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Equation of Collective Submanifold for Mixed States

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With the aim of giving a microscopic description of various nuclear phenomena observed in highly excited states, the equation of the collective submanifold for mixed states is presented. The basic idea is a possible TDHF-like variation in the enlarged space which is adopted in the thermo field dynamics formalism. A set of equations, which determines the collective submasifold, is obtained. The form is analogous to that given in the conventional TDHF theory. At the small amplitude limit, an equation, the form of which is similar to the conventional RPA equation, can be derived in a natural way.

§1. Introduction

One of the recent interests in study of the nuclear many-body theories may be to present a microscopic theory which enables us to describe nuclear phenomena observed in highly excited states and interpreted in the language of the concept of thermal equilibrium with the temperature $T \neq 0$. The references concerned with these phenomena can be found in Refs. 1) and 2). In these phenomena, individual highly excited states are equally populated and usually the average properties of the system are measured. Therefore, the statistical approach is necessary. In contrast to the above phenomena, low lying states are related to $T=0$. We know a powerful method for describing such states, i.e., the TDHF theory based on a single Slater determinant. The Slater determinant is an example of a pure state and the state of thermal equilibrium with $T \neq 0$ can be regarded as a mixed state. The TDHF theory formulated in terms of the equation of the collective submanifold enables us to describe collective motion as a pure state not only in the linear but also in the non-linear type.[3] Then, it may be interesting for describing the mixed states to extend the TDHF theory in the statistical sense.

In responce to the above-mentioned situation, the present authors (J. P. and C. F.) proposed a microscopic theory based on the density matrix formalism.[1] With the help of this theory, a variational derivation of static and dynamical mean field theories for the mixed states is possible in terms of a thermal boson expansion. As the lowest approximation, the RPA equation for the mixed states can be derived and by picking up higher order corrections, the anharmonicities can be treated. Then, it is desirable to describe the anharmonicities in the frame of a small number of the degrees of freedom, for example, one collective degree of freedom in the same way as in the TDHF theory.[3]

On the other hand, Tanabe formulated the thermal RPA and the second thermal RPA method in a new version in terms of the quasi-particles.[2] Further, Hatsuda also gave a theory in which the RPA and the boson expansion are formulated under the thermal HFB approximation.[4] A characteristic common to the above two works is the use of the thermo field dynamics formalism.[5] 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. For example, the enlarged space is constructed from a set of the quasi-particle operators (α_i^*, α_i) and another set $(\tilde{\alpha}_i^*, \tilde{\alpha}_i)$. By taking into account all possible bi-linear combinations of the quasi-particles $(\alpha_i^*, \alpha_i, \tilde{\alpha}_i^*, \tilde{\alpha}_i)$, the thermal RPA method is formulated. Also, the second thermal RPA method is given by including the higher order products of the quasi-particles.[2] Further, the bi-linear forms can be expressed in terms of the boson operators, i.e., the boson expansion can be formulated.[4]

From the reason mentioned later on, the approach based on the thermo field dynamics formalism is quite interesting. However, this approach, as it stands, contains an unnatural feature. As was already mentioned, this formalism is given in the enlarged space. This means that the number of degrees of freedom exceeds that of the many-fermion system under investigation. Therefore, if we make any exact calculation after the boson expansion, there does not exist any trouble. However, if we make any approximation, then, the degrees of freedom which do not correspond to those in the original system have some influence on the results. The approach presented in Ref. 1) does not contain such an unnatural point, because, in this case, the fermion space is not enlarged.

Main aim of this paper is to present a classical microscopic theory, with the aid of which the mixed states can be described. The basic idea is the extended use of the TDHF thoery for the pure state[3] in the enlarged space given in the thermo field dynamics formalism. As is well known, bi-linear forms of fermion operators form a closed algebra and they can be expressed in terms of boson operators, i.e., boson expansion theory. Further, c-number replacement of the boson in the boson expansion theory reduces to the TDHF theory parametrized in terms of canonical variables. Then, we obtain the TDHF theory in a small number of the variables by solving the equation of the collective submanifold.[3] From the above consideration, we can obtain the boson expansion theory in the enlarged space for the thermo field dynamics formalism[4] and, then, the c-number replacement reduces to the TDHF theory in the enlarged space. Under the above scheme, we can express the mixed states in terms of small number of the canonical variables. However, we must pay attention to the number of degrees of freedom in the enlarged space. Many of them do not correspond to those given in the original fermion space. Therefore, we must introduce a certain additional condition, which plays a role of constraint in the classical phase space. This is a new feature which is not contained in Refs. 2) and 4). The above is our basic idea.

In the next section, as preliminaries for the later discussion, basic relations obtained in the TDHF theory are given and general viewpoint of our treatment is described. In § 3, a possible formalism of constrained canonical form for the mixed states is given in a form analogous to the TDHF theory. Section 4 is devoted to the derivation of equation of collective submanifold for the mixed states. In § 5, as the zero-th order approximation, the RPA equation is derived. Finally, in § 6, some concluding remarks are mentioned for future problems. In this paper, we give our basic idea for the case of particle-hole type collective motion, therefore, we cannot make direct comparison with the RPA equation given in Refs. 2) and 4) where the pairing correlation is included.

§ 2. Preliminaries

2. 1. *Hamiltonian and Slater determinant as an approximate pure state*

We investigate an N-fermion system, the Hamiltonian of which is given by

$$\dot{H}=\sum_{ij} t_{ij}\dot{c}_i^*\dot{c}_j+(1/4)\sum_{ijkl} v_{ijkl}\dot{c}_i^*\dot{c}_j^*\dot{c}_l\dot{c}_k\,. \tag{2·1}$$

Here, the first term denotes the kinetic energy and the second represents the interaction energy. The single-particle states, the total number of which is M, are specified by the Latin subscripts $i, j, k, l\cdots$. The matrix elements t_{ij} and v_{ijkl} are real and have the following properties:

$$t_{ij}=t_{ji}\,,\quad v_{ijkl}=-v_{jikl}=-v_{ijlk}=v_{klij}\,. \tag{2·2}$$

The operators $\dot{c}_i^*$ and $\dot{c}_i$ denote, respectively, the fermion creation and the annihilation operator in the single-particle state i, which obey the anti-commutation relations

$$\{\dot{c}_i, \dot{c}_j^*\}=\delta_{ij}\,,\qquad \{\dot{c}_i, \dot{c}_j\}=\{\dot{c}_i^*, \dot{c}_j^*\}=0\,. \tag{2·3}$$

For the preparation of the later discussion, first, we will list up some relations given in the TDHF theory. The TDHF theory starts from a single time-dependent Slater determinant as an approximate of pure state $|p(t)\rangle$, which is denoted by $|s(t)\rangle$. The state $|s(t)\rangle$ can be expressed by $|s(t)\rangle=U^0(t)|0\rangle$, where $U^0(t)$ is a certain time-dependent unitary operator and $|0\rangle$ denotes a static HF vacuum. The exact pure state $|p(t)\rangle$ should satisfy the Schrödinger equation exactly and if the form of trial function is arbitrary, the pure state $|p(t)\rangle$ can be determined by the following variation:

$$\delta I^0=0,\quad I^0=\int_{t_0}^{t_1}\langle p(t)|i\partial/\partial t-\dot{H}|p(t)\rangle dt\,. \tag{2·4}$$

In the TDHF theory, the trial function in the above variation is a single time-dependent Slater determinant as a restricted form. Therefore, $|s(t)\rangle$ is an approximate pure state. In this case, the expectation value of the operator $\dot{c}_i^*\dot{c}_j$ is given by the following expression:

$$\left.\begin{aligned}&\langle s(t)|\dot{c}_i^*\dot{c}_j|s(t)\rangle=\langle 0|\dot{c}_i^*\dot{c}_j|0\rangle+F_{ij}^0\,,\\ &\langle 0|\dot{c}_i^*\dot{c}_j|0\rangle=n_i^0\delta_{ij}\,.\end{aligned}\right\} \tag{2·5}$$

Under an appropriate choice of the quantum numbers specifying the single-particle states, $\langle 0|\dot{c}_i^*\dot{c}_j|0\rangle$ is diagonal for the indices i and j so that it is written as $n_i^0\delta_{ij}$, where n_i^0 takes the value 1 or 0, depending on occupied or unoccupied states:

$$n_i^0=1\quad\text{or}\quad 0\,. \tag{2·6}$$

The second term F_{ij}^0 represents the fluctuation around n_i^0. The expectation value of $\dot{H}$ for the state $|s(t)\rangle$ is given by

$$\left.\begin{aligned}&\langle s(t)|\dot{H}|s(t)\rangle=\langle 0|\dot{H}|0\rangle+F^0\,,\\ &\langle 0|\dot{H}|0\rangle=E^0=\sum_i t_{ii}n_i^0+(1/2)\sum_{ij} v_{ijij}n_i^0 n_j^0\,.\end{aligned}\right\} \tag{2·7}$$

A main problem of the TDHF theory is how to determine the form of F_{ij}^0 and F^0. Further, the following relation is added in the TDHF theory: The quantity $t_{ij}+\sum_k v_{ikjk}n_k^0$ is diagonal with respect to the indices i and j in the form

$$t_{ij}+\sum_k v_{ikjk}n_k^0=\varepsilon_i^0\delta_{ij}\,. \tag{2·8}$$

2. 2. *A possible time-dependent variational approach to mixed states*

Our present problem is how to treat the case of mixed states, for example, statistical superpositions of various Slater determinants. In this case, n_i is not equal to 1 or 0. Let the mixed states under consideration give us the statistical ensemble average of the operator $\dot{c}_i^*\dot{c}_j$ in the following form:

$$\langle\!\langle \dot{c}_i^*\dot{c}_j\rangle\!\rangle_{m(t)}=n_i\delta_{ij}+F_{ij}(m)\,, \tag{2·9}$$

$$0\leq n_i\leq 1\,. \tag{2·10}$$

Hereafter, we call n_i the occupation probability of the state i. Depending on the type of equilibrium in which we are interested for the system under investigation, the occupation probabilities are determined. As was mentioned in Ref. 1), for statistical equilibrium, these probabilities are given by the Fermi-Dirac distribution, but in general they may be given by some other prescription, if situations of non-thermal equilibrium are under consideration. We describe the fluctuation $F_{ij}(m)$ around a given set of the occupation probabilities n_i for the mixed states. Further, let the statistical average value of the Hamiltonian $\dot{H}$ for the mixed states satisfy the same form as that given in Eq. (2·7):

$$\left.\begin{aligned}&\langle\!\langle \dot{H}\rangle\!\rangle_{m(t)}=E+F(m)\,,\\ &E=\sum_i t_{ii}n_i+(1/2)\sum_{ij} v_{ijij}n_i n_j\,.\end{aligned}\right\} \tag{2·11}$$

Of course, our problem is how to obtain concrete expressions for $F_{ij}(m)$ and $F(m)$. The quantity $t_{ij}+\sum_k v_{ikjk}n_k$ is assumed to be also diagonal with respect to the indices i and j in the form

$$t_{ij}+\sum_k v_{ikjk}n_k=\varepsilon_i\delta_{ij}\,. \tag{2·12}$$

Here, n_i is not always 1 or 0. The relations (2·11) and (2·12) can be found in Ref. 1). In the case of Eq. (2·6), a possible form of the fluctution can be described in the frame of the TDHF theory, if the Slater determinant as an approximate form of the pure state $|p(t)\rangle$ is determined through the variation (2·4). However, in the case $0<n_i<1$, the TDHF theory is powerless, because the mixed states cannot be expressed in terms of a Slater determinant. In this paper, we will show that if the system is transcribed in a certain fermion space, the fluctuation around any value of n_i can be described under the same scheme as that of the TDHF theory. Of course, a certain new condition, which does not exist in the TDHF theory, is added.

Let us describe basic idea of our approach in a rather general form, which is similar to the thermo field dynamics formalism.[5] We prepare two spaces, the dimensions of which are the same, and call c- and d-space, respectively. The orthonormal sets of both spaces are denoted by $\{|p\rangle\}$ and $\{|p\rangle\!\rangle\}$, respectively. In the product of these spaces, i.e., in the enlarged space, we introduce the following time-dependent state $|m(t)\rangle\!\rangle$ which is normalized as 1:

$$\left.\begin{aligned}&|m(t)\rangle\!\rangle=\sum_p \Gamma_p|p(t)\rangle\otimes|p\rangle\!\rangle\,,\\&\sum_p|\Gamma_p|^2=1\,,\quad \langle p(t)|p(t)\rangle=1\,.\end{aligned}\right\}\qquad(2\cdot13)$$

Here, Γ_p and $|p\rangle\!\rangle$ do not depend on t. The states of the set $\{|p(t)\rangle\}$, which depend on t, are not always orthogonal, but, are in a one to one correspondence with the states of the set $\{|p\rangle\!\rangle\}$. It should be noted that $|p(0)\rangle$ is not always $|p\rangle$.

For any operator $\hat{O}$ given in the c-space, we can prove the following relation:

$$\begin{aligned}\langle\!\langle m(t)|\hat{O}|m(t)\rangle\!\rangle&=\sum_p|\Gamma_p|^2\langle p(t)|\hat{O}|p(t)\rangle\\&=\mathrm{Tr}(\hat{D}(t)\hat{O})\,.\end{aligned}\qquad(2\cdot14)$$

Here, $\hat{D}(t)$ is a time-dependent density matrix given by

$$\hat{D}(t)=\sum_p|p(t)\rangle|\Gamma_p|^2\langle p(t)|\,.\quad(\mathrm{Tr}\hat{D}(t)=1)\qquad(2\cdot15)$$

The relation (2·14) shows that quantum mechanical calculation of the expectation value of $\hat{O}$ for the state $|m(t)\rangle\!\rangle$ is equivalent to the procedure of statistical ensemble average. The quantity $|\Gamma_p|^2$ plays a role of the statistical weight.

Now, let us consider the following variation for the Hamiltonian acting on the c-space:

$$\delta I=0\,,\quad I=\int_{t_0}^{t_1}\langle\!\langle m(t)|i\partial/\partial t-\hat{H}|m(t)\rangle\!\rangle dt\,.\qquad(2\cdot16)$$

The variation δI under arbitrary form of $|m(t)\rangle\!\rangle$ gives us the time-dependent Schrödinger equation:

$$i\partial/\partial t|m(t)\rangle\!\rangle=\hat{H}|m(t)\rangle\!\rangle\,.\qquad(2\cdot17)$$

From Eqs. (2·13) and (2·17), we can prove that the state $|p(t)\rangle$ satisfies the following Schrödinger equation:

$$i\partial/\partial t|p(t)\rangle=\hat{H}|p(t)\rangle\,.\qquad(2\cdot18)$$

The definition of the density matrix (2·15) and the Schrödinger equation (2·18) give us the Liouville-von Neumann equation:

$$-i\dot{\hat{D}}(t)=[\hat{D}(t),\hat{H}]\,.\qquad(2\cdot19)$$

The above equation (2·19) is a starting relation of Ref. 1).

From the above fact, it can be concluded that the approach based on the variation (2·16) is equivalent to the conventional density matrix approach. The preparation of two spaces is the basic idea for treating the case of the mixed states. Under a certain restricted form of the state $|m(t)\rangle\!\rangle$ in the same sense as that in the TDHF theory, we can perform the variation (2·16). In this case, we should take into account the following identity for any operator $\tilde{O}$ acting on the d-space: From Eqs. (2·13) and (2·14), we get the relation

$$\langle\!\langle m(t)|\tilde{O}|m(t)\rangle\!\rangle=\langle\!\langle m(0)|\tilde{O}|m(0)\rangle\!\rangle\,.\qquad(2\cdot20)$$

The above relation means that the expectation value of $\tilde{O}$ for $|m(t)\rangle\!\rangle$ does not depend on t. Then, when we perform an approximate procedure for the variation, the identity (2·20) should not be forgotten. This is a new feature which cannot be found in Refs. 2) and 4). Under the above preliminaries, we will investigate our problem.

§ 3. Constrained canonical form for mixed states

Our basic viewpoint is the idea of transcribing the original system in a fermion space, which is constructed by two kinds of fermions ($\tilde{a}_i^*$, $\tilde{a}_i$) and ($\tilde{b}_i^*$, $\tilde{b}_i$). Here, the numbers of the operators $\tilde{a}_i$ and $\tilde{b}_i$ are the same as that of the operators c_i, respectively, i.e., M. Any anti-commutation relation between ($\tilde{a}^*$, $\tilde{a}$) and ($\tilde{b}^*$, $\tilde{b}$) vanishes, and between the same kind of fermions, the anti-commutation relations are given by

$$\left.\begin{aligned}&\{\tilde{a}_i,\tilde{a}_j^*\}=\delta_{ij}\,,\quad\{\tilde{a}_i,\tilde{a}_j\}=\{\tilde{a}_i^*,\tilde{a}_j^*\}=0\,,\\&\{\tilde{b}_i,\tilde{b}_j^*\}=\delta_{ij}\,,\quad\{\tilde{b}_i,\tilde{b}_j\}=\{\tilde{b}_i^*,\tilde{b}_j^*\}=0\,.\end{aligned}\right\}\qquad(3\cdot1)$$

In this fermion space, we can define the following operators:

$$\tilde{c}_i^*=u_i\tilde{a}_i^*+v_i\tilde{b}_i\,,\quad\tilde{c}_i=u_i\tilde{a}_i+v_i\tilde{b}_i^*\,.\qquad(3\cdot2)$$

Here, u_i and v_i are given by

$$u_i=\sqrt{1-n_i}\,,\qquad v_i=\sqrt{n_i}\,.\quad(u_i^2+v_i^2=1)\qquad(3\cdot3)$$

By using the relations (3·1) and (3·3), it can be shown that the operators defined in Eq. (3·2) satisfy the same anti-commutation relations as those given in Eq. (1·3). In this sense, we regard $\tilde{c}_i^*$ and $\tilde{c}_i$ as the counterparts of $\hat{c}_i^*$ and $\hat{c}_i$, respectively. Associated with the above operators, we can define the operators $\tilde{d}_i^*$ and $\tilde{d}_i$, which are independent of $\tilde{c}_i^*$ and $\tilde{c}_i$, in the form

$$\tilde{d}_i^*=-v_i\tilde{a}_i+u_i\tilde{b}_i^*\,,\quad\tilde{d}_i=-v_i\tilde{a}_i^*+u_i\tilde{b}_i\,.\qquad(3\cdot4)$$

The operators $\tilde{d}_i^*$ and $\tilde{d}_i$ satisfy also the same anti-commutation relations as those given in Eq. (2·3) and they are anti-commutable with any $\tilde{c}_i^*$ and $\tilde{c}_i$. Further, it is noted that $\tilde{d}_i^*$ and $\tilde{d}_i$ have no counterparts in the original fermion space. In the thermo field dynamics formalism,[2),4)] the relations (3·2) and (3·4) are used in terms of the quasi-particles.

With the aid of the relation (3·1), the operators $\tilde{c}_i^*\tilde{c}_j$ can be expressed in the following form:

$$\hat c_i^* \hat c_j = n_i\delta_{ij} + \hat F_{ij}\,, \tag{3·5}$$

$$\hat F_{ij} = u_iv_j\hat a_i^*\hat b_j^* + v_iu_j\hat b_i\hat a_j + u_iu_j\hat a_i^*\hat a_j - v_iv_j\hat b_j^*\hat b_i\,. \tag{3·6}$$

Let the vacuum for the fermion operators $(\hat a_i^*, \hat a_i)$ and $(\hat b_i^*, \hat b)$ be $|0\rangle\!\rangle$:

$$\hat a_i|0\rangle\!\rangle = \hat b_i|0\rangle\!\rangle = 0\,. \tag{3·7}$$

Then, the expectation value of $\hat c_i^* \hat c_j$ for $|0\rangle\!\rangle$ is given by

$$\langle\!\langle 0|\hat c_i^* \hat c_j|0\rangle\!\rangle = n_i\delta_{ij}\,. \tag{3·8}$$

Further, it can be shown that the expectation value of the Hamiltonian $\hat H$ obtained by replacing $\dot c_i^*$ and $\dot c_i$ with $\hat c_i^*$ and $\hat c_i$ in the Hamiltonian $\dot H$ given by Eq. (2·1), for the state $|0\rangle\!\rangle$, is of the same form as that given in Eq. (2·11):

$$\langle\!\langle 0|\hat H|0\rangle\!\rangle = E\,. \tag{3·9}$$

From the above relations, we can see that the calculation of the expectation values of the operators $\hat c_i^* \hat c_j$ and $\hat H$ for the vacuum $|0\rangle\!\rangle$ gives us the procedure of statistical averaging for the mixed state with $F_{ij}(m) = F(m) = 0$. In the same way as is given in the above, we can obtain the following operators composed from $\hat d_i^*$ and $\hat d_i$:

$$\hat d_j^* \hat d_i = n_i\delta_{ij} + \tilde G_{ij}\,, \tag{3·10}$$

$$\tilde G_{ij} = v_iu_j\hat a_i^*\hat b_j^* + u_iv_j\hat b_i\hat a_j - v_iv_j\hat a_i^*\hat a_j + u_iu_j\hat b_j^*\hat b_i\,. \tag{3·11}$$

The expectation value of $\hat d_j^* \hat d_i$ for the state $|0\rangle\!\rangle$ gives us the following relation which plays an essential role in the later discussion:

$$\langle\!\langle 0|\hat d_j^* \hat d_i|0\rangle\!\rangle = n_i\delta_{ij}\,. \tag{3·12}$$

Our present system consists of the two kinds of fermions. Then, if we regard $(\hat a_i^*, \hat a_i)$ and $(\hat b_i^*, \hat b_i)$ as the operators which play the same role as that of the particle and the hole operators in the static HF theory, the fluctuation $\hat F_{ij}$ given in Eq. (3·6) is expressed in terms of a combination of the particle and the hole-pair operators. The fact that the fluctuation can be expressed in terms of the particle and the hole-pair operators permits us to use the canonical form of the TDHF theory for the description of the fluctuation.[3] As was already mentioned, in the original fermion space, it is impossible to describe the fluctuation in the frame of the TDHF theory.

In the present enlarged space, we introduce the following state which is of the same form as that of the Slater determinant:

$$\left.\begin{aligned} &|c(t)\rangle\!\rangle = U(t)|0\rangle\!\rangle\,,\\ &U(t) = \exp\sum_{ij}[\Gamma_{ji}\hat a_i^*\hat b_j^* - \Gamma_{ij}^*\hat b_i\hat a_j]\,.\end{aligned}\right\} \tag{3·13}$$

Here, $U(t)$ is unitary and Γ_{ji} and Γ_{ij}^* are time-dependent parameters, which are expressed in terms of the other parameters C_{ji} and C_{ij}^* in the following form:

$$\begin{aligned}\Gamma_{ji} &= [\sin^{-1}\sqrt{CC^\dagger}\cdot\sqrt{CC^\dagger}^{-1}\cdot C]_{ji}\\ &= [C\cdot\sqrt{C^\dagger C}^{-1}\cdot\sin^{-1}\sqrt{C^\dagger C}]_{ji}\,.\end{aligned} \tag{3·14}$$

We regard the state $|c(t)\rangle\!\rangle$ as a trial function for the variation (2·16). The operators $(\hat a_i^*, \hat a_i)$ and $(\hat b_i^*, \hat b_i)$ can be expressed in terms of the operators $(\hat c_i^*, \hat c_i)$ and $(\hat d_i^*, \hat d_i)$ in the form

$$\hat a_i^* = u_i\hat c_i^* - v_i\hat d_i\,, \quad \hat b_i = v_i\hat c_i^* + u_i\hat d_i\,. \tag{3·15}$$

Then, the vacuum $|0\rangle\!\rangle$ can be given by

$$|0\rangle\!\rangle = \prod_i(u_i + v_i\hat c_i^*\hat d_i^*)|\phi\rangle\otimes|\phi\rangle\!\rangle\,, \tag{3·16}$$

where $|\phi\rangle$ and $|\phi\rangle\!\rangle$ satisfy, respectively,

$$\hat c_i|\phi\rangle = 0\,, \quad \hat d_i|\phi\rangle\!\rangle = 0\,. \tag{3·17}$$

Then, the state $|c(t)\rangle\!\rangle$ can be written down as

$$|c(t)\rangle\!\rangle = \exp\sum_i(\Gamma_{ii}^* - \Gamma_{ii})u_iv_i\cdot\exp K\cdot\prod_i(u_i + v_i\hat c_i^*\hat d_i^*)|\phi\rangle\otimes|\phi\rangle\!\rangle\,, \tag{3·18}$$

$$\begin{aligned} K = \sum_{ij}[&(\Gamma_{ji}u_iu_j + \Gamma_{ij}^* v_iv_j)\hat c_i^*\hat d_j^* - (\Gamma_{ji}^* u_iu_j + \Gamma_{ij}v_iv_j)\hat d_j\hat c_i\\ &+ (\Gamma_{ji}u_iv_j - \Gamma_{ij}^* v_iu_j)\hat c_i^*\hat c_j + (\Gamma_{ji}v_iu_j - \Gamma_{ij}^* u_iv_j)\hat d_j^*\hat d_i]\,.\end{aligned} \tag{3·19}$$

Therefore, $|c(t)\rangle\!\rangle$ can be expressed in terms of

$$|c(t)\rangle\!\rangle = \sum_{i_1,\cdots,i_L}\Gamma_{i_1,\cdots,i_L}\cdot|i_1,\cdots,i_L(t)\rangle\otimes|i_1,\cdots,i_L\rangle\!\rangle\,, \tag{3·20}$$

where the set of the states $\{|i_1,\cdots,i_L\rangle\!\rangle\}$ is an orthonormal set given by

$$|i_1,\cdots,i_L\rangle\!\rangle = 1/\sqrt{L!}\cdot\hat d_{i_1}^*\cdots\hat d_{i_L}^*|\phi\rangle\!\rangle\,. \tag{3·21}$$

The state $|i_1,\cdots,i_L(t)\rangle$ is an L-fermion state for $\hat c^*$, which is a certain superposition of the orthonormal set given by

$$|j_1,\cdots,j_L\rangle\!\rangle = 1/\sqrt{L!}\cdot\hat c_{j_1}^*\cdots\hat c_{j_L}^*|\phi\rangle\!\rangle\,. \tag{3·22}$$

By comparing Eq. (3·20) with Eq. (2·13), we identify the spaces spanned by the sets (3·22) and (3·21) as the c- and the d-space, respectively. This is the reason why we can adopt the state $|c(t)\rangle\!\rangle$ given by Eq. (3·13) as the trial function for the variation (2·16).

The trial function (3·18) is of the restricted form. Therefore, $\Gamma_{i_1,\cdots,i_L}$ in Eq. (3·20) may not be a constant but depend on t and the state $|i_1\cdots i_L(t)\rangle$ may not be exact solution of the Schrödinger equation (2·18). In this sense, as the constraint, we should impose the relation (2·20), which is an identity in the case of the exact solution, for expectation value of any operator composed only of $\hat d_i^*$ and $\hat d_i$, with respect to $|c(t)\rangle\!\rangle$. We can see from Eq. (3·20) that the expectation value of any operator such as $\hat d_{i_1}^*,\cdots\hat d_{j_L}^*\cdot d_{i_L}\cdots d_{i_1}$ vanishes automatically for $|c(t)\rangle\!\rangle$ if $L\neq L'$. In the case $L=L'$, the expectation value can be expressed in terms of the product of the type $\langle\!\langle c(t)|\hat d_j^*\hat d_i|c(t)\rangle\!\rangle$, because $|c(t)\rangle\!\rangle$ is of the form of the Slater determinant and the Wick theorem is applicable. Therefore, it is enough to take into account only the case of $\langle\!\langle c(t)|\hat d_j^*\hat d_i|c(t)\rangle\!\rangle$. Further, if $n_i = n_i^0 = 1$ or 0, the state $|c(t)\rangle\!\rangle$ should be reduced to a single Slater determinant as an approximate pure state $|s(t)\rangle$. This reduction is realized automatically if $\langle\!\langle c(t)|\tilde{d}_j^*\tilde{d}_i|c(t)\rangle\!\rangle=\langle\!\langle 0|\tilde{d}_j^*\tilde{d}_i|0\rangle\!\rangle=n_i^0\delta_{ij}$. From the above argument, we impose the following relation:

$$\langle\!\langle c(t)|\tilde{d}_j^*\tilde{d}_i|c(t)\rangle\!\rangle=\langle\!\langle 0|\tilde{d}_j^*\tilde{d}_i|0\rangle\!\rangle=n_i\delta_{ij}\,. \tag{3·23}$$

The above relation plays a role of the constraint in our treatment. There does not exist the condition (3·23) in the thermo field dynamics formalism.[2),4)]

As can be shown in the TDHF theory, the expectation values of fermion-pair operators for the state $|c(t)\rangle\!\rangle$ are given in the following form:

$$\left.\begin{aligned}\langle\!\langle c(t)|\tilde{a}_i^*\tilde{b}_j^*|c(t)\rangle\!\rangle&=(a_i^*b_j^*)_C=\sum_k C_{jk}^*(\sqrt{1-C^\dagger C})_{ik}\,,\\ \langle\!\langle c(t)|\tilde{b}_i\tilde{a}_j|c(t)\rangle\!\rangle&=(b_ia_j)_C=\sum_k(\sqrt{1-C^*C^T})_{ki}C_{kj}\,,\end{aligned}\right\} \tag{3·24}$$

$$\left.\begin{aligned}\langle\!\langle c(t)|\tilde{a}_i^*\tilde{a}_j|c(t)\rangle\!\rangle&=(a_i^*a_j)_C=\sum_k C_{ki}^*C_{kj}\,,\\ \langle\!\langle c(t)|\tilde{b}_j^*\tilde{b}_i|c(t)\rangle\!\rangle&=(b_j^*b_i)_C=\sum_k C_{jk}^*C_{ik}\,.\end{aligned}\right\} \tag{3·25}$$

The parameters C_{ij}^* and C_{ij} play a role of canonical variables in the canonical form of the TDHF theory and satisfy so-called canonicity condition:

$$\left.\begin{aligned}\langle\!\langle c(t)|\partial/\partial C_{ij}|c(t)\rangle\!\rangle&=+C_{ij}^*/2\,,\\ \langle\!\langle c(t)|\partial/\partial C_{ij}^*|c(t)\rangle\!\rangle&=-C_{ij}/2\,.\end{aligned}\right\} \tag{3·26}$$

We can see that $(a_i^*b_j^*)_C$, $(b_ia_j)_C$, $(a_i^*a_j)_C$ and $(b_j^*b_i)_C$ given in Eqs. (3·24) and (3·25) satisfy the same algebra as that governing the operators $\tilde{a}_i^*\tilde{b}_j^*$, $\tilde{b}_i\tilde{a}_j$, $\tilde{a}_i^*\tilde{a}_j$ and $\tilde{b}_j^*\tilde{b}_i$, if we regard the Poisson bracket defined in the following as the counterpart of the commutator:

$$[A,B]_P=\sum_{ij}(\partial A/\partial C_{ij}\cdot\partial B/\partial C_{ij}^*-\partial B/\partial C_{ij}\cdot\partial A/\partial C_{ij}^*)\,. \tag{3·27}$$

With the use of the relations (3·24) and (3·25), we can express the expectation values of various quantities, for example, the Hamiltonian H as functions of all C^* and C:

$$H=\langle\!\langle c(t)|\tilde{H}|c(t)\rangle\!\rangle\,. \tag{3·28}$$

Thus, we could complete a possible canonical formulation for the mixed states in the form analogous to the TDHF theory for the pure state. The existence of the constraint (3·23) is characteristic of the present formulation.

§ 4. TDHF-like variation and equation of the collective submanifold

Following the principle of the TDHF theory, we start from the variation defined by

$$\delta I=0\,,\qquad I=\int_{t_0}^{t_1}\langle\!\langle c(t)|i\partial/\partial t-(\tilde{H}-\sum_{ij}\lambda_{ij}\tilde{G}_{ij})|c(t)\rangle\!\rangle dt\,. \tag{4·1}$$

Here, it is noted that the above variation should be performed under the constraints

$$G_{ij}=\langle\!\langle c(t)|\tilde{G}_{ij}|c(t)\rangle\!\rangle=0\,,\quad (G_{ij}^*=G_{ji}) \tag{4·2}$$

$$G_{ij}=v_iu_j(a_i^*b_j^*)_C+u_iv_j(b_ia_j)_C-v_iv_j(a_i^*a_j)_C+u_iu_j(b_j^*b_i)_C\,. \tag{4·2a}$$

As is shown in Eq. (3·23), our present system is governed by the constraint $G_{ij}=0$. Therefore, the variation (4·1) contains the Lagrange multipliers λ_{ij} which satisfies

$$\lambda_{ij}^*=\lambda_{ji}\,. \tag{4·3}$$

The variation (4·1) gives us the following equation of motion:

$$\left.\begin{aligned}+i\dot{C}_{ij}-(\partial/\partial C_{ij}^*)(H-\sum_{kl}\lambda_{kl}G_{kl})&=0\,,\\ -i\dot{C}_{ij}^*-(\partial/\partial C_{ij})(H-\sum_{kl}\lambda_{kl}G_{kl})&=0\,.\end{aligned}\right\} \tag{4·4}$$

Since the constraint should satisfy the condition $\dot{G}_{ij}=0$, we have the following relations:

$$\begin{aligned}i\dot{G}_{ij}&=[G_{ij},H-\sum_{kl}\lambda_{kl}G_{kl}]_P\\ &=\lambda_{ij}(n_i-n_j)-\sum_k\lambda_{ki}G_{kj}+\sum_k\lambda_{jk}G_{ik}-\sum_{kl}[G_{ij},\lambda_{kl}]_PG_{kl}=0\,.\end{aligned} \tag{4·5}$$

Here, we used the relations

$$\left.\begin{aligned}&[G_{ij},H]_P=0\,,\\ &[G_{ij},G_{kl}]_P=\delta_{il}\delta_{jk}(n_j-n_i)+\delta_{il}G_{kj}-\delta_{kj}G_{il}\,.\end{aligned}\right\} \tag{4·6}$$

Under the constraint $G_{ij}=0$, Eq. (4·5) gives us

$$\lambda_{ij}=0\,,\quad(\text{if } n_i\neq n_j)\qquad \lambda_{ij}\neq 0\,.\quad(\text{if } n_i=n_j) \tag{4·7}$$

In the above treatment, it is impossible to determine λ_{ij} for the case $n_i=n_j$. For the determination, we must find a convenient method. The expectation value of $\tilde{F}_{ij}$, $\langle\!\langle c(t)|\tilde{F}_{ij}|c(t)\rangle\!\rangle$ $(=F_{ij})$ can be written in the following form:

$$F_{ij}=f_{ij}\,,\qquad(\text{for } n_i\neq n_j)$$

$$f_{ij}=u_iv_j(a_i^*b_j^*)_C+v_iu_j(b_ia_j)_C+u_iu_j(a_i^*a_j)_C-v_iv_j(b_j^*b_i)_C\,, \tag{4·8}$$

$$F_{ij}=f_{ij}+G_{ij}\,,\qquad(\text{for } n_i=n_j)$$

$$f_{ij}=(a_i^*a_j)_C-(b_j^*b_i)_C\,. \tag{4·9}$$

Then, the Hamiltonian H can be expressed in the form

$$\begin{aligned}H=E&+\sum_i\varepsilon_if_{ii}+(1/2)\sum_{ijkl}v_{ikjl}f_{ij}f_{kl}\\ &+(1/2)\sum_{ij}{}''\sum_{kl}{}''v_{ikjl}G_{ij}G_{kl}+\sum_{ij}{}''(\varepsilon_i\delta_{ij}+\sum_{kl}v_{ikjl}f_{kl})G_{ij}\,.\end{aligned} \tag{4·10}$$

Here, the symbol $\sum_{ij}''$ denotes the sum with the restriction $n_i=n_j$. We choose λ_{ij} in the following form for the case $n_i=n_j$:

$$\lambda_{ij}=\varepsilon_i\delta_{ij}+\sum_{kl}v_{ikjl}f_{kl}\,. \tag{4·11}$$

Of course, λ_{ij} given in Eq. (4·11) satisfies the condition (4·3). The reason why we choose the form (4·11) is as follows: Our description is based on the picture that the particle-hole pair type variables C_{ij}^* and C_{ij} describe our system. In the case $n_i \neq n_j$, we can imagine that these variables are of the particle-hole pair type. However, in the case $n_i = n_j$, the occupation probabilities are the same and, then, we cannot provide an interpretation of these quantities as the particle-hole pair amplitudes. If λ_{ij} is chosen as the form shown in Eq. (4·11), the interaction term starts with the quadratic terms for C_{ij}^* and C_{ij} with $n_i \neq n_j$. Then, the leading terms in the equation of motion do not contain any C_{ij}^* and C_{ij} with $n_i = n_j$. This is the reason why we have adopted the form (4·11). Then, the Hamiltonian is given by

$$H - \sum_{ij} \lambda_{ij} G_{ij} = H_c$$

$$= E + \sum_i \varepsilon_i f_{ii} + (1/2) \sum_{ijkl} v_{ikjl} f_{ij} f_{kl} + (1/2) \sum_{ij}'' \sum_{kl}'' v_{ikjl} G_{ij} G_{kl} . \qquad (4\cdot12)$$

Of course, the last term does not contribute any effect to the result. The equation of motion (4·4) is written down as

$$\left. \begin{array}{l} +i\dot{C}_{ij} - \partial H_c / \partial C_{ij}^* = 0 , \\ -i\dot{C}_{ij}^* - \partial H_c / \partial C_{ij} = 0 . \end{array} \right\} \qquad (4\cdot13)$$

The canonicity condition (3·26), the constraint (4·2) and the equation of motion (4·13) form a set of basic relations in our approach. By solving these equations, we can determine the time-dependence of the parameters C^* and C, i.e., Γ^* and Γ. Then, the state $|c(t)\rangle\!\rangle$ can be given as a function of t and we can calculate the ensemble average values of various quantities.

In the formalism developed above, all degrees of freedom permitted are contained in the treatment. Then, we investigate to describe the system in terms of small number of degrees of freedom, which is analogous to that given in the case of the pure state. For simplicity, we consider the case of only one degree of freedom and we call it as collective degree of freedom. For this aim, we separate all degrees of freedom into collective and non-collective degrees of freedom. First, we introduce new canonical variables (X^*, X) and $(y_r^*, y_r$: $r = 1, 2, \cdots, f)$, where f is equal to $M^2 - 1$. The former are for the collective motion and the latter for the non-collective ones. These variables are connected with C_{ij}^* and C_{ij}, the number of which is M^2, under canonical transformation. It is clear that variables (C^*, C) are functions for the variables (X^*, X) and (y^*, y). A possible definition of the collective submanifold can be given by the following requirement: On a certain submanifold, all $\dot{y}_r^*$ and $\dot{y}_r$ are equal to 0 under an appropriate choice of initial condition. We can set up all $y_r^* = y_r = 0$ without violating the equation of motion. We introduce new notations:

$$\left. \begin{array}{l} C_{ij}^*(X^*, X, \text{all } y_r^* = 0, y_r = 0) = C_{ij}^*(X^*, X) , \\ C_{ij}(X^*, X, \text{all } y_r^* = 0, y_r = 0) = C_{ij}(X^*, X) . \end{array} \right\} \qquad (4\cdot14)$$

For any function of the variables C^* and C, $F = \Phi(C^*, C)$, we adopt the notation $F = \Phi(C^*, C)$. With the use of the above notations, the following formulae are obtained:

$$\left. \begin{array}{l} (\partial C_{ij}^* / \partial X^*)_{y^* = y = 0} = \partial C_{ij}^* / \partial X^* , \text{ etc.,} \\ (\partial F / \partial C_{ij})_{C^* = C^*, C = C} = \partial F / \partial C_{ij} , \text{ etc.} \end{array} \right\} \qquad (4\cdot15)$$

Let us write down our basic equations which determine the collective submanifold. Since the new variables are also canonical, they should obey the canonicity condition (3·26) and, from the conditions for the old and the new variable, (C^*, C) and (X^*, X), we can get the following relations:

$$\left. \begin{array}{l} \sum_{ij} (C_{ij}^* \cdot \partial C_{ij} / \partial X - C_{ij} \cdot \partial C_{ij}^* / \partial X) = X^* , \\ \sum_{ij} (C_{ij} \cdot \partial C_{ij}^* / \partial X^* - C_{ij}^* \cdot \partial C_{ij} / \partial X^*) = X . \end{array} \right\} \qquad (4\cdot16)$$

The constraint (4·2) gives us

$$G_{ij} = 0 , \qquad (4\cdot17)$$

where the explicit form is obtained by replacing C^* and C by C^* and C in the constraint (4·2). From the equation of motion (4·13), we have the following equation, which is called equation of the collective submanifold:

$$\left. \begin{array}{l} +\lambda \partial C_{ij} / \partial X - \lambda^* \partial C_{ij} / \partial X^* = \partial H_c / \partial C_{ij}^* , \\ -\lambda \partial C_{ij}^* / \partial X + \lambda^* \partial C_{ij}^* / \partial X^* = \partial H_c / \partial C_{ij} . \end{array} \right\} \qquad (4\cdot18)$$

Here, λ and λ^* are given by

$$\lambda = i\dot{X} = \partial H_{col} / \partial X^* , \quad \lambda^* = -i\dot{X}^* = \partial H_{col} / \partial X . \qquad (4\cdot19)$$

The set of the relations (4·16)~(4·18) determines the collective submanifold. Of course, H_c is given by replacing C^* and C with C^* and C in H_c shown in Eq. (4·12). The Hamiltonian H_{col} is a function of X^* and X and obtained from H_c through C^* and C as functions of X^* and X. By solving the equation of motion (4·19) under an appropriate initial condition, we can determine the time-dependence of X^* and X. Then, the time-dependence of C^* and C is determined and we can obtain the state $|c(t)\rangle\!\rangle$.

§ 5. Small amplitude limit and the RPA equation

Let us give an approximate solution of the set of Eqs. (4·16)~(4·18) in the case of the small amplitude limit. This solution gives us a boundary condition for the exact solution of the above equations. The quantities C_{ij}^* and C_{ij} are related to the fluctuation around n_i and, then, in the limit of $X^* = X = 0$, they should vanish. Therefore, they start linearly in X^* and X and, as the zero-th order approximation, we can set up

$$\left. \begin{array}{l} C_{ij}^* = v_i u_j (U_{ij} X^* - V_{ji}^* X) , \\ C_{ij} = -v_i u_j (V_{ji} X^* - U_{ij}^* X) . \end{array} \right\} \qquad (5\cdot1)$$

The coefficients U and V should be determined in the frame of our basic equations. The canonicity condition (4·16) reduces to

$$\sum_{ij} u_i^2 v_j^2 (U_{ji}^* U_{ji} - V_{ij}^* V_{ij}) = 1 . \tag{5·2}$$

The constraint (4·17) gives us the following relation:

$$\begin{aligned} G_{ij} &= v_i u_j C_{ji}^* + u_i v_j C_{ij} \\ &= u_i v_i u_j v_j [(U_{ji} - V_{ji}) X^* + (U_{ij}^* - V_{ij}^*) X] \\ &= 0 . \end{aligned} \tag{5·3}$$

From the relation (5·3), we have

$$U_{ij} = V_{ij} . \quad (= W_{ij}) \tag{5·4}$$

Therefore, Eqs. (5·1) and (5·2) reduce to

$$\left. \begin{aligned} C_{ij}^* &= v_i u_j (W_{ij} X^* - W_{ji}^* X) , \\ C_{ij} &= - v_i u_j (W_{ji} X^* - W_{ij}^* X) , \end{aligned} \right\} \tag{5·5}$$

$$\sum_{ij} (n_i - n_j) W_{ij}^* W_{ij} = 1 . \tag{5·6}$$

Finally, we investigate the equation of collective submanifold (4·18). The right-hand side of Eq. (4·18) reduces, under the present approximation, to the following relation: For $n_i \neq n_j$, we have

$$\begin{aligned} \partial H_c / \partial C_{ij}^* &= (\varepsilon_i - \varepsilon_j) C_{ij} + v_i u_j {\sum_{kl}}' v_{ijkl} (u_k v_l C_{lk}^* + v_k u_l C_{kl}) \\ &= + v_i u_j [(\varepsilon_i - \varepsilon_j)(W_{ji} X^* - W_{ij}^* X) + {\sum_{kl}}' v_{ijkl} (n_l - n_k)(W_{lk} X^* - W_{kl}^* X)] , \end{aligned} \tag{5·7a}$$

$$\begin{aligned} \partial H_c / \partial C_{ij} &= (\varepsilon_i - \varepsilon_j) C_{ij}^* + v_i u_j {\sum_{kl}}' v_{ijkl} (v_k u_l C_{kl}^* + u_k v_l C_{lk}) \\ &= - v_i u_j [(\varepsilon_i - \varepsilon_j)(W_{ij} X^* - W_{ji}^* X) + {\sum_{kl}}' v_{ijkl} (n_l - n_k)(W_{kl} X^* - W_{lk}^* X)] , \end{aligned} \tag{5·7b}$$

where the symbol ${\Sigma}'_{ij}$ denotes the sum with the restriction $n_i \neq n_j$. For $n_i = n_j$, we have

$$\begin{aligned} \partial H_c / \partial C_{ij}^* &= (\varepsilon_j - \varepsilon_i) C_{ij} \\ &= u_i v_j [(\varepsilon_i - \varepsilon_j)(W_{ji} X^* - W_{ij}^* X)] , \end{aligned} \tag{5·8a}$$

$$\begin{aligned} \partial H_c / \partial C_{ij} &= (\varepsilon_j - \varepsilon_i) C_{ij}^* \\ &= - u_i v_j [(\varepsilon_i - \varepsilon_j)(W_{ij} X^* - W_{ji}^* X)] . \end{aligned} \tag{5·8b}$$

On the other hand, the left-hand side of Eq. (4·18) can be expressed in the following form:

$$+ \lambda \partial C_{ij} / \partial X - \lambda^* \partial C_{ij} / \partial X^* = v_i u_j [(\mu W_{ji} - \nu W_{ij}^*) X^* + (\mu W_{ij}^* - \nu^* W_{ji}) X] , \tag{5·9a}$$

$$- \lambda \partial C_{ij}^* / \partial X + \lambda^* \partial C_{ij}^* / \partial X^* = v_i u_j [(\mu W_{ij} - \nu W_{ji}^*) X^* + (\mu W_{ji}^* - \nu^* W_{ij}) X] . \tag{5·9b}$$

Here, μ and ν are constants contained in H_{col}, which is, under the present approximation, quadratic with respect to (X^*, X):

$$H_{col} = \mu X^* X - 1/2 \cdot (\nu X^{*2} + \nu^* X^2) . \tag{5·10}$$

Therefore, μ and ν are real and complex numbers, respectively. Of course, our problem is how to determine the values. By equating both sides of Eqs. (5·7) and (5·9), we can obtain the following set of equations for the case $n_i \neq n_j$:

$$\mu W_{ij} - \nu W_{ji}^* = (\varepsilon_j - \varepsilon_i) W_{ij} + {\sum_{kl}}' v_{ijkl} (n_k - n_l) W_{kl} , \tag{5·11a}$$

$$\nu^* W_{ij} - \mu W_{ji}^* = (\varepsilon_j - \varepsilon_i) W_{ji}^* + {\sum_{kl}}' v_{ijkl} (n_k - n_l) W_{lk}^* . \tag{5·11b}$$

Equation (5·11b) is the complex conjugate of Eq. (5·11a). Also, from Eqs. (5·8) and (5·9), we have the following set of equations for the case $n_i = n_j$:

$$\mu W_{ij} - \nu W_{ji}^* = (\varepsilon_j - \varepsilon_i) W_{ij} , \tag{5·12a}$$

$$\nu^* W_{ij} - \mu W_{ji}^* = (\varepsilon_j - \varepsilon_i) W_{ji}^* . \tag{5·12b}$$

Equations (5·6), (5·11) and (5·12) are our basic relations in the present treatment and problem is reduced to searching a solution of the equations which is expected to be the most suitable for the problem under investigation.

In order to investigate properties of the above equations, we introduce the quantities ψ_{ij} and ϕ_{ij} defined by

$$\left. \begin{aligned} + \sqrt{n_i - n_j}\, W_{ij} &= \psi_{ij} , \quad (\text{for } n_i > n_j) \\ - \sqrt{n_j - n_i}\, W_{ij} &= \phi_{ji} . \quad (\text{for } n_i < n_j) \end{aligned} \right\} \tag{5·13}$$

Further, we define the following quantities:

$$\left. \begin{aligned} \sqrt{n_i - n_j}\, v_{ijlk} \sqrt{n_k - n_l} &= u_{ij,kl} , \\ \sqrt{n_i - n_j}\, v_{iklj} \sqrt{n_k - n_l} &= w_{ij,kl} . \end{aligned} \right\} \tag{5·14}$$

Then, Eq. (5·6) is rewritten in the form

$$\sum_{ij} (\psi_{ij}^* \psi_{ij} - \phi_{ij}^* \phi_{ij}) = 1 . \tag{5·15}$$

Equation (5·11a) is also rewritten as

$$\left. \begin{aligned} + \mu \psi_{ij} + \nu \phi_{ij}^* &= (\varepsilon_j - \varepsilon_i) \psi_{ij} + \sum_{kl} (u_{ij,kl} \psi_{kl} + w_{ij,kl} \phi_{kl}) , \\ - \nu \psi_{ij}^* - \mu \phi_{ij} &= (\varepsilon_j - \varepsilon_i) \phi_{ij} + \sum_{kl} (w_{ij,kl} \psi_{kl} + u_{ij,kl} \phi_{kl}) . \end{aligned} \right\} \tag{5·16}$$

Equation (5·11b) reduces to the complex conjugate of Eq. (5·16). We can see that if ν is equal to zero, Eq. (5·16) reduces to the RPA equation and Eq. (5·15) gives us the normalization condition.[1] However, as was discussed by the present authors (M. Y. and A. K.),[6] the presence of ν is essential for the unified treatment of the stable, the critical and the unstable solution.

In order to give some concrete insight concerning the above equation, we treat a rather special system, in which the interaction matrix elements satisfy the following condition:

$$v_{iUk} = s v_{ikjl} = s v_{jlik} . \quad (s = \pm 1) \tag{5·17}$$

Examples of the matrix elements obeying the condition (5·17) can be found in the case of the quadrupole interaction for $s = +1$ and the spin-spin interaction for $s = -1$, respectively. Therefore, the condition (5·17) is not so restrictive as it may be imagined. Further, we assume the following relation:

$$\varepsilon_j > \varepsilon_i . \quad (\text{if } n_j < n_i) \tag{5·18}$$

The above condition represents that if ε_i increases, n_i decreases and this is also not so strong condition. Under the above conditions, we define the following quantities:

$$\psi_U + s\phi_U = \Psi_U(+s) , \quad \psi_U - s\phi_U = \Psi_U(-s) , \tag{5·19}$$

$$(\varepsilon_j - \varepsilon_i)\delta_{jk}\delta_{jl} + u_{U,kl} + s w_{U,kl} = (\varepsilon_j - \varepsilon_i)\delta_{jk}\delta_{jl} + 2\sqrt{n_i - n_j}\, v_{iUk}\sqrt{n_k - n_l}$$
$$= E_{U,kl}(+s) , \tag{5·20a}$$

$$(\varepsilon_j - \varepsilon_i)\delta_{jk}\delta_{jl} = E_{U,kl}(-s) . \tag{5·20b}$$

Then, Eq. (5·16) is rewritten in the form

$$\left.\begin{aligned} \mu\Psi_U(-s) - s\nu\Psi_U(-s)^* &= \sum_{kl} E_{U,kl}(+s)\Psi_{kl}(+s) , \\ \mu\Psi_U(+s) + s\nu\Psi_U(+s)^* &= \sum_{kl} E_{U,kl}(-s)\Psi_{kl}(-s) . \end{aligned}\right\} \tag{5·21}$$

The above equation and its complex conjugate are reduced to

$$\kappa\Psi_U(-s) = \sum_{kl}[E(+s)E(-s)]_{U,kl}\Psi_{kl}(-s) , \tag{5·22}$$

where κ is given by

$$\kappa = \mu^2 - |\nu|^2 . \tag{5·23}$$

In order to solve Eq. (5·22), let us investigate the following equation:

$$\kappa\Phi_U(-s) = \sum_{kl}[\sqrt{E(-s)}E(+s)\sqrt{E(-s)}]_{U,kl}\Phi_{kl}(-s) . \tag{5·24}$$

It should be noted that from the condition (5·18), the matrix $E(-s)$ is positive definite and, then, the matrix $\sqrt{E(-s)}$ exists. Equation (5·24) can be regarded as an eigenvalue equation for the real symmetric matrix $\sqrt{E(-s)}E(+s)\sqrt{E(-s)}$ and, then, the eigenvalue κ is real. For any eigenvalue of Eq. (5·24), we can normalize $\Phi_U(-s)$ in such a way as

$$\sum_U \Phi_U(-s)^2 = 1 . \tag{5·25}$$

Equation (5·22) is identical to Eq. (5·24), if $\Psi_U(\pm s)$ is connected to $\Phi_U(-s)$ in the form

$$\left.\begin{aligned} \Psi_U(-s) &= e^{-i\chi}N(-s)[\sqrt{E(-s)}^{-1}\Phi(-s)]_U , \\ \Psi_U(+s) &= e^{-i\chi}N(-s)/(\mu + s\nu_0)[\sqrt{E(-s)}\Phi(-s)]_U . \end{aligned}\right\} \tag{5·26}$$

Here, $N(-s)$ is the normalization constant, which is real. From the condition (5·15), the definition (5·19) and the normalization (5·25), we can determine $N(-s)$ in the form

$$N(-s)^2 = \mu + s\nu_0 \ (>0) , \quad \text{i.e.,} \quad N(-s) = \sqrt{\mu + s\nu_0} , \tag{5·27}$$

where ν_0 denotes $\pm|\nu|$ and the sign $\pm$ is determined through the condition $\mu + s\nu_0 > 0$. Therefore, we have

$$\nu_0 = \pm|\nu| , \quad \text{i.e.,} \quad \mu^2 - \nu_0^2 = \kappa . \tag{5·28}$$

The phase factor $e^{-i\chi}$ is related to

$$\nu = \nu_0 e^{-2i\chi} . \tag{5·29}$$

By substituting Eq. (5·27) into Eq. (5·26), we have

$$\left.\begin{aligned} \Psi_U(-s) &= e^{-i\chi}\sqrt{\mu + s\nu_0}[\sqrt{E(-s)}^{-1}\Phi(-s)]_U , \\ \Psi_U(+s) &= e^{-i\chi}\sqrt{\mu + s\nu_0}^{-1}[\sqrt{E(-s)}\Phi(-s)]_U . \end{aligned}\right\} \tag{5·30}$$

Then, W_U is given in the form

$$W_U = e^{-i\chi}/2\sqrt{n_i - n_j}$$
$$\times[(\sqrt{\mu + s\nu_0}\sqrt{E(-s)}^{-1} + \sqrt{\mu + s\nu_0}^{-1}\sqrt{E(-s)})\Phi(-s)]_U , \quad (n_i > n_j) \tag{5·31a}$$

$$W_U = e^{-i\chi}/2\sqrt{n_j - n_i}$$
$$\times[(\sqrt{\mu + s\nu_0}\sqrt{E(-s)}^{-1} - \sqrt{\mu + s\nu_0}^{-1}\sqrt{E(-s)})\Phi(-s)]_U . \quad (n_i < n_j) \tag{5·31b}$$

In order to get a solution $W_U \neq 0$ to Eq. (5·12), κ should be equal to $(\varepsilon_i - \varepsilon_j)^2$. However, in general, the value is different from the eigenvalue of Eq. (5·22). Therefore, we have the following solution for the case $n_i = n_j$:

$$W_U = 0 . \quad (n_i = n_j) \tag{5·31c}$$

The above is an approximate solution of our basic equation for the small amplitude limit and it provides the boundary condition for solving the large amplitude case.

As is clear from the above treatment, our result can be applied to the case $\kappa \lesseqgtr 0$. The amplitudes can be normalized in the conventional condition. The reason why the treatment is possible is as follows: In our treatment, κ is expressed as $(\mu + s\nu_0) \times (\mu - s\nu_0)$ in terms of two parameters μ and ν_0. The factor $(\mu + s\nu_0)$ can be chosen as positive and the normalization of the amplitude is performed by this factor. Therefore, the sign of κ is determined by the factor $(\mu - s\nu_0)$. In the conventional treatment, ν_0 is equal to zero at the beginning. Then, it is impossible to give $\kappa = 0$ under non-vanishing number and, further, $\kappa < 0$ under real number.

With the use of the method mentioned above, we can give a solution at the small amplitude limit for the case of the stable, the critical and the unstable situation. However, there exist two parameters which cannot be fixed in the frame of the starting equations. In principle, their values cannot be determined, but, this does not lead to any trouble. Let us explain the reason why this is so. With this aim, we introduce the following canonical transformation (symplectic):

$$X=a^*X'+bX'^*, \quad X^*=b^*X'+aX'^*. \quad (|a|^2-|b|^2=1) \tag{5·32}$$

As is shown in the sequel, the Hamiltonian H_{col} should be invariant under the transformation (5·32):

$$\begin{aligned} H_{col}&=\mu X^*X-1/2\cdot(\nu X^{*2}+\nu^*X^2) \\ &=\mu'X'^*X'-1/2\cdot(\nu'X'^{*2}+\nu'^*X'^2). \end{aligned} \tag{5·33}$$

Then, the parameters μ' and ν' in the new coordinate system are connected to μ and ν in the old system in the form

$$\left.\begin{aligned} \mu'&=\mu(|a|^2+|b|^2)-(\nu ab^*+\nu^*a^*b), \\ \nu'&=(\nu a^2+\nu^*b^2)-2\mu ab. \end{aligned}\right\} \tag{5·34}$$

From the above relations, we have $\mu'^2-|\nu'|^2=\mu^2-|\nu|^2$. This means that κ is an invariant for the transformation (5·32). Then, two coordinate systems connected with each other under the transformation (5·32) are equivalent to each other. Therefore, if we adopt a possible coordinate system, then, referring to the system, we can determine the unknown parameters. For example, in the case $\kappa>0$, putting $\nu_0=0$, we have $\mu=\sqrt{\kappa}$. As a possible choice, we can put $\chi=0$. This procedure corresponds to the conventional RPA. However, in order to give a unified expression for the stable, the critical and the unstable solution, it is desirable to express the Hamiltonian and the other quantities only in terms of the invariant given above. For this aim, we introduce the following canonical variables Q and P:

$$\left.\begin{aligned} Q&=(s_+-is_-)/\sqrt{2(\mu+s\nu_0)}\cdot(e^{-i\chi}X^*+se^{i\chi}X), \\ P&=(s_-+is_+)\sqrt{(\mu+s\nu_0)/2}\cdot(e^{-i\chi}X^*-se^{i\chi}X), \end{aligned}\right\} \tag{5·35}$$

$$s_\pm=(1\pm s)/2. \quad (s_\pm{}^2=s_\pm, \quad s_+s_-=0) \tag{5·36}$$

The variables Q and P satisfy the conditions

$$Q^*=Q, \quad P^*=P, \quad [Q,P]_P=i. \tag{5·37}$$

The relations (5·37) mean that Q and P are coordinate and its canonical conjugate momentum variable, respectively. By picking up a solution which is the most interesting for the problem under investigation, the Hamiltonian H_{col} and C_{ij} can be expressed in the following form:

$$H_{col}=P^2/2+\kappa Q^2/2, \tag{5·38}$$

$$\begin{aligned} C_{ij}&=v_iu_j/\sqrt{2(n_i-n_j)}\cdot\{(s_+-is_-)[\sqrt{E(-s)}\,\Phi(-s)]_{ij}Q \\ &\quad+(s_-+is_+)[\sqrt{E(-s)}^{-1}\Phi(-s)]_{ij}P\}, \qquad (n_i>n_j) \end{aligned} \tag{5·39a}$$

$$\begin{aligned} C_{ij}&=-v_iu_j/\sqrt{2(n_j-n_i)}\cdot\{(s_++is_-)[\sqrt{E(-s)}\,\Phi(-s)]_{ji}Q \\ &\quad+(s_--is_+)[\sqrt{E(-s)}^{-1}\Phi(-s)]_{ji}P\}, \qquad (n_i<n_j) \end{aligned} \tag{5·39b}$$

$$C_{ij}=0. \qquad (n_i=n_j) \tag{5·39c}$$

Thus, we can search an approximate solution of our basic equations (4·16)~(4·18) at the small amplitude limit. Starting from this lowest approximate solution, we can proceed the approximation to higher order, as has been done in the study of the large amplitude collective motion based on the TDHF theory.

§ 6. Concluding remarks

In this paper, we presented a classical microscopic theory, with the aid of which the mixed states can be described systematically. The basic idea is the natural extension of the TDHF theory for the pure states to the case of the mixed states. Therefore, the quantization scheme should be given and in the future we will contact with this problem.

As the concluding remarks, we will mention that our treatment is also applicable to the case of many collective variables, for example, the case given by the present authors (J. P. and C. F.).[1] Let us introduce the variables X_{ij} satisfying the conditions

$$\begin{aligned} &X_{ij}^*=X_{ji}, \\ &[X_{ij}, X_{kl}]_P=\delta_{jk}\delta_{il}(n_i-n_j), \qquad (\text{for } n_i\neq n_j) \\ &X_{ij}=0. \qquad (\text{for } n_i=n_j) \end{aligned} \tag{6·1}$$

Instead of the relation (4·16), we set up the following canonicity condition:

$$\sum_{ij}(C_{ij}^*\cdot\partial C_{ij}/\partial X_{kl}-C_{ij}\cdot\partial C_{ij}^*/\partial X_{kl})=X_{lk}/(n_k-n_l). \tag{6·2}$$

Combining the canonicity condition (6·2) with the constraint (4·17), we obtain the following expressions for $(c_i{}^*c_j)_C$:

$$(c_i{}^*c_j)_C=n_i\delta_{ij}+\sum_k 1/(n_k-n_i)\cdot X_{ik}X_{kj}+\cdots, \qquad (\text{for } n_i=n_j) \tag{6·3a}$$

$$\begin{aligned} (c_i{}^*c_j)_C&=X_{ij}+\sum_k[(1-n_i)(1-n_j)n_k/(n_k-n_i)(n_k-n_j) \\ &\quad-n_in_j(1-n_k)/(n_k-n_i)(n_k-n_j)]\cdot X_{ik}X_{kj}+\cdots. \qquad (\text{for } n_i\neq n_j) \end{aligned} \tag{6·3b}$$

The expression (6·3) is equivalent to that obtained by the present authors (J. P and C. F.).[1] The RPA equation is also equivalent to their result.

As is shown above, our basic idea may be applied to many other cases. Of course, some modification may be necessary. In this sense, it is very interesting to formulate the equation of the collective submanifold for the mixed states based on the

TDHB theory and to compare with the results obtained in Refs. 2) and 4). In a forthcoming paper, we will report these points.

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