follows:

$$\Psi^{(ab)}_{ij}+\Phi^{(ab)}_{ij}=0\,, \qquad (\text{for} \quad (ij)\neq(ab)) \quad (3\cdot34a)$$

$$\Psi^{(ab)}_{ij}+\Phi^{(ab)}_{ij}\neq0\,. \qquad (\text{for} \quad (ij)=(ab)) \quad (3\cdot34b)$$

Combining the solutions (3·34) with (3·31), we have

$$\Psi^{(ab)}_{ij}=\Phi^{(ab)}_{ij}=0\,, \qquad (\text{for} \quad (ij)\neq(ab)) \quad (3\cdot35a)$$

$$[\Psi^{(ab)}_{ij}]^2-[\Phi^{(ab)}_{ij}]^2\neq0\,. \qquad (\text{for} \quad (ij)=(ab)) \quad (3\cdot35b)$$

Then, Eq. (3·15b) leads us to

$$(\varepsilon_i-\varepsilon_j)[U^{(ab)}_{ij}-V^{(ab)}_{ij}]-\chi q_{ij}\sum_{kl}{}' q_{kl}(n_l-n_k)[U^{(ab)}_{kl}-V^{(ab)}_{kl}]$$
$$-2\chi q_{ij}q_{ab}u_av_a[\Psi^{(ab)}_{ab}-\Phi^{(ab)}_{ab}]$$
$$=(\varepsilon_a-\varepsilon_b)[U^{(ab)}_{ij}-V^{(ab)}_{ij}]\,. \quad (3\cdot36)$$

Equations (3·32) and (3·36) give us

$$U^{(ab)}_{ij}=-V^{(ab)}_{ij}$$
$$=M^{(ab)}q_{ij}/[(\varepsilon_i-\varepsilon_j)-(\varepsilon_a-\varepsilon_b)]\,. \quad (3\cdot37)$$

Here, $M^{(ab)}$ is a normalization constant which is given by

$$M^{(ab)}=\chi q_{ab}u_a v_a[\Psi_{ab}^{(ab)}-\Phi_{ab}^{(ab)}]\cdot[1-\chi F(\varepsilon_a-\varepsilon_b)]^{-1}\,. \tag{3·38}$$

Thus, we have the following forms:

$$\hat{B}_{ab}^{*}=M^{(ab)}\sum_{ij}{}' q_{ij}(\hat{X}_{ij}-\hat{Y}_{ij})/[(\varepsilon_i-\varepsilon_j)-(\varepsilon_a-\varepsilon_b)]+\Psi_{ab}^{(ab)}\hat{C}_{ba}^{*}+\Phi_{ab}^{(ab)}\hat{C}_{ab}\,. \tag{3·39}$$

The quantities $\Psi_{ab}^{(ab)}$ and $\Phi_{ab}^{(ab)}$, further, the normalization constants $M^{(ab)}$ are determined by the condition $[\hat{B}_{ab}, \hat{B}_{ab}^{*}]=1$, which gives us the relation $[\Psi_{ab}^{(ab)}]^2-[\Phi_{ab}^{(ab)}]^2=1$. Then, we can put

$$\Psi_{ab}^{(ab)}=1\,, \qquad \Phi_{ab}^{(ab)}=0\,. \tag{3·40}$$

The above treatment is also valid for the case $a=b$.

With the use of the results (3·28) and (3·29), the Hamiltonian $\hat{K}$ is expressed as

$$\hat{K}=\sum_{n=1,2,\cdots}{}' \omega_n(\hat{B}_{+n}^{*}\hat{B}_{+n}-\hat{B}_{-n}^{*}\hat{B}_{-n})+\sum_{\varepsilon_a>\varepsilon_b}{}'' (\varepsilon_a-\varepsilon_b)(\hat{B}_{ab}^{*}\hat{B}_{ab}-\hat{B}_{ba}^{*}\hat{B}_{ba})\,. \tag{3·41}$$

Therefore, the excitation energies are given by ω_n and $(\varepsilon_a-\varepsilon_b)$ (>0). The above is the TFRPA (B) formalism. In § 5, we will discuss again the approach (B).

§ 4. The TFRPA equation in the approach (C)

As was mentioned in § 1, the approach (C) has been initiated by the present authors.[4)] The basic idea is based on the TDHF-like variational principle and it is a classical theory. First, let us give some basic parts of this theory. A characteristic point, in contrast to the approaches (A) and (B), is the existence of the constraint (2·10), the explicit form of which is

$$G_{ij}=+v_i u_j(a_i^{*}b_j^{*})_C+u_i v_j(b_i a_j)_C+u_i u_j(b_j^{*}b_i)_C-v_i v_j(a_i^{*}a_j)_C=0\,. \tag{4·1}$$

Here, $(a_i^{*}b_j^{*})_C$, etc., denote the expectation value of the operators $\hat{a}_i^{*}\hat{b}_j^{*}$, etc., for the mixed state $|m(t)\rangle\rangle$ which is a Slater determinant-like state for the Schrödinger equation (2·3). These expectation values can be expressed in the classical correspondences of the relation (2·16). In this case, $\hat{C}_{ij}$ and $\hat{C}_{ji}^{*}$ are replaced with the c-number variables $\boldsymbol{C}_{ij}$ and $\boldsymbol{C}_{ji}^{*}$:

$$\hat{C}_{ij}\rightarrow \boldsymbol{C}_{ij}\,, \qquad \hat{C}_{ji}^{*}\rightarrow \boldsymbol{C}_{ji}^{*}\,. \tag{4·2}$$

The variables $\boldsymbol{C}_{ij}$ and $\boldsymbol{C}_{ji}^{*}$ are canonical if the constraint is suppressed. The constraint (4·1) is explicitly given by

$$\begin{aligned} G_{ij}&=+v_i u_j\sum_k \boldsymbol{C}_{jk}^{*}(\sqrt{1-\boldsymbol{C}^{\dagger}\boldsymbol{C}})_{ik}+u_i v_j\sum_k(\sqrt{1-\boldsymbol{C}^{*}\boldsymbol{C}^{T}})_{ki}\boldsymbol{C}_{kj}\\ &\quad+u_i u_j\sum_k \boldsymbol{C}_{jk}^{*}\boldsymbol{C}_{ik}-v_i v_j\sum_k \boldsymbol{C}_{ki}^{*}\boldsymbol{C}_{kj}\\ &=v_i u_j\boldsymbol{C}_{ji}^{*}+u_i v_j\boldsymbol{C}_{ij}+u_i u_j\sum_k \boldsymbol{C}_{jk}^{*}\boldsymbol{C}_{ik}-v_i v_j\sum_k \boldsymbol{C}_{ki}^{*}\boldsymbol{C}_{kj}+\cdots=0\,. \end{aligned} \tag{4·3}$$

The above relation means that, on the submanifold governed by the constraint

$G_{ij}=0$, these variables are not canonical. Therefore, we introduce the boson-type canonical variables D_m and $D_m{}^*$ on the submanifold, where m denotes the index specifying the variables. At the present stage, we do not know the total number of the variables.

Our problem is to express C_{ij} and C_{ji}^* as functions of the new canonical variables, D_m and $D_m{}^*$. We impose the following relation, which is called the canonicity condition:

$$1/2\cdot\sum_{ij}(C_{ij}^*\partial C_{ij}/\partial D_m - C_{ji}\partial C_{ji}^*/\partial D_m) = D_m{}^*/2 - i\cdot\partial S/\partial D_m\,. \tag{4·4}$$

Of course, we also consider the complex conjugate of the relation (4·4). Here, S is a function of $(D_m, D_m{}^*)$ and satisfies $S^*=S$. Let us note that the state $|m(t)\rangle\!\rangle$ satisfies

$$\langle\!\langle m(t)|\partial/\partial C_{ij}|m(t)\rangle\!\rangle = C_{ij}^*/2\,. \tag{4·5}$$

The complex conjugate of the above relation will be also used. Then, combining Eq. (4·4) with Eq. (4·5), we have

$$\langle\!\langle m(t)|i\partial/\partial t|m(t)\rangle\!\rangle = i/2\cdot\sum_m(\dot{D}_m D_m{}^* - \dot{D}_m{}^* D_m) + dS/dt\,. \tag{4·6}$$

The variation for determining $|m(t)\rangle\!\rangle$ can be expressed in the following form:

$$\delta\int_{t_0}^{t_1} L dt = 0\,, \tag{4·7}$$

$$L = \langle\!\langle m(t)|i\partial_t - \hat{H}|m(t)\rangle\!\rangle$$

$$= i/2\cdot\sum_m(\dot{D}_m D_m{}^* - \dot{D}_m{}^* D_m) - H + dS/dt\,, \tag{4·8}$$

$$H = \langle\!\langle m(t)|\hat{H}|m(t)\rangle\!\rangle = H(D, D^*)\,. \tag{4·9}$$

The term dS/dt does not give any effect on the variation (4·7) and from this variation, we have the Hamilton equations of motion.

Now, on the basis of the relations (4·3) and (4·4), let us determine C_{ij} and C_{ji}^* as functions of the canonical variables D_m and $D_m{}^*$. We expand G_{ij}, C_{ij} and C_{ji}^* in the following forms:

$$G_{ij} = G_{ij}^{(1)} + G_{ij}^{(2)} + \cdots\,, \tag{4·10}$$

$$C_{ij} = C_{ij}^{(1)} + C_{ij}^{(2)} + \cdots\,,$$

$$C_{ji}^* = C_{ji}^{(1)*} + C_{ji}^{(2)*} + \cdots\,. \tag{4·11}$$

The first and the second order of G_{ij} are determined by

$$G_{ij}^{(1)} = v_i u_j C_{ji}^{(1)*} + u_i v_j C_{ij}^{(1)} = 0\,, \tag{4·12}$$

$$G_{ij}^{(2)} = v_i u_j C_{ji}^{(2)*} + u_i v_j C_{ij}^{(2)} + u_i u_j \sum_k C_{jk}^{(1)*} C_{ik}^{(1)} - v_i v_j \sum_k C_{ki}^{(1)*} C_{kj}^{(1)} = 0\,. \tag{4·13}$$

From the relation (4·12), we can put

$$C_{ij}^{(1)} = +v_i u_j Z_{ij}\,, \qquad C_{ji}^{(1)*} = -u_i v_j Z_{ij}\,. \tag{4·14}$$

Since $(\boldsymbol{C}_{ij}^{(1)})^* = \boldsymbol{C}_{ij}^{(1)*}$, $\boldsymbol{Z}_{ij}$ should satisfy

$$\boldsymbol{Z}_{ji}^* = -\boldsymbol{Z}_{ij} . \tag{4·15}$$

Then, by substituting the relation (4·14) into Eq. (4·13), we have

$$v_i u_j \boldsymbol{C}_{ji}^{(2)*} + u_i v_j \boldsymbol{C}_{ij}^{(2)} = u_i v_i u_j v_j \sum_k (1-2n_k) \boldsymbol{Z}_{ik} \boldsymbol{Z}_{kj} . \tag{4·16}$$

From the relation (4·16), we can put

$$\boldsymbol{C}_{ij}^{(2)*} = v_i u_j \sum_k w_{ij,k} \boldsymbol{Z}_{ik} \boldsymbol{Z}_{kj} ,$$

$$\boldsymbol{C}_{ji}^{(2)} = u_i v_j \sum_k w_{ji,k} \boldsymbol{Z}_{ik} \boldsymbol{Z}_{kj} . \tag{4·17}$$

The above relations satisfy $(\boldsymbol{C}_{ij}^{(2)})^* = \boldsymbol{C}_{ij}^{(2)*}$ and $w_{ij,k}$ and $w_{ji,k}$ should satisfy

$$w_{ij,k} + w_{ji,k} = 1 - 2n_k . \tag{4·18}$$

The quantity $w_{ij,k}$ is a function of n_i, n_j and n_k: $w_{ij,k} = w(n_i, n_j, n_k)$. Through a procedure similar to the above case, the higher order terms can be determined.

Next, in order to determine $\boldsymbol{Z}_{ij}$ and $w_{ij,k}$, we use the canonicity condition (4·4). Under the present approximation, the condition (4·4) can be expressed by

$$\begin{aligned} &1/2 \cdot \sum_{ij} (n_i - n_j) [\boldsymbol{Z}_{ij} \partial \boldsymbol{Z}_{ji} / \partial \boldsymbol{D}_m - \boldsymbol{Z}_{ji} \partial \boldsymbol{Z}_{ij} / \partial \boldsymbol{D}_m] \\ &\quad + \sum_{ijk} [n_i (1-n_j) w_{ij,k} + n_j (1-n_i) w_{ji,k}] \\ &\qquad \cdot [(\boldsymbol{Z}_{ik} \boldsymbol{Z}_{kj}) \partial \boldsymbol{Z}_{ji} / \partial \boldsymbol{D}_m - \boldsymbol{Z}_{ji} \partial (\boldsymbol{Z}_{ik} \boldsymbol{Z}_{kj}) / \partial \boldsymbol{D}_m] \\ &= \boldsymbol{D}_m^* - 2i \cdot \partial S / \partial \boldsymbol{D}_m . \end{aligned} \tag{4·19}$$

For the above relation, we impose the following relations:

$$n_i (1-n_j) w_{ij,k} + n_j (1-n_i) w_{ji,k} = 0 , \quad (\text{for} \quad n_i \neq n_j , \quad n_i \neq n_k , \quad n_j \neq n_k) \tag{4·20}$$

$$n_i (1-n_j) w_{ij,k} + n_j (1-n_i) w_{ji,k} = n_i (1-n_i)(1-2n_j) . \quad (\text{for} \quad n_i \neq n_j , \quad n_i = n_k) \tag{4·21}$$

Then, the relation (4·19) can be rewritten as

$$\begin{aligned} &1/2 \cdot \sum_{ij} (n_i - n_j)(\boldsymbol{A}_{ij} \partial \boldsymbol{A}_{ji} / \partial \boldsymbol{D}_m - \boldsymbol{A}_{ji} \partial \boldsymbol{A}_{ij} / \partial \boldsymbol{D}_m) \\ &\quad - \partial / \partial \boldsymbol{D}_m \cdot \sum_{ijk} [n_i (1-n_i)(1-2n_k) \boldsymbol{\alpha}_{ij} \boldsymbol{A}_{ik} \boldsymbol{A}_{kj} \\ &\qquad + 1/3 \cdot n_i (1-n_i)(1-2n_i) \boldsymbol{\alpha}_{ji} \boldsymbol{\alpha}_{ik} \boldsymbol{\alpha}_{kj}] \\ &= \boldsymbol{D}_m^* - 2i \cdot \partial S / \partial \boldsymbol{D}_m . \end{aligned} \tag{4·22}$$

Here, $\boldsymbol{A}_{ij}$ and $\boldsymbol{\alpha}_{ij}$ are defined by

$$\boldsymbol{Z}_{ij} = \boldsymbol{A}_{ij} , \quad (\text{for} \quad n_i \neq n_j) \qquad \boldsymbol{\alpha}_{ij} . \quad (\text{for} \quad n_i = n_j) \tag{4·23}$$

The relation (4·23) gives us

$$1/2\cdot\sum_{ij}(n_i-n_j)(\boldsymbol{A}_{ij}\partial\boldsymbol{A}_{ji}/\partial\boldsymbol{D}_m-\boldsymbol{A}_{ji}\partial\boldsymbol{A}_{ij}/\partial\boldsymbol{D}_m)=\boldsymbol{D}_m^*\,, \tag{4·24}$$

$$iS=1/2\cdot\sum_{ijk}[n_i(1-n_i)(1-2n_k)\boldsymbol{\alpha}_{ij}\boldsymbol{A}_{ik}\boldsymbol{A}_{kj} +1/3\cdot n_i(1-n_i)(1-2n_k)\boldsymbol{\alpha}_{ji}\boldsymbol{\alpha}_{ik}\boldsymbol{\alpha}_{kj}]\,. \tag{4·25}$$

Of course, S given in Eq. (4·25) satisfies $S^*=S$. A possible solution of Eq. (4·24) and its complex conjugate is given by

$$\boldsymbol{A}_{ij}=\begin{cases}+\boldsymbol{D}_{i>j}/\sqrt{n_i-n_j}\,, & (\text{for}\quad n_i>n_j)\\ -\boldsymbol{D}^*_{j>i}/\sqrt{n_j-n_i}\,. & (\text{for}\quad n_i<n_j)\end{cases} \tag{4·26}$$

Here, the index of the canonical variables $\boldsymbol{D}_m$ and $\boldsymbol{D}_m{}^*$, m , is defined by the ordered pair of the single-particle states such as denoted $i>j$ if $n_i>n_j$. From the solution (4·26), we can see that $\boldsymbol{Z}_{ij}$ for every combination (i, j) except $n_i=n_j(\boldsymbol{A}_{ij})$ can be expressed as function of $\boldsymbol{D}_{i>j}$ and $\boldsymbol{D}^*_{i>j}$ and $\boldsymbol{Z}_{ij}$ for $n_i=n_j(\boldsymbol{\alpha}_{ij})$ exists only in S, which does not give any influence on the equation of motion. This means that the many-body system under investigation can be described only in terms of $\boldsymbol{A}_{ij}$. Therefore, the number of the variables is determined by the ordered pairs of the single-particle states. With the use of the relations (4·18), (4·20) and (4·21), we can determine $w_{ij,k}$:

$$w_{ij,k}=\begin{cases} n_j(1-n_i)(1-2n_k)/(n_j-n_i)\,, & \\ & (\text{for}\quad n_i\neq n_j\,,\quad n_i\neq n_k\,,\quad n_j\neq n_k)\\ 1-n_k\,, & (\text{for}\quad n_i\neq n_j\,,\quad n_i=n_k)\\ -n_k\,, & (\text{for}\quad n_i\neq n_j\,,\quad n_j=n_k)\\ (1-2n_k)/2\,. & (\text{for}\quad n_i=n_j)\end{cases} \tag{4·27}$$

Then, we have

$$\boldsymbol{C}_{ij}=v_iu_j[\boldsymbol{A}_{ij}+\sum_k n_j(1-n_i)(1-2n_k)/(n_j-n_i)\boldsymbol{A}_{ik}\boldsymbol{A}_{kj} +\sum_k(1-n_k)\boldsymbol{\alpha}_{ik}\boldsymbol{A}_{kj}-\sum_k n_k\boldsymbol{A}_{ik}\boldsymbol{\alpha}_{kj}]\,, \quad (\text{for}\quad n_i\neq n_j) \tag{4·28a}$$

$$\boldsymbol{C}_{ij}=v_iu_j[\boldsymbol{\alpha}_{ij}+\sum_k(1-2n_k)/2\cdot(\boldsymbol{A}_{ik}\boldsymbol{A}_{kj}+\boldsymbol{\alpha}_{ik}\boldsymbol{\alpha}_{kj})]\,. \quad (\text{for}\quad n_i=n_j) \tag{4·28b}$$

Now, it is possible to express the Hamiltonian in terms of the canonical variables. We first give the expression for $(c_i{}^*c_j)_C$:

$$(c_i{}^*c_j)_C=n_i\delta_{ij}+\sum_k(n_i-n_k)\boldsymbol{Z}_{ik}\boldsymbol{Z}_{kj}+\cdots\,, \quad (\text{for}\quad n_i=n_j) \tag{4·29a}$$

$$(c_i{}^*c_j)_C=(n_i-n_j)\boldsymbol{Z}_{ij}+\sum_k[n_in_j(1-n_k)-(1-n_i)(1-n_j)n_k +n_i(1-n_j)w_{ij,k}+n_j(1-n_i)w_{ij,k}]\boldsymbol{Z}_{ik}\boldsymbol{Z}_{kj}+\cdots\,. \quad (\text{for}\quad n_i\neq n_j) \tag{4·29b}$$

Substituting the relation (4·23) into Eqs. (4·29), we have

$$(c_i{}^*c_j)_C=n_i\delta_{ij}+\sum_k(n_i-n_k)\boldsymbol{A}_{ik}\boldsymbol{A}_{kj}+\cdots\,, \quad (\text{for}\quad n_i=n_j) \tag{4·30a}$$

$$(c_i{}^*c_j)_C=(n_i-n_j)\boldsymbol{A}_{ij}$$
$$+\sum_k[n_in_j(1-n_k)-(1-n_i)(1-n_j)n_k]\boldsymbol{A}_{ik}\boldsymbol{A}_{kj}+\cdots. \quad (\text{for } n_i\neq n_j) \tag{4·30b}$$

It should be noted that the quantity $(c_i{}^*c_j)_C$, in terms of which the Hamiltonian $\boldsymbol{H}$ is expressed, does not contain the quantity $\boldsymbol{\alpha}_{ij}$ ($\boldsymbol{Z}_{ij}$ for $n_i=n_j$). Therefore, the Hamiltonian can be expressed only in terms of the canonical variables introduced in Eq. (4·26):

$$\boldsymbol{H}=E_0+1/2\cdot\sum_{ij}(\varepsilon_j-\varepsilon_i)(n_i-n_j)\boldsymbol{A}_{ij}\boldsymbol{A}_{ji}-\chi/2\cdot[\sum_{ij}q_{ij}(n_i-n_j)\boldsymbol{A}_{ij}]^2. \tag{4·31}$$

With the use of $\boldsymbol{D}_{i>j}$ and $\boldsymbol{D}^*_{i>j}$, the Hamiltonian is

$$\boldsymbol{H}=E_0+\sum_{ij}(\varepsilon_i-\varepsilon_j)\boldsymbol{D}^*_{i>j}\boldsymbol{D}_{i>j}-\chi/2\cdot[\sum_{ij}q_{ij}\sqrt{n_i-n_j}(\boldsymbol{D}_{i>j}+\boldsymbol{D}^*_{i>j})]^2. \tag{4·32}$$

We can see that the Hamiltonian (4·32) is of the familiar to the standard understanding of the RPA. From the equation of motion for the above Hamiltonian, the TFRPA (C) equation is obtained and in the next section, we will give it explicitly.

§ 5. Discussion

First of all, we will show that the Hamiltonian $\boldsymbol{H}$ given in Eq. (4·32) can be rewritten as

$$\boldsymbol{H}=E_0+\sum_{ij}{}'(\varepsilon_j-\varepsilon_i)/2(n_i-n_j)\cdot\boldsymbol{X}_{ji}\boldsymbol{X}_{ij}-\chi/2\cdot[\sum_{ij}{}'q_{ij}\boldsymbol{X}_{ij}]^2. \tag{5·1}$$

Here, $\boldsymbol{X}_{ij}$ is defined by

$$\boldsymbol{X}_{ij}=\begin{cases}\sqrt{n_i-n_j}\,\boldsymbol{D}_{i>j}, & (\text{for } n_i>n_j)\\ \sqrt{n_j-n_i}\,\boldsymbol{D}^*_{j>i} & (\text{for } n_i<n_j)\end{cases} \tag{5·2}$$

and satisfies the relations

$$\boldsymbol{X}^*_{ij}=\boldsymbol{X}_{ji}, \qquad [\boldsymbol{X}_{ij},\boldsymbol{X}_{kl}]_P=\delta_{jk}\delta_{il}(n_i-n_j). \tag{5·3}$$

Here, $[\ ,\ ]_P$ denotes the Poisson bracket for $\boldsymbol{D}_{i>j}$ and $\boldsymbol{D}^*_{i>j}$. We can see that, under the correspondence between the relations (3·6a) and (5·3), the Hamiltonian $\boldsymbol{H}$ corresponds to the term $\hat{K}_X$ given in Eq. (3·8a). Further, if we rewrite Eqs. (4·30) in terms of $\boldsymbol{X}$, the quantities $(c_i{}^*c_j)_C$ recover the same forms as those given in Eqs. (6·3) of Ref. 4). Of course, the properties of $\boldsymbol{X}$ given in Eq. (5·3) are also the same as those given in Eq. (6·1) of Ref. 4).

The Hamilton equation of motion gives us the TFRPA (C) eigenvalue equation and it is of the same form as that given in Eq. (3·13a) for the case $\Psi_{kl}=\Phi_{kl}=0$. It is also equivalent to that given in Eq. (5·11) of Ref. 4). With the use of the notations shown in § 3, we can express H in the form

$$\boldsymbol{H}=E_0+\sum_{n=1,2,\cdots}{}'\omega_n\boldsymbol{B}^*_{+n}\boldsymbol{B}_{+n}, \tag{5·4}$$

$$\boldsymbol{B}^*_{+n} = N^{(+n)} \sum_{ij}{}' q_{ij} \boldsymbol{X}_{ij} / (\varepsilon_i - \varepsilon_j - \omega_n) . \tag{5·5}$$

Here, ω_n is the positive n-th solution of Eq. (3·18) and $N^{(+n)}$ is given by Eq. (3·29).

On the basis of the above result, let us compare the approach (C) with the approach (A) or (B). As one of the merits of the use of the thermo field dynamics formalism, we can find the following statement on page 2805 of Ref. 2), which is the original paper of the approach (A): This enlarged space provides us with the new possibility of supplying more variational parameters than those in the variational derivation of the TRPA equation. This statement is quite interesting, but, concerning the construction of the RPA, the thermo field dynamics formalism does not realize this expectation. As was already mentioned, the approach (A) cannot give us the standard form of the RPA. The solution given in the approach (B) can be classified into two types: The first and the second solution are related with the frequencies ω_n and $(\varepsilon_a - \varepsilon_b)$, respectively. The first is nothing but the solution in the TRPA equation. In some sense, the second corresponds to the single-particle excitation. Therefore, the approach (B) does not lead us to the solution with new correlations which do not exist in the TRPA equation. Further, in the approach (C), only the first type solution of the approach (B) is obtained. Therefore, the approach (C) also cannot lead us to the solution with the new correlations.

From the above statement, we must note the existence of the second type solution in the approach (B). In order to investigate the meaning of the solution, here, we will recapitulate the RPA at the pure state limit where we have $n_i = 0$ or 1. The former and the latter correspond to the single-particle and the single-hole states, respectively, which are denoted by the notations (p, p', p'') and (h, h', h''), respectively. The creation and the annihilation operators of the particle and the hole are defined by

$$\hat{c}_i = \begin{cases} \hat{a}_p , \\ \hat{b}_h^* , \end{cases} \qquad c_i^* = \begin{cases} \hat{a}_p^* , & (\text{for} \quad i=p) \\ \hat{b}_h^* . & (\text{for} \quad i=h) \end{cases} \tag{5·6}$$

Further, we introduce the following operators:

$$\hat{A}_{hp} = \hat{b}_h \hat{a}_p , \quad \hat{B}_{pp'} = \hat{a}_p^* \hat{a}_{p'} , \quad \hat{B}_{hh'} = \hat{b}_h^* \hat{b}_{h'} . \tag{5·7}$$

With the use of the above operators, the Hamiltonian (2·1) can be rewritten as

$$\hat{H} = E_0{}^0 + \sum_p \varepsilon_p{}^0 \hat{B}_{pp} - \sum_h \varepsilon_h{}^0 \hat{B}_{hh} - \chi/2 \cdot [\sum_{ph} q_{ph} (\hat{A}^*_{hp} + \hat{A}_{hp})$$
$$+ \sum_{pp'} q_{pp'} \hat{B}_{pp'} - \sum_{hh'} q_{hh'} \hat{B}_{hh'}]^2 . \tag{5·8}$$

Here, $E_0{}^0$, $\varepsilon_p{}^0$ and $\varepsilon_h{}^0$ are given by

$$E_0{}^0 = \sum_h t_{hh} - \chi/2 \cdot [\sum_h q_{hh}]^2 , \tag{5·8a}$$

$$\varepsilon_p{}^0 = t_{pp} - \chi q_{pp} [\sum_{h'} q_{h'h'}] ,$$

$$\varepsilon_h{}^0 = t_{hh} - \chi q_{hh} [\sum_{h'} q_{h'h'}] . \tag{5·8b}$$

The above is the solution of the conventional Hartree equation. If we pick up the linear terms for $\hat{A}^*_{hp}$, $\hat{A}_{hp}$, $\hat{B}_{pp'}$ and $\hat{B}_{hh'}$, the equations of motion for the above operators are approximately given by

$$[\hat{H}, \hat{A}^*_{ph}]=(\varepsilon_p{}^0-\varepsilon_h{}^0)\hat{A}^*_{hp}-\chi q_{ph}\sum_{p'h'}q_{p'h'}(\hat{A}^*_{h'p'}+\hat{A}_{h'p'})$$

$$-\chi q_{ph}[\sum_{p'p''}q_{p'p''}\hat{B}_{p'p''}-\sum_{h'h''}q_{h'h''}\hat{B}_{h'h''}]\,, \tag{5·9a}$$

$$[\hat{H}, \hat{A}_{hp}]=-(\varepsilon_p{}^0-\varepsilon_h{}^0)\hat{A}_{hp}+\chi q_{ph}\sum_{p'h'}q_{p'h'}(\hat{A}^*_{h'p'}+\hat{A}_{h'p'})$$

$$+\chi q_{ph}[\sum_{p'p''}q_{p'p''}\hat{B}_{p'p''}-\sum_{h'h''}q_{h'h''}\hat{B}_{h'h''}]\,, \tag{5·9b}$$

$$[\hat{H}, \hat{B}_{pp'}]=(\varepsilon_p{}^0-\varepsilon^0_{p'})\hat{\boldsymbol{B}}_{pp'}\,, \tag{5·10a}$$

$$[\hat{H}, \hat{B}_{hh'}]=(\varepsilon_h{}^0-\varepsilon^0_{h'})\hat{\boldsymbol{B}}_{hh'}\,. \tag{5·10b}$$

Concerning the above equations, there exist two interpretations for the linearization for the operators $\hat{A}_{hp}$, $\hat{B}_{pp'}$ and $\hat{B}_{hh'}$. One is the following: Regarding the operators (5·7) as independent of each other, Eqs. (5·9) and (5·10) are fundamental in the RPA. In this case, from Eqs. (5·10), we can get the solutions with the single-particle exicitations. Further, from Eqs. (5·9), we obtain the well-known RPA frequencies. However, in the boson expansion theory, it is questionable to regard $\hat{B}_{pp'}$ and $\hat{B}_{hh'}$ as independent of $\hat{A}_{hp}$ and $\hat{A}^*_{hp}$. In the first order expansion, $\hat{A}_{hp}$ and $\hat{A}^*_{hp}$ are regarded as boson operators A_{hp} and $\hat{A}^*_{hp}$. The operators $B_{pp'}$ and $\hat{B}_{hh'}$ can be expressed in the forms $\hat{B}_{pp'}=\sum_h\hat{A}^*_{hp}\hat{A}_{hp'}$ and $\hat{B}_{hh'}=\sum_p\hat{A}^*_{hp}\hat{A}_{h'p}$. Therefore, $\hat{B}_{pp'}$ and $\hat{B}_{hh'}$ are quadratic in the bosons. In this sense, the equations of motion (2·9) contain non-linear terms, which are linear for $\hat{B}_{p'p''}$ and $\hat{B}_{h'h''}$. Therefore, for the linearization, such terms should be rejected from Eqs. (5·9). Further, Eqs. (5·10) are quadratic with respect to the bosons and we can pick up the other quadratic terms from the exact equation of motion for $\hat{B}_{pp'}$ and $\hat{B}_{hh'}$. This means that Eqs. (5·10) are not consistent to the order of the approximation. Therefore, they should not be included in the set of equations in the RPA. Further, on the basis of Eqs. (5·9) and (5·10), it may be impossible to investigate the higher order effects systematically. If we start only from Eqs. (5·9), no trouble arises under the boson expansion. From the above-mentioned reason, the RPA at the pure state limit should be restricted to the forms (5·9) with $\hat{B}_{pp'}=\hat{B}_{hh'}=0$.

Now, we will go back to our starting problem. As was shown in § 3, the TFRPA (B) equation contains the solution which gives us the excitation energy $(\varepsilon_a-\varepsilon_b)$. At the pure state limit, its value is reduced to $(\varepsilon_p{}^0-\varepsilon_h{}^0)$, which cannot be accepted in the RPA at the pure state limit. This means that such solutions should be rejected from those of the TFRPA equation. The approach (C) does not contain such solutions and all solutions are reduced to those given under the condition $\hat{B}_{pp'}=\hat{B}_{hh'}=0$ at the pure state limit. In this sense, we can conclude that, in the thermo field dynamics formalism, the constraints introduced in the approach (C) play an essential role for rejecting the solution which does not have any physical meaning. In contrast to the above case, the approaches (A) and (B) do not contain such constraints and the variables $\hat{C}_{ij}$ and $\hat{C}^*_{ji}$ $(n_i = n_j)$ are independent of the others and this fact leads to the trouble discussed in this paper. Further, we again remark that the TFRPA (C) equation coincides with that based on the use of the Liouville-von Neumann equation by the present authors (J. P. and C. F.).[7] In conclusion, in spite of an interesting approach, the thermo field dynamics formalism cannot give any extended TRPA equation under the standard form of the RPA. In this sense, the merit of the thermo field dynamics formalism may appear at the case where the approximation is higher than that of the TFRPA. In this paper, we have shown only the expressions up to the quadratic order terms. In the subsequent paper, under careful investigation on the constraints, we will give a method which makes possible to calculate straightforwardly the terms with any order.

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