Progress of Theoretical Physics, Vol. 75, No. 3, March 1986

Equations of Collective Submanifold for Large Amplitude Collective Motion and Its Coupling with Intrinsic Degrees of Freedom. II

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(Received October 21, 1985)

Various properties of the equations of collective submanifold derived in part I are investigated. Especially, it is stressed that the equations are invariant for any canonical transformation of collective coordinate system and for symplectic transformation of intrinsic coordinate system. Further, initial condition for solving the equations is shown.

§ 1. Introduction

In part I, equations of collective submanifold were given with the help of the time-dependent Hartree-Fock theory in a canonical form which is combined with a certain canonical transformation.[1] They consist of two types. One is called the first equation and, by solving it, we can pick up the collective degree of freedom from a many-body system. The other is called the second one. If the solution is obtained, we can determine the intrinsic degrees of freedom. As was mentioned in part I, the first equation is of the same form as that we already obtained in a method different from that in part I.[2] The second is a set of linear partial differential equations. On the other hand, the second equation which we obtained previously is non-linear.[2] Therefore, a new one is expected to be practically useful.

As was stressed by the present authors, the first equation is canonically invariant with respect to any canonical transformation for the collective variables.[3] From this fact, we could derive a unique solution in contrast to the discussion, for example, given by Mukherjee and Pal.[4] If we follow their discussion, we cannot get the unique solution. The reason comes from the lack of the viewpoint of canonical invariance. This suggests that it is inevitable for obtaining the solution to investigate the property of the equations in relation to the canonical transformation.

The main aim of part II is to investigate various properties of the second equations. As was clear from the experience on the first equations,[3] such an investigation gives us important help for obtaining the solution of the second equations. In the present case, not only the canonical invariance for the collective degree of freedom but also that for the intrinsic degrees of freedom are interesting. As an important conclusion, the second equations are invariant with respect to arbitrary canonical transformation for the collective and the symplectic transformation for the intrinsic degrees of freedom. From this conclusion, we have an idea how the coordinate system is specified. Through solving the first equations, we could specify the collective coordinate system.[3] In the same way, the intrinsic coordinate system is specified through the solution of the second equations.

In the next section, we will make a discussion on the canonical invariance of our basic relations. In § 3, the second equation of collective submanifold obtained in part I will be

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transformed. From this transform, the relation between the second equation of collective submanifold and the second condition of canonical transformation is clarified. Section 4 will be devoted to general discussion on the specification of coordinate system. Finally, in § 5, we will give the initial condition for the second equation. The present paper is the second part of the series. Then, hereafter, part I will be referred to as (I).

§ 2. Canonical invariance

By solving the first and the second equations of collective submanifold given in Eqs. (I·4·17) and (I·4·19), respectively, we can separate the whole degrees of freedom into the collective and the intrinsic ones. Needless to say, the first and the second conditions of canonical transformation shown in Eqs. (I·4·2) and (I·4·4), respectively, are also necessary. Therefore, our present main interest is concerned with the problem how to solve them. For the preparation of this task, we will investigate canonical invariance property of the equations of collective submanifold.

In (I), we mentioned that coordinate systems obeying the condition $H_d=0$ are connected with one another through relations (I·4·14), (I·4·15) and (I·4·16) for (q_f, p_f), $(q_m, p_m; m\neq f)$ and (α, π), respectively. Further, we introduced new variables (Q, P), which we called collective variables, through Eqs. (I·4·22). Under the approximation adopted in (I), we can prove the following relation:

$$\frac{\partial Q'}{\partial Q}\cdot\frac{\partial P'}{\partial P}-\frac{\partial Q'}{\partial P}\cdot\frac{\partial P'}{\partial Q}=1\,. \qquad (2\cdot1)$$

Here, Q' and P' are defined by

$$Q'=\alpha'+q_f'\,,\qquad P'=\pi'+p_f'\,. \qquad (2\cdot2)$$

Relation (2·1) means that the transformation $(Q, P)\rightarrow(Q', P')$ is canonical. On the other hand, as is clear from Eqs. (I·4·15), the transformation $(q_m, p_m; m\neq f)\rightarrow(q_m', p_m'; m\neq f)$ is also canonical, i.e., symplectic transformation. This fact tells us that the coordinate systems obeying $H_d=0$ are connected through arbitrary canonical transformation for the collective and symplectic transformation for the intrinsic degrees of freedom. Main aim of this section is to investigate transformation property of the equations of collective submanifold and the conditions of canonical transformation with respect to the above-mentioned two types of the canonical transformations.

Let us start from the discussion concerning the collective degrees of freedom. It is enough to investigate the case $(\alpha, \pi)\rightarrow(\alpha', \pi')$, which obeys relations (I·4·16). Under the relation (I·4·16), the following relation can be easily derived:

$$Z(\alpha\pi)\equiv\frac{\partial X}{\partial\alpha}\cdot\frac{\partial Y}{\partial\pi}-\frac{\partial X}{\partial\pi}\cdot\frac{\partial Y}{\partial\alpha}=\frac{\partial X'}{\partial\alpha'}\cdot\frac{\partial Y'}{\partial\pi'}-\frac{\partial X'}{\partial\pi'}\frac{\partial Y'}{\partial\alpha'}\,. \qquad (2\cdot3)$$

Here, X and Y are arbitrary functions of (α, π) and, for example, X' represents

$$X\equiv X(\alpha\pi)=X(\alpha(\alpha'\pi')\pi(\alpha'\pi'))=X'(\alpha'\pi')\equiv X'\,. \qquad (2\cdot4)$$

Relations (2·3) mean that the form $Z(\alpha\pi)$ is invariant for any canonical transformation of (α, π). The left-hand sides of Eqs. (I·4·2b) and (I·4·17) are three examples of the form $Z(\alpha\pi)$. Therefore, they are invariant under the transformation $(\alpha, \pi)\rightarrow(\alpha', \pi')$.

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In other words, the first equations are canonically invariant for the collective degrees of freedom. Next, we contact with the second equations. The unknown functions A_{rm}, B_{rm}, C_{rm} and D_{rm} ($r=1, \cdots, f$; $m=1, \cdots, f-1$) are determined by Eqs. (I·4·4) and (I·4·19). The first terms of the left-hand sides of Eqs. (I·4·19) are the examples of the form $Z(\alpha\pi)$ and the coefficients of A_{sm}, etc., in the second terms are also of the form $Z(\alpha\pi)$. Therefore, Eqs. (I·4·19) are invariant for the transformation $(\alpha, \pi)\to(\alpha', \pi')$. If A_{rm}, etc., satisfy Eqs. (I·4·4) in the coordinate system (α, π), they also obey Eqs. (I·4·4) in (α', π'). Therefore, we can conclude that the second equations are also canonically invariant for $(\alpha, \pi)\to(\alpha', \pi')$.

Next, we investigate the case of the intrinsic degrees of freedom. In this case, as was already mentioned, the symplectic transformation is essential. Since the first equations do not connect with this transformation, we investigate the second equations. We express $\tilde{Q}_r^{(1)}$ and $\tilde{P}_r^{(1)}$, which are given in Eqs. (I·4·7) for the (q, p) coordinate system, as the following forms for the (q', p') coordinate system:

$$\left.\begin{aligned} \tilde{Q}_r^{(1)} &= \sum_{m=1}^{f-1}(A'_{rm}q_m' + C'_{rm}p_m') , \\ \tilde{P}_r^{(1)} &= \sum_{m=1}^{f-1}(B'_{rm}q_m' + D'_{rm}p_m') . \end{aligned}\right\} \tag{2·5}$$

With the use of relations (I·4·15), the following equations are obtained from Eqs. (I·4·7) and (2·5):

$$\left.\begin{aligned} A'_{rm} &= \sum_{n=1}^{f-1}(A_{rn}\bar{D}_{mn} - C_{rn}\bar{B}_{mn}) , \\ B'_{rm} &= \sum_{n=1}^{f-1}(B_{rn}\bar{D}_{mn} - D_{rn}\bar{B}_{mn}) , \\ C'_{rm} &= \sum_{n=1}^{f-1}(C_{rn}\bar{A}_{mn} - A_{rn}\bar{C}_{mn}) , \\ D'_{rm} &= \sum_{n=1}^{f-1}(D_{rn}\bar{A}_{mn} - B_{rn}\bar{C}_{mn}) . \end{aligned}\right\} \tag{2·6}$$

Further, we impose the conditions

$$\Lambda\bar{A}_{mn} = \Lambda\bar{B}_{mn} = \Lambda\bar{C}_{mn} = \Lambda\bar{D}_{mn} = 0 . \tag{2·7}$$

Then, we can see that A'_{rm}, etc., satisfy the same forms as those given in Eqs. (I·4·19). The operator Λ' is equal to Λ and, for example, $\Lambda'A'_{rm}$ is given as follows:

$$\Lambda'A'_{rm} = \sum_n(\Lambda A_{rn}\cdot\bar{D}_{mn} - \Lambda C_{rn}\cdot\bar{B}_{mn}) . \tag{2·8}$$

Here, the conditions (2·7) were used. Substituting Eqs. (I·4·19) into the parts of ΛA_{rn} and ΛC_{rn} and, then, using Eqs. (2·6), we can see that $\Lambda'A'_{rm}$ is of the linear combination of A'_{sm} and B'_{sm} and the coefficients are identical to those of ΛA_{rm}. Further, with the use of relations (I·4·15a) and (2·6), we can prove that relations (I·4·4) hold for A'_{rm}, etc. For the above-mentioned reason, the second equations are canonically invariant for the symplectic transformation with conditions (2·7). Conditions (2·7) will play an essential role for the determination of A_{rm}.

Thus, we learned that the first and the second equations are invaricnt under any canonical transformation for the collective and the symplectic transformation for the

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intrinsic coordinate system. This fact is quite important: The collective submanifold is independent of the choice of coordinate system. Therefore, as was already stressed by the present authors,[3] we have freedom of choosing the coordinate system, with the use of which the collective submanifold is expressed.

§ 3. Transform of the second equation of collective submanifold

The quantites A_{rm}, B_{rm}, C_{rm} and D_{rm} are determined by solving Eqs. (I·4·4) and (I·4·19). However, the number of the equations is excess of that of the unknown quantities. Therefore, it is necessary to investigate if these equations are compatible or not.

For this aim, we introduce the following set of partial differential equations:

$$\left.\begin{aligned}
&\Lambda\mathcal{A}_{rm}+\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]\mathcal{A}_{sm}-\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]\mathcal{B}_{sm}=0\,,\\
&\Lambda\mathcal{B}_{rm}+\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]\mathcal{A}_{sm}-\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]\mathcal{B}_{sm}=0\,,\\
&\Lambda\mathcal{C}_{rm}+\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]\mathcal{C}_{sm}-\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]\mathcal{D}_{sm}=0\,,\\
&\Lambda\mathcal{D}_{rm}+\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]\mathcal{C}_{sm}-\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]\mathcal{D}_{sm}=0\,.
\end{aligned}\right\}\tag{3·1}$$

It can be proved from Eqs. (3·1) that $\mathcal{A}_{rm}$, $\mathcal{B}_{rm}$, $\mathcal{C}_{rm}$ and $\mathcal{D}_{rm}$ satisfy

$$\left.\begin{aligned}
&\Lambda\sum_r\left(\mathcal{A}_{rm}\frac{\partial P_r}{\partial\alpha}-\mathcal{B}_{rm}\frac{\partial Q_r}{\partial\alpha}\right)=0\,,\quad \Lambda\sum_r\left(\mathcal{A}_{rm}\frac{\partial P_r}{\partial\pi}-\mathcal{B}_{rm}\frac{\partial Q_s}{\partial\pi}\right)=0\,,\\
&\Lambda\sum_r\left(\mathcal{C}_{rm}\frac{\partial P_r}{\partial\alpha}-\mathcal{D}_{rm}\frac{\partial Q_r}{\partial\alpha}\right)=0\,,\quad \Lambda\sum_r\left(\mathcal{C}_{rm}\frac{\partial P_r}{\partial\pi}-\mathcal{D}_{rm}\frac{\partial Q_r}{\partial\pi}\right)=0\,.
\end{aligned}\right\}\tag{3·2a}$$

Further, under relations (3·2a), we have

$$\left.\begin{aligned}
&\Lambda\sum_r(\mathcal{A}_{rm}\mathcal{B}_{rn}-\mathcal{B}_{rm}\mathcal{A}_{rn})=0\,,\\
&\Lambda\sum_r(\mathcal{C}_{rm}\mathcal{D}_{rn}-\mathcal{D}_{rm}\mathcal{C}_{rn})=0\,,\\
&\Lambda\sum_r(\mathcal{A}_{rm}\mathcal{D}_{rn}-\mathcal{B}_{rm}\mathcal{C}_{rn})=0\,.
\end{aligned}\right\}\tag{3·2b}$$

The set of partial differential equations (3·1) can be rewritten in terms of the variables (H, τ) obtained from (α, π) through the relation

$$\frac{\partial H}{\partial\alpha}\cdot\frac{\partial\tau}{\partial\pi}-\frac{\partial H}{\partial\pi}\cdot\frac{\partial\tau}{\partial\alpha}=1\,.\tag{3·3}$$

The variable H denotes the Hamiltonian determined by the first equations in terms of (α, π) and, therefore, τ is a momentum conjugate to H. In the variables (H, τ), the operator Λ is expressed by

$$\Lambda=-\frac{\partial}{\partial\tau}\,.\tag{3·4}$$

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The coefficients of the linear combinations for $\mathcal{A}_{rm}$, etc., are functions of (H, τ). However, Eqs. (3·1) are ordinary differential equations for the variable τ and H plays a role of parameter in these equations. Then, by solving Eqs. (3·1), we have the following type of solution:

$$\left.\begin{aligned}\mathcal{A}_{rm}&=\mathcal{A}_{rm}(\tau;\, H|\alpha_{1m}\cdots\alpha_{rf}\beta_{1m}\cdots\beta_{fm})\,,\\ \mathcal{B}_{rm}&=\mathcal{B}_{rm}(\tau;\, H|\alpha_{1m}\cdots\alpha_{fm}\beta_{1m}\cdots\beta_{fm})\,,\\ \mathcal{C}_{rm}&=\mathcal{C}_{rm}(\tau;\, H|\gamma_{1m}\cdots\gamma_{fm}\delta_{1m}\cdots\delta_{fm})\,,\\ \mathcal{D}_{rm}&=\mathcal{D}_{rm}(\tau;\, H|\gamma_{1m}\cdots\gamma_{fm}\delta_{1m}\cdots\delta_{fm})\,.\end{aligned}\right\} \tag{3·5}$$

Here, α_{rm}, β_{rm}, γ_{rm} and δ_{rm} $(r=1, \cdots, f)$ are the integral constants and they are fixed, for example, by equating the values of $\mathcal{A}_{rm}$, etc., at $\tau=0$ to certain values which we denote $\mathcal{A}_{rm}^{(0)}$, $\mathcal{B}_{rm}^{(0)}$, $\mathcal{C}_{rm}^{(0)}$ and $\mathcal{D}_{rm}^{(0)}$. This is nothing but the initial condition for Eqs. (3·1). Thus, we can determine $\mathcal{A}_{rm}$, etc. Let $\mathcal{A}_{rm}^{(0)}$, etc., satisfy the same relations as Eqs. (I·4·4) with $\partial Q_r/\partial\alpha$, $\partial Q_r/\partial\pi$, $\partial P_r/\partial\alpha$ and $\partial P_r/\partial\pi$ at $\tau=0$:

$$\left.\begin{aligned}&\sum_r\left(\mathcal{A}_{rm}^{(0)}\left(\frac{\partial P_r}{\partial\alpha}\right)_0-\mathcal{B}_{rm}^{(0)}\left(\frac{\partial Q_r}{\partial\alpha}\right)_0\right)=0\,,\quad \sum_r\left(\mathcal{A}_{rm}^{(0)}\left(\frac{\partial P_r}{\partial\pi}\right)_0-\mathcal{B}_{rm}^{(0)}\left(\frac{\partial Q_r}{\partial\pi}\right)_0\right)=0\,,\\ &\sum_r\left(\mathcal{C}_{rm}^{(0)}\left(\frac{\partial P_r}{\partial\alpha}\right)_0-\mathcal{D}_{rm}^{(0)}\left(\frac{\partial Q_r}{\partial\alpha}\right)_0\right)=0\,,\quad \sum_r\left(\mathcal{C}_{rm}^{(0)}\left(\frac{\partial P_r}{\partial\pi}\right)_0-\mathcal{D}_{rm}^{(0)}\left(\frac{\partial Q_r}{\partial\pi}\right)_0\right)=0\,,\end{aligned}\right\} \tag{3·1a}$$

$$\left.\begin{aligned}&\sum_r(\mathcal{A}_{rm}^{(0)}\mathcal{B}_{rn}^{(0)}-\mathcal{B}_{rm}^{(0)}\mathcal{A}_{rn}^{(0)})=0\,,\\ &\sum_r(\mathcal{C}_{rm}^{(0)}\mathcal{D}_{rn}^{(0)}-\mathcal{D}_{rm}^{(0)}\mathcal{C}_{rn}^{(0)})=0\,,\\ &\sum_r(\mathcal{A}_{rm}^{(0)}\mathcal{D}_{rn}^{(0)}-\mathcal{B}_{rm}^{(0)}\mathcal{C}_{rn}^{(0)})=\delta_{mn}\,.\end{aligned}\right\} \tag{3·6a}$$

Here, $(\partial P_r/\partial\alpha)_0$, etc., denote the values of $\partial P_r/\partial\alpha$, etc., at $\tau=0$. Then, noting the differential operator (3·4) and Eqs. (3·2), we can see that $\mathcal{A}_{rm}$, etc., at any value of τ satisfy also the same forms as Eqs. (I·4·4). From the above discussion, we get a conclusion that the set of Eqs. (3·1) has a solution which is compatible with Eqs. (I·4·19).

Under the above preparation, we contact with the second equation (I·4·19). The set of equations can be rewritten as

$$\begin{aligned}\Lambda A_{rm}&+\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]A_{sm}-\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]B_{sm}\\ &+\left(\frac{\partial Q_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\pi^2}-\frac{\partial Q_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}\right)\sum_s\left(A_{sm}\frac{\partial P_s}{\partial\alpha}-B_{sm}\frac{\partial Q_s}{\partial\alpha}\right)\\ &-\left(\frac{\partial Q_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}-\frac{\partial Q_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha^2}\right)\sum_s\left(A_{sm}\frac{\partial P_s}{\partial\pi}-B_{sm}\frac{\partial Q_s}{\partial\pi}\right)=0\,,\end{aligned}$$

$$\begin{aligned}\Lambda B_{rm}&+\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]A_{sm}-\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]B_{sm}\\ &+\left(\frac{\partial P_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\pi^2}-\frac{\partial P_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}\right)\sum_s\left(A_{sm}\frac{\partial P_s}{\partial\alpha}-B_{sm}\frac{\partial Q_s}{\partial\alpha}\right)\\ &-\left(\frac{\partial P_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}-\frac{\partial P_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha^2}\right)\sum_s\left(A_{sm}\frac{\partial P_s}{\partial\pi}-B_{sm}\frac{\partial Q_s}{\partial\pi}\right)=0\,,\end{aligned}$$

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$$\Lambda C_{rm}+\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]C_{sm}-\sum_s\left[\frac{\partial Q_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial Q_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]D_{sm}$$
$$+\left(\frac{\partial Q_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\pi^2}-\frac{\partial Q_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}\right)\sum_s\left(C_{sm}\frac{\partial P_s}{\partial\alpha}-D_{sm}\frac{\partial Q_s}{\partial\alpha}\right)$$
$$-\left(\frac{\partial Q_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}-\frac{\partial Q_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha^2}\right)\sum_s\left(C_{sm}\frac{\partial P_s}{\partial\pi}-D_{sm}\frac{\partial Q_s}{\partial\pi}\right)=0\,,$$

$$\Lambda D_{rm}+\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial P_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial P_s}{\partial\alpha}\right]C_{sm}-\sum_s\left[\frac{\partial P_r}{\partial\alpha}\Lambda\frac{\partial Q_s}{\partial\pi}-\frac{\partial P_r}{\partial\pi}\Lambda\frac{\partial Q_s}{\partial\alpha}\right]D_{sm}$$
$$+\left(\frac{\partial P_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\pi^2}-\frac{\partial P_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}\right)\sum_s\left(C_{sm}\frac{\partial P_s}{\partial\alpha}-D_{sm}\frac{\partial Q_s}{\partial\alpha}\right)$$
$$-\left(\frac{\partial P_r}{\partial\alpha}\cdot\frac{\partial^2 H}{\partial\alpha\partial\pi}-\frac{\partial P_r}{\partial\pi}\cdot\frac{\partial^2 H}{\partial\alpha^2}\right)\sum_s\left(C_{sm}\frac{\partial P_s}{\partial\pi}-D_{sm}\frac{\partial Q_s}{\partial\pi}\right)=0\,. \tag{3·7}$$

From the comparison of Eqs. (3·7) with Eqs. (3·1), we can see that, as a possible set of solutions of Eqs. (I·4·19), there exists the following:

$$A_{rm}=\mathcal{A}_{rm},\quad B_{rm}=\mathcal{B}_{rm},\quad C_{rm}=\mathcal{C}_{rm},\quad D_{rm}=\mathcal{D}_{rm}\,. \tag{3·8}$$

Clearly, $\mathcal{A}_{rm}$, etc., are the solutions of Eqs. (3·1) with the initial conditions (3·6). Since the solutions satisfy Eqs. (I·4·4), Eqs. (I·4·4) and (I·4·19) are compatible with each other.

§ 4. Specification of coordinate system

In § 2, we have shown that the equations of collective submanifold are canonically invariant. This is a quite natural fact, because the collective submanifold does not depend on the choice of its coordinate system. However, it is necessary to fix the coordinate system in order to express the Hamiltonian in a concrete form. For the case of the collective coordinate system, we have already discussed our basic idea in some papers.[2),3)] Then, for the completeness of the paper, first, we will mention briefly the specification of the collective coordinate system.

Let us discuss a typical example. We note $H(\alpha,\pi)$ (or $H(Q,P)$) given in Eq. (I·4·20) (or Eq. (I·4·21)). This is a function of only (α,π) (or (Q,P)) through $Q_r(\alpha\pi)$ and $P_r(\alpha\pi)$ (or $Q_r(QP)$ and $P_r(QP)$). Therefore, we call H the collective Hamiltonian and, hereafter, we denote it as $H_{\rm coll}$. Our task is to determine $H_{\rm coll}$ concretely. A practical method is to obtain it successively from the lower to the higher terms in the framework of power series expansion for π:

$$H_{\rm coll}=V(\alpha)+\frac{\pi^2}{2M(\alpha)}+\sum_{n=3}^{\infty}h_n(\alpha)\pi^n\,. \tag{4·1}$$

Here, we assumed that $H_{\rm coll}$ is stationary at the point $\alpha=\pi=0$. Practically, we have to stop the expansion at a finite power. Therefore, it is undesirable that the power, at which we stop the expansion, changes if we view from another coordinate system. Of course, it connects to the original by a canonical transformation. The point transformation, which is shown in the following, satisfies this condition:

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$$\alpha'=f(\alpha)\,,\quad \pi'=\frac{\pi}{\dfrac{df(\alpha)}{d\alpha}}\,, \tag{4·2}$$

where $f(\alpha)$ is an arbitrary function.

Keeping the invariance property of expansion (4·1) in mind, let us consider how to solve the first equations (I·4·2b) and (I·4·17). As was already mentioned, they are invariant for any canonical transformation. Therefore, in the framework of Eqs. (I·4·2b) and (I·4, 17), it is impossible to specify the coordinate system in one special type. Then, instead of Eq. (I·4·2b), we adopt Eqs. (I·4·2a), from which Eq. (I·4·2b) is derived. In this case, Eqs. (I·4·17) and (I·4·2a) with $W=0$ are not invariant for any canonical transformation, but the point transformation (4·2). Therefore, in the framework of Eqs. (I·4·17) and (I·4·2a) with $W=0$, we can specify the coordinate system except the choice of the function $f(\alpha)$ in Eqs. (4·2). In order to fix $f(\alpha)$, we set up $M(\alpha)=1$, where $M(\alpha)$ appears in expansion (4·1). By adopting the condition that the small amplitude limit is reduced to the random phase approximation, we can solve the first equations. This is the outline of the specification of the collective coordinate system, which we have discussed in other papers.[2),3)]

Main interest of this paper is how to specify the intrinsic coordinate system. As an interpretation of the solution (3·5), we mentioned that, in order to solve the second equations, it is necessary to give, as the initial condition, $\mathcal{A}_{rm}^{(0)}$, etc, satisfying Eqs. (3·6). The total number of $\mathcal{A}_{rm}^{(0)}$, etc., is $4f(f-1)$ and the number of Eqs. (3·6) is $2(f-1)^2+3(f-1)$. Therefore, $2(f-1)^2+(f-1)$ of $\mathcal{A}_{rm}^{(0)}$, etc., are free and we cannot fix all of $\mathcal{A}_{rm}^{(0)}$, etc. Further, we do not have any additional condition for fixing all of them. It seems for us that our theory is not self-contained. However, this question can be solved. We should remember that, if a set of certain A_{rm}, etc., is a solution of the second equations, the set of A'_{rm}, etc., satisfying relations (2·6) and (2·7) is also a solution. The parameters $\bar{A}_{mn}$, $\bar{B}_{mn}$, $\bar{C}_{mn}$ and $\bar{D}_{mn}$, which are independent of τ, are related to the symplectic transformation (I·4·15) and obey relations (I·4·15a). The number of $\bar{A}_{mn}$, etc., is $4(f-1)^2$ and the number of the relations (4·15a) is $2(f-1)^2-(f-1)$. Therefore, $2(f-1)^2+(f-1)$ of $\bar{A}_{mn}$, etc., are free. The number $2(f-1)^2+(f-1)$ is equal to that in the case of $\mathcal{A}_{mn}^{(0)}$, etc. This means that, as a result of the canonical invariance, a general solution of the second equations contains $2(f-1)^2+(f-1)$ parameters and our theory is self-contained. From the above analysis, it is necessary to introduce a condition for fixing all of $\mathcal{A}_{rm}^{(0)}$, etc., from the outside. With the aid of the condition, we can specify the intrinsic coordinate system.

§ 5. Initial condition for the second equation

As was already mentioned in § 4, the specification of the intrinsic coordinate system is reduced to giving all of $\mathcal{A}_{rm}^{(0)}$, $\mathcal{B}_{rm}^{(0)}$, $\mathcal{C}_{rm}^{(0)}$ and $\mathcal{D}_{rm}^{(0)}$ which play a role of the initial condition for the second equation. Needless to say, they obey the conditions (3·6). Main aim of this section is to give a concrete form of the set $\mathcal{A}_{rm}^{(0)}$, etc., obeying Eqs. (3·6).

First, we introduce the following $2f$-dimensional matrix Γ:

$$\Gamma=\begin{bmatrix} K & L \\ M^T & K^T \end{bmatrix}\,. \tag{5·1}$$

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Here, K, L and M are f-dimensional matrices, the elements of which are given by

$$K_{rs}=\delta_{rs}-\left[\left(\frac{\partial Q_r}{\partial \alpha}\right)_0\left(\frac{\partial P_s}{\partial \pi}\right)_0-\left(\frac{\partial Q_r}{\partial \pi}\right)_0\left(\frac{\partial P_s}{\partial \alpha}\right)_0\right], \tag{5·2a}$$

$$L_{rs}=\left(\frac{\partial Q_r}{\partial \alpha}\right)_0\left(\frac{\partial Q_s}{\partial \pi}\right)_0-\left(\frac{\partial Q_r}{\partial \pi}\right)_0\left(\frac{\partial Q_s}{\partial \alpha}\right)_0, \tag{5·2b}$$

$$M_{rs}=\left(\frac{\partial P_r}{\partial \alpha}\right)_0\left(\frac{\partial P_s}{\partial \pi}\right)_0-\left(\frac{\partial P_r}{\partial \pi}\right)_0\left(\frac{\partial P_s}{\partial \alpha}\right)_0. \tag{5·2c}$$

Clearly, L and M satisfy

$$L^T=-L\,,\quad M^T=-M\,. \tag{5·3}$$

With the use of the first condition of canonical transformation (I·4·2b), we can prove

$$\Gamma^2=\Gamma\,,\quad \mathrm{Tr}\Gamma=2(f-1)\,. \tag{5·4}$$

The above relations tell us that the matrix Γ is an idempotent matrix and 2 and $2(f-1)$ eigenvalues are zero and one, respectively. The following relations are easily derived:

$$\Gamma\begin{bmatrix}\left(\frac{\partial Q}{\partial \alpha}\right)_0\\ \left(\frac{\partial P}{\partial \alpha}\right)_0\end{bmatrix}=0\,,\qquad \Gamma\begin{bmatrix}\left(\frac{\partial Q}{\partial \pi}\right)_0\\ \left(\frac{\partial P}{\partial \pi}\right)_0\end{bmatrix}=0\,. \tag{5·5}$$

Here, the column vectors consist of $(\partial Q_1/\partial\alpha)_0\cdots(\partial Q_f/\partial\alpha)_0$, $(\partial P_1/\partial\alpha)_0\cdots(\partial P_f/\partial\alpha)_0$ and $(\partial Q_1/\partial\pi)_0\cdots(\partial Q_f/\partial\pi)_0$, $(\partial P_1/\partial\pi)_0\cdots(\partial P_f/\partial\pi)_0$. Further, $\mathcal{A}^{(0)}_{rm}$, etc., satisfying the conditions (3·6a) obey

$$\Gamma\begin{bmatrix}\mathcal{A}_m{}^{(0)}\\ \mathcal{B}_m{}^{(0)}\end{bmatrix}=\begin{bmatrix}\mathcal{A}_m{}^{(0)}\\ \mathcal{B}_m{}^{(0)}\end{bmatrix},\quad \Gamma\begin{bmatrix}\mathcal{C}_m{}^{(0)}\\ \mathcal{D}_m{}^{(0)}\end{bmatrix}=\begin{bmatrix}\mathcal{C}_m{}^{(0)}\\ \mathcal{D}_m{}^{(0)}\end{bmatrix}. \tag{5·6}$$

The interpretation of the notations may not be necessary.

Now, let us suppose that $\mathcal{A}_m{}^{(0)}$, etc., satisfy the following relations:

$$\Gamma^T\mathcal{H}^{(0)}\Gamma\begin{bmatrix}\mathcal{A}_m{}^{(0)}\\ \mathcal{B}_m{}^{(0)}\end{bmatrix}=\Omega_m\begin{bmatrix}\mathcal{D}_m{}^{(0)}\\ -\mathcal{C}_m{}^{(0)}\end{bmatrix}, \tag{5·7a}$$

$$\Gamma^T\mathcal{H}^{(0)}\Gamma\begin{bmatrix}\mathcal{C}_m{}^{(0)}\\ \mathcal{D}_m{}^{(0)}\end{bmatrix}=\begin{bmatrix}-\mathcal{B}_m{}^{(0)}\\ \mathcal{A}_m{}^{(0)}\end{bmatrix}. \tag{5·7b}$$

Here, $\mathcal{H}^{(0)}$ is a $2f$-dimensional matrix defined by

$$\mathcal{H}^{(0)}=\begin{bmatrix}\mathcal{H}^{(0)}_{QQ}\,, & \mathcal{H}^{(0)}_{QP}\\ \mathcal{H}^{(0)}_{PQ}\,, & \mathcal{H}^{(0)}_{PP}\end{bmatrix}, \tag{5·8}$$

$$\left.\begin{aligned}(\mathcal{H}^{(0)}_{QQ})_{rs}&=\left(\frac{\partial^2\mathcal{H}}{\partial Q_r\partial Q_s}\right)_0, & (\mathcal{H}^{(0)}_{QP})_{rs}&=\left(\frac{\partial^2\mathcal{H}}{\partial Q_r\partial P_s}\right)_0,\\ (\mathcal{H}^{(0)}_{PQ})_{rs}&=\left(\frac{\partial^2\mathcal{H}}{\partial P_r\partial Q_s}\right)_0, & (\mathcal{H}^{(0)}_{PP})_{rs}&=\left(\frac{\partial^2\mathcal{H}}{\partial P_r\partial P_s}\right)_0.\end{aligned}\right\} \tag{5·8a}$$

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The quantities of the right-hand sides of Eqs. (5·8a) are given by substituting $\tau=0$ to those shown in Eq. (I·4·10c). Later, we will determine Ω_m. For a moment, we assume that if $m\neq n$, $\Omega_m\neq\Omega_n$ and all $\Omega_m\neq 0$. Then, with the use of the transpose of relations (5·5) and Eqs. (5·7), relations (3·6a) can be derived. Further, if $m\neq n$, we can prove relations (3·6b). In the case $m=n$, the first and the second of Eqs. (3·6b) are trivial and the the third is used for the normalization. Therefore, the solution of Eqs. (5·7) gives us the initial condition for the second equation.

Thus, our problem is reduced to solving Eqs. (5·7). These equations become the following eigenvalue equations for the eigenvalue Ω_m:

$$J^T\Gamma^T\mathcal{H}^{(0)}\Gamma J\Gamma^T\mathcal{H}^{(0)}\Gamma\begin{bmatrix}\mathcal{A}_m^{(0)}\\ \mathcal{B}_m^{(0)}\end{bmatrix}=\Omega_m\begin{bmatrix}\mathcal{A}_m^{(0)}\\ \mathcal{B}_m^{(0)}\end{bmatrix}, \tag{5·9a}$$

$$J^T\Gamma^T\mathcal{H}^{(0)}\Gamma J\Gamma^T\mathcal{H}^{(0)}\Gamma\begin{bmatrix}\mathcal{C}_m^{(0)}\\ \mathcal{D}_m^{(0)}\end{bmatrix}=\Omega_m\begin{bmatrix}\mathcal{C}_m^{(0)}\\ \mathcal{D}_m^{(0)}\end{bmatrix}. \tag{5·9b}$$

Here, J is a $2f$-dimensional matrix defined by

$$J=\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}. \tag{5·10}$$

The symbols 0 and 1 denote f-dimensional null and unit matrices, respectively. Therefore, if we solve the eigenvalue equations (5·9), our task finishes. As is clear from Eqs. (5·9), there exist two independent eigenvectors for each eigenvalue. Also, Eqs. (5·5) tell us that the matrix $J^T\Gamma^T\mathcal{H}^{(0)}\Gamma J\Gamma^T\mathcal{H}^{(0)}\Gamma$ has two independent eigenvectors with eigenvalue 0. Therefore, it is enough to pick up the eigenvectors with non-vanishing eigenvalues.

Finally, we will mention briefly the small amplitude limit of the initial condition. In this limit, $(Q_r/\partial\alpha)_0$ and $(\partial P_r/\partial\pi)_0$ become certain constants which relate to the collective solution of the random phase approximation for the first equation. Further, $(\partial Q_r/\partial\pi)_0$ and $(\partial P_r/\partial\alpha)_0$ vanish.[2] Then, relations (3·6) are reduced to the ortho-normalization conditions of the random phase approximation. Therefore, in the small amplitude limit, the initial condition becomes non-collective solution of the random phase approximation automatically. In the near future, we will report some numerical results based on the present method.

Acknowledgements

This work has been performed as a part of the Annual Research Project for "Large Amplitude Collective Motions in Nuclei" organized by the Research Institute for Fundamental Physics, Kyoto in 1985.

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