Progress of Theoretical Physics, Vol. 64, No. 4, October 1980

Self-Consistent Collective-Coordinate Method for the Large-Amplitude Nuclear Collective Motion

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(Received April 24, 1980)

This is the second in a series of papers which intends to develop a new microscopic theory capable by itself to select the "optimum" collective path or, more generally, the "optimum" collective submanifold in the many-particle Hilbert space. The main content of this paper consists of i) a restatement of the basic equations of the theory, derived from the fundamental principle which leads us to the "maximal decoupling" between the collective and intrinsic modes and is called the "invariance principle of the Schrödinger equation", and ii) a proposal of a method of solving the basic equations in an appropriate way for the large-amplitude and highly non-linear collective vibrations about the Hartree-Fock ground state with a spherically symmetric equilibrium.

§ 1. Introduction

This is the second in a series of papers which intends to develop a new microscopic theory capable by itself to select the "optimum" collective path (or, more generally, the "optimum" collective submanifold in the many-particle Hilbert space), consistent with the specified boundary condition on the collective motion. In Paper I,[1] the basic equations of the theory (within the framework of the Hartree-Fock approximation) were derived at some length with a major effort directed toward making clear the physical meaning of the fundamental principle to derive the equations, which was called the "invariance principle of the Schrödinger equation" and led us to the "maximal decoupling" between the collective and the intrinsic modes.

The main content of this paper is i) a restatement of the basic equations of the theory with further discussion from a different point of view[2] and ii) a proposal of a new method of solving the basic equations, consistently with such a specified condition on the collective motion that we are considering the large amplitude collective vibrations about the Hartree-Fock ground state with a spherically sym-

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metric equilibrium. The first part consists of §§ 2 and 3, and the second part is contained in § 4.

Since the purpose of this paper is to formulate the basic idea in a simple and systematic way, in this paper we dispense with the complications of the pairing correlations, and will use the pure Hartree-Fock theory instead of the use of the Hartree-Fock-Bogoliubov theory.

§ 2. Generalized moving frame associated with time-dependent self-consistent mean field

It may never be an overstatement to say that the history in the study of nuclear dynamics has been the struggle to find the proper place for the complementary concepts referring to the independent particle motion inside the nucleus and the collective behavior of the nucleus as a whole.[3] A starting point in exploring the nuclear dynamics involving such two modes of motion was the collective model of Bohr and Mottelson. The basic idea underlying this model is the following: In the shell model, the mean field in which the particles move independently is assumed to be of spherical shape and to be impossible to deform its shape. If we allow the mean field to be time-dependent and deformable, then the mean field is capable by itself to move self-consistently with the action of the particles. This is just the collective mode of motion.

In investigating the dynamics underlying the collective mode of motion, therefore, an essential element is the "particle-collective coupling" *which represents the variations in the mean field.* It must be emphasized that this coupling is just what organizes the self-consistent collective modes out of the particle excitations. A basis for such an investigation of the nuclear dynamics is provided by the cranking model[4] for the collective rotation. In the cranking model, one considers the particle motion in such a mean field with a deformed equilibrium that is uniformly rotating with frequency $\boldsymbol{\omega}_{\rm rot}$. In the rotating (time-dependent) coordinate frame the "particle-collective coupling", which organizes the collective rotation, manifests itself as the Coriolis coupling $-\boldsymbol{\omega}_{\rm rot}\cdot\boldsymbol{J}$. (Here and hereafter we use $\hbar=1$.) This coupling in the rotating frame gives rise to an increase in the energy of the particle motion, which is identified with the collective rotational energy,

$$\mathcal{H}_{\rm rot}(\omega_{\rm rot})=\langle\phi(\omega_{\rm rot})|H|\phi(\omega_{\rm rot})\rangle_\beta-\langle\phi_0|H|\phi_0\rangle_\beta\,. \tag{2·1}$$

Here $|\phi_0\rangle_\beta$ is the Hartree-Fock ground state with the deformation β and $|\phi(\omega_{\rm rot})\rangle_\beta$ is the Hartree-Fock state in the rotating frame satisfying

$$\delta\langle\phi(\omega_{\rm rot})|H-\boldsymbol{\omega}_{\rm rot}\cdot\boldsymbol{J}|\phi(\omega_{\rm rot})\rangle=0\,, \tag{2·2}$$

where $H'=H-\boldsymbol{\omega}_{\rm rot}\cdot\boldsymbol{J}$ is the time-displacement operator describing the time-evolution of the system in the rotating (time-dependent) frame.

Now let us generalize this idea in order to describe the large-amplitude collective vibration about the Hartree-Fock ground state $|\phi_0\rangle$ with a spherically symmetric equilibrium. An essential difference of this case from the above cranking model is in the fact that we do not know, in advance, the "particle-collective coupling" organizing the large amplitude collective vibration under consideration, out of the particle excitations. In order to find the "particle-collective coupling" in this case, we therefore introduce a generalized moving frame called a *vibrating frame* hereafter by a time-dependent unitary transformation with a complex parameter $\eta(t)$ and its complex conjugate $\eta^*(t)$,

$$|\phi(\eta^*(t),\eta(t))\rangle = U^{-1}(\eta^*(t),\eta(t))\,|\phi_0\rangle\,. \tag{2·3}$$

Here $|\phi(\eta^*(t),\eta(t))\rangle$ is the Hartree-Fock state in the vibrating frame and the pair of parameters $(\eta^*(t),\eta(t))$ specifies the time-dependent variations of the self-consistent field, associated with the collective vibration described by a collective coordinate $\alpha(t)$ and its conjugate $\pi(t)$,

$$\alpha=\frac{1}{\sqrt{2}}\{\eta^*+\eta\},\quad \pi=i\frac{1}{\sqrt{2}}\{\eta^*-\eta\}\,. \tag{2·4a}$$

In order to simplify the presentation of the theory, here we have restricted ourselves to a single pair of parameters $(\eta^*,\eta)\equiv(\alpha,\pi)$, although a set of pairs of parameters may be generally necessary to specify the realistic collective mode.*) An extension of the theory to any finite number of pairs of parameters is, of course, straightforward.

Since the time-dependence of the pair of parameters $(\eta^*(t),\eta(t))$ specifies the time-dependence of $|\phi(\eta^*,\eta)\rangle$, we obtain

$$\begin{aligned} i\frac{\partial}{\partial t}|\phi(\eta^*,\eta)\rangle &= i\dot\eta\frac{\partial}{\partial\eta}|\phi(\eta^*,\eta)\rangle + i\dot\eta^*\frac{\partial}{\partial\eta^*}|\phi(\eta^*,\eta)\rangle \\ &= i\dot\eta\cdot\mathring{O}^\dagger(\hat z(\eta),\eta^*\eta)\,|\phi(\eta^*,\eta)\rangle - i\dot\eta^*\cdot\mathring{O}(\hat z(\eta),\eta^*\eta)\,|\phi(\eta^*,\eta)\rangle\,, \end{aligned} \tag{2·5}$$

where the operators $\mathring{O}^\dagger(\hat z(\eta),\eta^*\eta)$ and $\mathring{O}(\hat z(\eta),\eta^*\eta)$ are the *local* infinitesimal generators with respect to η and η^* respectively, defined by

$$\left.\begin{aligned} \frac{\partial}{\partial\eta}U^{-1}(\eta^*,\eta) &= \mathring{O}^\dagger(\hat z(\eta),\eta^*\eta)\,U^{-1}(\eta^*,\eta)\,,\\ \frac{\partial}{\partial\eta^*}U^{-1}(\eta^*,\eta) &= -\mathring{O}(\hat z(\eta),\eta^*\eta)\,U^{-1}(\eta^*,\eta)\,. \end{aligned}\right\} \tag{2·6}$$

Here and hereafter we use the notation $\hat z$ to collectively denote a set of all the

*) For the case of the shape vibrations of order $\lambda=2$, we need five pairs of parameters $(\eta_\mu^*,\eta_\mu;\mu=-2,-1,0,1,2)$ associated with the collective coordinates and their conjugates,

$$\alpha_{2\mu}=\frac{1}{\sqrt{2}}\{\eta_\mu^*+(-)^\mu\eta_{-\mu}\},\qquad \pi_{2\mu}=i\frac{1}{\sqrt{2}}\{(-)^\mu\eta^*_{-\mu}-\eta_\mu\}\,. \tag{2.4b}$$

normal products of the one-body fermion pair operators under consideration, with respect to the Hartree-Fock ground state $|\phi_0\rangle$,

$$\hat{z}=\{:c_\alpha{}^\dagger c_\beta:\}.^{*)} \tag{2·7}$$

We also use the notation $\hat{z}(\eta)$ to denote the same set of all the normal products of the one-body fermion pair operators with respect to the Hartree-Fock state $|\phi(\eta^*,\eta)\rangle$ in the vibrating frame,

$$\hat{z}(\eta)=U^{-1}(\eta^*,\eta)\hat{z}U(\eta^*,\eta). \tag{2·8}$$

In order that the state $|\phi(\eta^*,\eta)\rangle$ is the Hartree-Fock state, the local generators $\mathring{O}^\dagger(\hat{z}(\eta),\eta^*\eta)$ and $\mathring{O}(\hat{z}(\eta),\eta^*\eta)$ must be linear functions of the fermion pair operators $\hat{z}(\eta)$ and **1**.

Since, by definition, the state $|\phi(\eta^*,\eta)\rangle$ in the vibrating frame is completely specified by the values of (η^*,η), the generators must strictly satisfy the integrability condition

$$\Big\{\frac{\partial}{\partial\eta}\mathring{O}(\hat{z}(\eta),\eta^*\eta)+\frac{\partial}{\partial\eta^*}\mathring{O}^\dagger(\hat{z}(\eta),\eta^*\eta)$$
$$+[\mathring{O}(\hat{z}(\eta),\eta^*\eta),\mathring{O}^\dagger(\hat{z}(\eta),\eta^*\eta)]\Big\}U^{-1}(\eta^*,\eta)=0 \tag{2·9a}$$

which is derived from

$$\frac{\partial^2}{\partial\eta\partial\eta^*}U^{-1}(\eta^*,\eta)=\frac{\partial^2}{\partial\eta^*\partial\eta}U^{-1}(\eta^*,\eta). \tag{2·9b}$$

Since the discussion so far is not affected by any variable transformation $\eta'=f(\eta^*,\eta)$, it is convenient to set up the following expectation values with the use of this freedom:

$$\left.\begin{aligned}\langle\phi(\eta^*,\eta)|\mathring{O}^\dagger(\hat{z}(\eta),\eta^*\eta)|\phi(\eta^*,\eta)\rangle&=\frac{1}{2}\eta^*,\\ \langle\phi(\eta^*,\eta)|\mathring{O}(\hat{z}(\eta),\eta^*\eta)|\phi(\eta^*,\eta)\rangle&=\frac{1}{2}\eta.\end{aligned}\right\} \tag{2·10}$$

As is shown in Appendix C, it is generally possible to choose such parameters (η^*,η) that satisfy the condition (2·10). With the definition

$$\left.\begin{aligned}\mathring{O}^\dagger(\hat{z}(\eta),\eta^*\eta)&=U^{-1}(\eta^*,\eta)\mathring{O}^\dagger(\hat{z},\eta^*\eta)U(\eta^*,\eta),\\ \mathring{O}(\hat{z}(\eta),\eta^*\eta)&=U^{-1}(\eta^*,\eta)\mathring{O}(\hat{z},\eta^*\eta)U(\eta^*,\eta),\end{aligned}\right\} \tag{2·11a}$$

*) Throughout the paper, we adhere to the convention of denoting occupied single-particle orbits of $|\phi_0\rangle$ by the indices $i, j, \cdots$, and unoccupied single-particle orbits of $|\phi_0\rangle$ by the indices $\mu, \nu, \cdots$. We also use labels $\alpha, \beta, \cdots$ to indicate the single-particle orbits when we need not specify to be occupied or unoccupied.

i.e.,

$$\left.\begin{aligned}\mathring{O}^{\dagger}(\hat{z}, \eta^*\eta) &= U(\eta^*, \eta)\frac{\partial}{\partial\eta}U^{-1}(\eta^*, \eta),\\ \mathring{O}(\hat{z}, \eta^*\eta) &= -U(\eta^*, \eta)\frac{\partial}{\partial\eta^*}U^{-1}(\eta^*, \eta),\end{aligned}\right\} \qquad (2\cdot 11\text{b})$$

we then obtain from Eq. (2·10)

$$\begin{aligned}\frac{\partial}{\partial\eta}\left(\frac{1}{2}\eta\right)+\frac{\partial}{\partial\eta^*}\left(\frac{1}{2}\eta^*\right) &= -\frac{\partial}{\partial\eta}\langle\phi_0|U(\eta^*, \eta)\frac{\partial}{\partial\eta^*}U^{-1}(\eta^*, \eta)|\phi_0\rangle\\ &\quad+\frac{\partial}{\partial\eta^*}\langle\phi_0|U(\eta^*, \eta)\frac{\partial}{\partial\eta}U^{-1}(\eta^*, \eta)|\phi_0\rangle\\ &=\langle\phi(\eta^*, \eta)|[\mathring{O}(\hat{z}(\eta), \eta^*\eta), \mathring{O}^{\dagger}(\hat{z}(\eta), \eta^*\eta)]|\phi(\eta^*\eta)\rangle,\end{aligned}$$

i.e.,

$$\begin{aligned}&\langle\phi(\eta^*\eta)|[\mathring{O}(\hat{z}(\eta), \eta^*\eta), \mathring{O}^{\dagger}(\hat{z}(\eta), \eta^*\eta)]|\phi(\eta^*, \eta)\rangle\\ &\quad=\langle\phi_0|[\mathring{O}(\hat{z}, \eta^*\eta), \mathring{O}^{\dagger}(\hat{z}, \eta^*\eta)]|\phi_0\rangle=1,\end{aligned} \qquad (2\cdot 12\text{a})$$

where we have used Eq. (2·9b). Hereafter we call Eq. (2·10) the *canonical-variables condition* which leads to the "weak" canonical commutation relation

$$\langle\phi_0|[\mathring{q}(\hat{z}, \eta^*\eta), \mathring{p}(\hat{z}, \eta^*\eta)]|\phi_0\rangle=i \qquad (2\cdot 12\text{b})$$

with

$$\left.\begin{aligned}\mathring{q}(\hat{z}, \eta^*\eta) &= \sqrt{\frac{1}{2}}\{\mathring{O}^{\dagger}(\hat{z}, \eta^*\eta)+\mathring{O}(\hat{z}, \eta^*\eta)\},\\ \mathring{p}(\hat{z}, \eta^*\eta) &= i\sqrt{\frac{1}{2}}\{\mathring{O}^{\dagger}(\hat{z}, \eta^*\eta)-\mathring{O}(\hat{z}, \eta^*\eta)\},\end{aligned}\right\} \qquad (2\cdot 13\text{a})$$

where

$$\begin{aligned}\mathring{q}(\hat{z}(\eta), \eta^*\eta) &= U^{-1}(\eta^*, \eta)\mathring{q}(\hat{z}, \eta^*\eta)U(\eta^*, \eta),\\ \mathring{p}(\hat{z}(\eta), \eta^*\eta) &= U^{-1}(\eta^*, \eta)\mathring{p}(\hat{z}, \eta^*\eta)U(\eta^*, \eta),\end{aligned} \qquad (2\cdot 13\text{b})$$

are the local infinitesimal generators with respect to the collective coordinate α and its conjugate π defined by

$$\left.\begin{aligned}i\frac{\partial}{\partial\alpha}U^{-1}(\eta^*, \eta) &= \mathring{p}(\hat{z}(\eta), \eta^*\eta)U^{-1}(\eta^*, \eta),\\ -i\frac{\partial}{\partial\pi}U^{-1}(\eta^*, \eta) &= \mathring{q}(\hat{z}(\eta), \eta^*\eta)U^{-1}(\eta^*, \eta).\end{aligned}\right\} \qquad (2\cdot 14)$$

§ 3. Invariance principle of the Schrödinger equation

The next task is to determine the vibrational frame as well as the structure of the operators $\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)$ and $\mathring{O}(\hat{z}(\eta), \eta^*\eta)$. For this purpose, we use the *invariance principle of the Schrödinger equation*, which was explained in Paper I[1] in connection with the concept of "maximal decoupled" collective subspace. This principle can be simply stated as follows: The time-dependence of the parameters $(\eta^*(t), \eta(t))$, which specifies the time-variation of the vibrating frame, must be introduced in such a way that the Schrödinger equation always remains invariant. In the variational form, the principle is expressed as

$$\delta_0\langle\phi(\eta^*, \eta)|\left\{\left(i\frac{\partial}{\partial t}-H\right)|\phi(\eta^*, \eta)\rangle\right\}=0 \quad \text{and} \quad \text{h.c.} \tag{3·1}$$

with the boundary condition at $\eta=\eta^*=0$,

$$\left.\begin{aligned}&\delta\langle\phi_0|H|\phi_0\rangle=0, \quad \delta\langle\phi_0|\phi_0\rangle=0\,,\\ &U(\eta^*=0, \eta=0)=1\,,\end{aligned}\right\} \tag{3·2}$$

where the variation $|\delta_0\phi(\eta^*, \eta)\rangle$ is defined by

$$|\delta_0\phi(\eta^*, \eta)\rangle\equiv U^{-1}(\eta^*, \eta)|\delta\phi_0\rangle\,. \tag{3·3}$$

Needless to say, the uniformly rotating frame in the cranking model is one of the simplest which satisfies the invariance principle of the Schrödinger equation.

With the use of Eq. (2·5), Eq. (3·1) can be written as

$$\begin{aligned}&\delta_0\langle\phi(\eta^*, \eta)|H-i\dot{\eta}\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)+i\dot{\eta}^*\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)|\phi(\eta^*, \eta)\rangle\\ &\quad=\delta_0\langle\phi(\eta^*, \eta)|H-\dot{\alpha}\cdot\mathring{p}(\hat{z}(\eta), \eta^*\eta)+\dot{\pi}\cdot\mathring{q}(\hat{z}(\eta), \eta^*\eta)|\phi(\eta^*, \eta)\rangle=0\,.\end{aligned} \tag{3·4}$$

By taking $|\delta_0\phi(\eta^*, \eta)\rangle=i\mathring{q}(\hat{z}(\eta), \eta^*\eta)|\phi(\eta^*, \eta)\rangle$ and $|\delta_0\phi(\eta^*, \eta)\rangle=i\mathring{p}(\hat{z}(\eta), \eta^*\eta)\times|\phi(\eta^*, \eta)\rangle$ as variational directions, respectively, we obtain from Eq. (3·4)

$$\left.\begin{aligned}i\dot{\eta}\ &=-\langle\phi(\eta^*, \eta)|[H, \mathring{O}(\hat{z}(\eta), \eta^*\eta)]|\phi(\eta^*, \eta)\rangle=+\frac{\partial}{\partial\eta^*}\mathcal{H}_c(\eta^*, \eta),\\ i\dot{\eta}^*&=-\langle\phi(\eta^*, \eta)|[H, \mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)]|\phi(\eta^*, \eta)\rangle=-\frac{\partial}{\partial\eta}\mathcal{H}_c(\eta^*, \eta),\end{aligned}\right\} \tag{3·5a}$$

i.e.,

$$\dot{\alpha}=\frac{\partial}{\partial\pi}\mathcal{H}_c(\eta^*, \eta), \quad \dot{\pi}=-\frac{\partial}{\partial\alpha}\mathcal{H}_c(\eta^*, \eta) \tag{3·5b}$$

with

$$\mathcal{H}_c(\eta^*, \eta)\equiv\langle\phi(\eta^*, \eta)|H|\phi(\eta^*, \eta)\rangle-\langle\phi_0|H|\phi_0\rangle\,,$$

where we have used the weak canonical commutation relation (2·12) and the definition (2·6).

Equation (3·4) with Eq. (3·5) is just the generalization of Eq. (2·2) in the simple cranking model into the vibrating frame. The operator

$$H' = H - i\dot{\eta}\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta) + i\dot{\eta}^*\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)$$
$$= H - \dot{\alpha}\cdot\mathring{p}(\hat{z}(\eta), \eta^*\eta) + \dot{\pi}\cdot\mathring{q}(\hat{z}(\eta), \eta^*\eta) \quad (3\cdot6)$$

corresponds to the time-displacement operator describing the time-evolution of the system in the vibrating frame. In this frame, thus the "particle-collective coupling", which organizes the large-amplitude collective motion out of the particle excitations, manifests itself as the coupling $H'-H = -i\dot{\eta}\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta) + i\dot{\eta}^*\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)$. This coupling gives rise to an increase in the energy of the particle motion, which is identified with the collective vibrational energy

$$\mathscr{H}_c(\eta^*, \eta) \equiv \langle\phi(\eta^*, \eta)|H|\phi(\eta^*, \eta)\rangle - \langle\phi_0|H|\phi_0\rangle, \quad (3\cdot7)$$

and is compatible with the canonical equation of motion $(3\cdot5)$ of the collective coordinate and its conjugate.

The invariance principle $(3\cdot1)$ can also be expressed in a variational form for the local generators:

$$\delta_0\langle\phi(\eta^*+\delta\eta^*, \eta+\delta\eta)|\left\{\left(i\frac{\partial}{\partial t} - H\right)|\phi(\eta^*+\delta\eta^*, \eta+\delta\eta)\rangle\right\}$$
$$-\delta_0\langle\phi(\eta^*, \eta)|\left\{\left(i\frac{\partial}{\partial t} - H\right)|\phi(\eta^*, \eta)\rangle\right\} = 0 \quad (3\cdot8a).$$

with the boundary condition $(3\cdot2)$. Since $|\phi(\eta^*+\delta\eta^*, \eta+\delta\eta)\rangle = \{1+\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)\times\delta\eta - \mathring{O}(\hat{z}(\eta), \eta^*\eta)\delta\eta^*\}|\phi(\eta^*, \eta)\rangle$, this equation can be written as

$$\delta_0\langle\phi(\eta^*, \eta)|[H, \{\delta\eta\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta) - \delta\eta^*\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)\}]$$
$$-\left(\frac{\partial}{\partial t}\{i\delta\eta\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta) - i\delta\eta^*\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)\}\right)|\phi(\eta^*, \eta)\rangle = 0, \quad (3\cdot8b)$$

from which we obtain

$$\delta_0\langle\phi(\eta^*, \eta)|[H, \mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)] - \frac{\partial^2\mathscr{H}_c}{\partial\eta\partial\eta^*}\cdot\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)$$
$$-\frac{\partial^2\mathscr{H}_c}{\partial\eta^2}\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta) - \frac{\partial\mathscr{H}_c}{\partial\eta^*}\cdot\frac{\partial}{\partial\eta}\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)$$
$$+\frac{\partial\mathscr{H}_c}{\partial\eta}\cdot\frac{\partial}{\partial\eta^*}\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta)|\phi(\eta^*, \eta)\rangle = 0,$$

$$\delta_0\langle\phi(\eta^*, \eta)|[H, \mathring{O}(\hat{z}(\eta), \eta^*\eta)] + \frac{\partial^2\mathscr{H}_c}{\partial\eta\partial\eta^*}\cdot\mathring{O}(\hat{z}(\eta), \eta^*\eta)$$
$$+\frac{\partial^2\mathscr{H}_c}{(\partial\eta^*)^2}\mathring{O}^\dagger(\hat{z}(\eta), \eta^*\eta) - \frac{\partial\mathscr{H}_c}{\partial\eta^*}\cdot\frac{\partial}{\partial\eta}\mathring{O}(\hat{z}(\eta), \eta^*\eta)$$
$$+\frac{\partial\mathscr{H}_c}{\partial\eta}\cdot\frac{\partial}{\partial\eta^*}\mathring{O}(\hat{z}(\eta), \eta^*\eta)|\phi(\eta^*, \eta)\rangle = 0, \quad (3\cdot9)$$

where we have used Eq. (3·5a). Equation (3·9) is called the equation of path. Here it must be emphasized that Eq. (3·9) is essentially different from a set of fundamental equations of the "local harmonic approach"[5),6),7)] and is *completely equivalent* to Eq. (3·1) itself.

As has been shown in the above discussion, a set of the basic equation in our theory, which must be solved self-consistently, consists of:

(a) *the invariance principle* (3·1)

$$\delta\langle\phi_0|U(\eta^*,\eta)\left(i\frac{\partial}{\partial t}-H\right)U^{-1}(\eta^*,\eta)|\phi_0\rangle=0 \quad \text{and} \quad \text{h.c.,} \tag{I}$$

which is equivalently expressed in the form of the *equation of path* (3·9),

(b) *the canonical-variables condition* (2·10) which is written as

$$\langle\phi_0|\mathring{O}^\dagger(\hat{z},\eta^*\eta)|\phi_0\rangle=\frac{1}{2}\eta^*,$$

$$\langle\phi_0|\mathring{O}(\hat{z},\eta^*\eta)|\phi_0\rangle=\frac{1}{2}\eta, \tag{II}$$

where $\mathring{O}^\dagger(\hat{z},\eta^*\eta)$ and $\mathring{O}(\hat{z},\eta^*\eta)$ are defined by Eq. (2·11b) and satisfy the integrability condition (2·9a). The canonical equation of motion (3·5) is obtained from (I) and (II).

§ 4. A self-consistent solution of the basic equations

In Paper I, a method is given to solve the set of the basic equation (I) (which is expressed in the form of the equation of path (3·9)) and (II), with the explicit use of the integrability condition (2·9a). In this section we show a more general and simple method of solution consistent with the specified boundary condition on our collective motion.

This method is based on the following two lemmata:

Lemma 1 When the infinitesimal generators $\mathring{O}^\dagger(\hat{z},\eta^*\eta)$ and $\mathring{O}(\hat{z},\eta^*\eta)$ are linear functions of the one-body fermion-pair operators $\hat{z}$ and **1**, there exists such a hermitian operator $\widehat{F}(\hat{z},\eta^*\eta)$ that is a linear function of $\hat{z}$ and **1** and satisfies

$$U^{-1}(\eta^*,\eta)=\exp\ \{i\widehat{F}(\hat{z},\eta^*\eta)\}. \tag{4·1}$$

Definition $\hat{x}$ and $\hat{y}$ denote, respectively, a set of all the one-body particle-hole pairs and a set of all the one-body particle-particle and hole-hole pairs under consideration,

$$\hat{x}=\{c_\mu{}^\dagger c_i,\ c_i{}^\dagger c_\mu\},\quad \hat{y}=\{c_\mu{}^\dagger c_\nu,\ c_ic_j{}^\dagger\},\quad \hat{z}=\hat{x}\oplus\hat{y}\ . \tag{4·2}$$

Lemma 2

$$e^{i\hat{F}(\hat{z},\eta^*\eta)}=e^{i\hat{G}(\hat{x},\eta^*\eta)}\cdot e^{i\hat{G}_0(\hat{y},\eta^*\eta)}, \tag{4·3a}$$

where

$$\hat{F}(\hat{z},\eta^*\eta)\in\hat{z}\oplus\{\mathbf{1}\},$$
$$\hat{G}(\hat{x},\eta^*\eta)\in\hat{x},\quad \hat{G}_0(\hat{y},\eta^*\eta)\in\hat{y}\oplus\{\mathbf{1}\}. \tag{4·3b}$$

The proof of each lemma is given in Appendices A and B, respectively. Since $\hat{y}|\phi_0\rangle=0$, we obtain

$$e^{i\hat{G}_0(\hat{y},\eta^*\eta)}|\phi_0\rangle=e^{i\theta(\eta^*,\eta)}|\phi_0\rangle, \tag{4·4}$$

where $\theta(\eta^*,\eta)$ is a c-number function. Because the basic equation (I) is independent of the phase $\theta(\eta^*,\eta)$ by $\delta\langle\phi_0|\phi_0\rangle=0$, we may choose $\theta(\eta^*,\eta)=0$ so that we obtain

$$\delta\langle\phi_0|e^{-i\hat{G}(\hat{x},\eta^*\eta)}\left(i\frac{\partial}{\partial t}-H\right)e^{i\hat{G}(\hat{x},\eta^*\eta)}|\phi_0\rangle=0, \tag{4·5}$$

and the basic equation (II) becomes

$$\langle\phi_0|e^{-i\hat{G}(\hat{x},\eta^*\eta)}\frac{\partial}{\partial\eta}e^{i\hat{G}(\hat{x},\eta^*\eta)}|\phi_0\rangle=\frac{1}{2}\eta^*,$$
$$\langle\phi_0|e^{-i\hat{G}(\hat{x},\eta^*\eta)}\frac{\partial}{\partial\eta^*}e^{i\hat{G}(\hat{x},\eta^*\eta)}|\phi_0\rangle=-\frac{1}{2}\eta. \tag{4·6}$$

In Appendix C it is shown that such a choice of parameter (η^*,η) that satisfies Eq. (4·6) is generally possible. It is now clear that the problem to solve the set of the basic equations (I) and (II) self-consistently can be reduced to finding the hermitian operator $\hat{G}(\hat{x},\eta^*\eta)$ which satisfies Eqs. (4·5) and (4·6).

In order to choose a solution $\hat{G}(\hat{x},\eta^*\eta)$ appropriate for the collective motion under consideration, it is rather convenient to use the complete set of the RPA eigenmodes $\{X_\lambda^\dagger, X_\lambda\}$ instead of the set of the particle-hole pairs $\hat{x}\equiv\{c_\mu^\dagger c_i, c_i^\dagger c_\mu\}$,

$$X_\lambda^\dagger=\sum_{\mu i}\{\psi_\lambda(\mu i)c_\mu^\dagger c_i-\varphi_\lambda(\mu i)c_i^\dagger c_\mu\}$$
$$\langle\phi_0|[X_\lambda, X_{\lambda'}^\dagger]|\phi_0\rangle=\delta_{\lambda\lambda'},\quad \langle\phi_0|[X_\lambda, X_{\lambda'}]|\phi_0\rangle=0,$$
$$\langle\phi_0|[X_\lambda,[H,X_{\lambda'}^\dagger]]|\phi_0\rangle=\omega_\lambda\delta_{\lambda\lambda'}.\quad(\omega_\lambda>0) \tag{4·7}$$

In this case, Eq. (4·5) is written as

$$\langle\phi_0|\left[iX_\lambda^\dagger, e^{-i\hat{G}}\left(H-i\dot{\eta}\frac{\partial}{\partial\eta}-i\dot{\eta}^*\frac{\partial}{\partial\eta^*}\right)e^{i\hat{G}}\right]|\phi_0\rangle=0\quad\text{and}\quad\text{h.c.}, \tag{4·8}$$

which can be decomposed into

$$\langle\phi_0|\left[iX_\lambda^\dagger, e^{-i\hat{G}}\left(H-i\dot{\eta}\frac{\partial}{\partial\eta}-i\dot{\eta}^*\frac{\partial}{\partial\eta^*}\right)e^{i\hat{G}}\right]|\phi_0\rangle=0$$

$$\text{and h.c.,} \quad X_\lambda^\dagger \neq X_{\lambda_0}^\dagger, \tag{4·9a}$$

$$\langle\phi_0|[i\mathring{O}^\dagger, e^{-i\hat{G}}He^{i\hat{G}} - i\eta\cdot\mathring{O}^\dagger + i\eta^*\cdot\mathring{O}]|\phi_0\rangle = 0 \quad \text{and} \quad \text{h.c.,} \tag{4·9b}$$

where

$$\mathring{O}^\dagger \equiv \mathring{O}^\dagger(\hat{x}, \eta^*\eta) = e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}$$

and $X_{\lambda_0}^\dagger$ is the conventional RPA-phonon creation operator with the lowest eigenvalue ω_{λ_0}.*) Since Eq. (4·9b) with Eq. (4·6) leads to the canonical equation of motion (3·5) of the collective variables, Eq. (4·5) is finally reduced to

$$\langle\phi_0|\Bigg[iX_\lambda^\dagger, e^{-i\hat{G}}He^{i\hat{G}} - \left(\frac{\partial\mathcal{H}_c}{\partial\eta^*}\right)\cdot e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}$$

$$+\left(\frac{\partial\mathcal{H}_c}{\partial\eta}\right)\cdot e^{-i\hat{G}}\frac{\partial}{\partial\eta^*}e^{i\hat{G}}\Bigg]|\phi_0\rangle = 0 \quad \text{and h.c.,} \quad \lambda\neq\lambda_0, \tag{4·10}$$

where we have used Eq. (3·5).

With the use of the notations

$$\hat{G}(\hat{x}, \eta^*\eta) = \sum_\lambda\{G^{(\lambda)}(\eta^*\eta)\cdot X_\lambda + G^{(\lambda)*}(\eta^*\eta)\cdot X_\lambda^\dagger\}, \tag{4·11}$$

$$e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}} = i\frac{\partial\hat{G}}{\partial\eta} + \frac{1}{2!}\left[i\frac{\partial\hat{G}}{\partial\eta}, i\hat{G}\right] + \frac{1}{3!}\left[\left[i\frac{\partial\hat{G}}{\partial\eta}, i\hat{G}\right], i\hat{G}\right] + \cdots$$

$$\equiv i\frac{\partial\hat{G}}{\partial\eta} + \sum_{n\geq2}\frac{1}{n!}\Big[\cdots\Big[i\frac{\partial\hat{G}}{\partial\eta}, \overbrace{i\hat{G}\Big], \cdots\Big], i\hat{G}}^{(n-1)}\Big], \tag{4·12}$$

$$e^{-i\hat{G}}He^{i\hat{G}} = H + [H, i\hat{G}] + \frac{1}{2!}[[H, i\hat{G}], i\hat{G}] + \cdots$$

$$\equiv H + \sum_{n\geq1}\frac{1}{n!}[\cdots[H, \overbrace{i\hat{G}], \cdots], i\hat{G}}^{n}], \tag{4·13}$$

Eq. (4·10) is written as

$$\left\{\omega_\lambda G^{(\lambda)} + \frac{\partial G^{(\lambda)}}{\partial\eta}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta^*} - \frac{\partial G^{(\lambda)}}{\partial\eta^*}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta}\right\}$$

$$-\sum_{n\geq2}\frac{1}{n!}\langle\phi_0|[iX_\lambda^\dagger, \{[\cdots[H, \overbrace{i\hat{G}], \cdots], i\hat{G}}^{n}]\}]|\phi_0\rangle$$

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*) When Eq. (4·9a) is satisfied, Eq. (4·9b) becomes equivalent to the equation with the RPA-phonon mode $X_{\lambda_0}^\dagger$,

$$\langle\phi_0|\left[iX_{\lambda_0}, e^{-i\hat{G}}\left(H - i\eta\frac{\partial}{\partial\eta} - i\eta^*\frac{\partial}{\partial\eta^*}\right)e^{i\hat{G}}\right]|\phi_0\rangle = 0 \quad \text{and h.c.}$$

$$+\sum_{m\geq 1}\frac{1}{(2m+1)!}\langle\phi_0|\Big[iX_\lambda^+,\Big\{\Big[\cdots\Big[\Big(i\frac{\partial\hat{G}}{\partial\eta}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta^*}-i\frac{\partial\hat{G}}{\partial\eta^*}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta}\Big),\overbrace{i\hat{G}\Big],\cdots\Big],i\hat{G}}^{2m}\Big]\Big\}\Big]|\phi_0\rangle=0,^{*)}\ \lambda\neq\lambda_0. \tag{4·14}$$

In the same way, Eq. (4·6) is written as

$$\eta^*-\sum_\lambda\Big\{G^{(\lambda)}\cdot\frac{\partial G^{(\lambda)*}}{\partial\eta}-\frac{\partial G^{(\lambda)}}{\partial\eta}\cdot G^{(\lambda)*}\Big\}$$
$$-2\sum_{m\geq 2}\frac{1}{(2m)!}\langle\phi_0|\Big[\cdots\Big[i\frac{\partial\hat{G}}{\partial\eta},\overbrace{i\hat{G}\Big],\cdots\Big],i\hat{G}}^{(2m-1)}\Big]|\phi_0\rangle=0\,. \tag{4·15}$$

Thus, Eqs. (4·14) and (4·15), with

$$\mathcal{H}_c\equiv\langle\phi_0|e^{-i\hat{G}}He^{i\hat{G}}|\phi_0\rangle-\langle\phi_0|H|\phi_0\rangle$$
$$=\sum_{n\geq 1}\frac{1}{n!}\langle\phi_0|[\cdots[H,\overbrace{i\hat{G}],\cdots],i\hat{G}}^{n}]|\phi_0\rangle\,, \tag{4·16}$$

become the basic equations to specify the coefficients $G^{(\lambda)}(\eta^*\eta)$ of $\hat{G}(\hat{x},\eta^*\eta)$ in Eq. (4·11).

We are now at a position to determine the coefficients $G^{(\lambda)}(\eta^*\eta)$ as well as the collective Hamiltonian $\mathcal{H}_c$, which are appropriate for our specified collective motion. To do this, we make the following expansion of $G^{(\lambda)}(\eta^*\eta)$ with respect to (η^*,η):

$$\left.\begin{aligned}G^{(\lambda)}(\eta^*\eta)&=G^{(\lambda)}(1)+G^{(\lambda)}(2)+\cdots=\sum_{n\geq 1}G^{(\lambda)}(n)\,,\\ G^{(\lambda)}(n)&\equiv\sum_{\substack{r,s\\(r+s=n)}}G^{(\lambda)}_{rs}\cdot(\eta^*)^r(\eta)^s\,.\end{aligned}\right\} \tag{4·17}$$

Since the basic equations (4·14) and (4·15) with the (η^*,η)-expansion (4·17) are supposed to be valid for continuous ranges of η^* and η, we can equate the coefficients of each power of (η^*,η) in these equations to zero. Thus, by starting with the coefficients with the lowest power of (η^*,η) and by proceeding to the higher (η^*,η)-coefficients step by step, we can determine the unknown quantities $G^{(\lambda)}_{rs}$ of $G^{(\lambda)}(\eta^*\eta)$ in Eq. (4·17) as well as the collective Hamiltonian $\mathcal{H}_c$ self-consistently.

The important task in this expansion method is the choice of the lowest order term $G^{(\lambda)}(1)$ to satisfy our specified condition on the collective motion. Since the term with the lowest power of (η^*,η) in Eq. (4·15) leads us to

*) In Eq. (4·14) we have used the fact that each term of

$$\sum_{m\geq 1}\frac{1}{(2m)!}\langle\phi_0|\Big[iX_\lambda^+,\Big\{\Big[\cdots\Big[\Big(i\frac{\partial\hat{G}}{\partial\eta}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta^*}-i\frac{\partial\hat{G}}{\partial\eta^*}\cdot\frac{\partial\mathcal{H}_c}{\partial\eta}\Big)\Big],\overbrace{i\hat{G},\cdots\Big],i\hat{G}}^{2m-1}\Big]\Big\}\Big]|\phi_0\rangle$$

always vanishes.

$$\eta^* = \sum_\lambda \left\{ G^{(\lambda)}(1) \cdot \frac{\partial G^{(\lambda)*}(1)}{\partial \eta} - \frac{\partial G^{(\lambda)}(1)}{\partial \eta} \cdot G^{(\lambda)*}(1) \right\}, \tag{4·18}$$

and the term with the lowest power of (η^*, η) in the collective Hamiltonian (4·16) is

$$\begin{aligned} \mathcal{H}_c{}^{(0)} &\equiv \frac{1}{2} \langle \phi_0 | [[H, i\widehat{G}(1)], i\widehat{G}(1)] | \phi_0 \rangle \\ &= \sum_\lambda \omega_\lambda \cdot G^{(\lambda)}(1) G^{(\lambda)*}(1) \end{aligned} \tag{4·19}$$

with

$$\widehat{G}(1) \equiv \sum_\lambda \{ G^{(\lambda)}(1) \cdot X_\lambda + G^{(\lambda)*}(1) \cdot X_\lambda{}^\dagger \}, \tag{4·20}$$

we can choose

$$G^{(\lambda)}(1) = i \cdot \eta^* \cdot \delta_{\lambda\lambda_0}, \quad G^{(\lambda)*}(1) = -i \cdot \eta \cdot \delta_{\lambda\lambda_0} \tag{4·21}$$

so that Eq. (4·18) is satisfied and $\mathcal{H}_c{}^{(0)}$ becomes the RPA-phonon Hamiltonian

$$\mathcal{H}_c{}^{(0)} = \omega_{\lambda_0} \cdot \eta^* \eta \,. \tag{4·22}$$

With the use of (4·21) and (4·22), Eqs. (4·14) and (4·15) can be written in the following forms, respectively:

$$\begin{aligned} &\left\{ \omega_\lambda + \omega_{\lambda_0} \cdot \left(\eta \frac{\partial}{\partial \eta} - \eta^* \frac{\partial}{\partial \eta^*} \right) \right\} G^{(\lambda)} = \left\{ \frac{\partial G^{(\lambda)}}{\partial \eta^*} \cdot \frac{\partial \mathcal{H}_c{}^{(\text{int})}}{\partial \eta} - \frac{\partial G^{(\lambda)}}{\partial \eta} \cdot \frac{\partial \mathcal{H}_c{}^{(\text{int})}}{\partial \eta^*} \right\} \\ &\quad + \sum_{n \geq 2} \frac{1}{n!} \langle \phi_0 | [iX_\lambda{}^\dagger, \{ \overbrace{[\cdots [H, i\widehat{G}], \cdots], i\widehat{G}]}^{n} \}] | \phi_0 \rangle \\ &\quad - \sum_{m \geq 1} \frac{1}{(2m+1)!} \langle \phi_0 | \Bigg[iX_\lambda{}^\dagger, \Bigg\{ \Bigg[\cdots \Bigg[\Bigg(i \frac{\partial \widehat{G}}{\partial \eta} \cdot \frac{\partial \mathcal{H}_c}{\partial \eta^*} \\ &\quad - i \frac{\partial \widehat{G}}{\partial \eta^*} \cdot \frac{\partial \mathcal{H}_c}{\partial \eta} \Bigg), \overbrace{i\widehat{G} \Bigg], \cdots \Bigg], i\widehat{G}}^{2m} \Bigg] \Bigg\} \Bigg] | \phi_0 \rangle, \quad \lambda \neq \lambda_0 , \end{aligned} \tag{4·23}$$

$$\begin{aligned} &\left(1 - \eta \frac{\partial}{\partial \eta} \right) \{ \varDelta G^{(\lambda_0)} \} - \eta^* \frac{\partial}{\partial \eta} \{ \varDelta G^{(\lambda_0)*} \} \\ &\quad = i \cdot \left[\{ \varDelta G^{(\lambda_0)*} \} \cdot \frac{\partial}{\partial \eta} \{ \varDelta G^{(\lambda_0)} \} - \{ \varDelta G^{(\lambda_0)} \} \cdot \frac{\partial}{\partial \eta} \{ \varDelta G^{(\lambda_0)*} \} \right] \\ &\qquad + i \cdot \sum_{\lambda \neq \lambda_0} \left\{ \frac{\partial G^{(\lambda)}}{\partial \eta} \cdot G^{(\lambda)*} - G^{(\lambda)} \cdot \frac{\partial G^{(\lambda)*}}{\partial \eta} \right\} \\ &\qquad - 2i \cdot \sum_{m \geq 2} \frac{1}{(2m)!} \langle \phi_0 | \left[\cdots \left[i \frac{\partial \widehat{G}}{\partial \eta}, \overbrace{i\widehat{G} \right], \cdots \right], i\widehat{G}}^{(2m-1)} \right] | \phi_0 \rangle \equiv f \end{aligned} \tag{4·24}$$

with

$$\varDelta G^{(\lambda_0)} \equiv \sum_{n\geq 2} G^{(\lambda_0)}(n) . \tag{4·25}$$

The quantity $\mathcal{H}_c^{(\text{int})}$ in Eq. (4·23) is defined by

$$\begin{aligned}
\mathcal{H}_c{}^{(\text{int})} &\equiv \mathcal{H}_c - \mathcal{H}_c{}^{(0)} = \omega_0 \cdot \{i\eta^* \varDelta G^{(\lambda_0)*} - i\eta \varDelta G^{(\lambda_0)}\} \\
&\quad + \omega_0 \cdot \varDelta G^{(\lambda_0)} \cdot \varDelta G^{(\lambda_0)*} + \sum_{\lambda\neq\lambda_0} \omega_\lambda \cdot G^{(\lambda)} G^{(\lambda)*} \\
&\quad + \sum_{n\geq 3} \frac{1}{n!} \langle \phi_0 | [\overbrace{\cdots [H, i\widehat{G}], \cdots], i\widehat{G}}^{n}] | \phi_0 \rangle \\
&= h(3) + h(4) + \cdots = \sum_{n\geq 3} h(n) , \\
h(n) &\equiv \sum_{\substack{r,s \\ (r+s=n)}} h_{rs} (\eta^*)^r (\eta)^s .
\end{aligned} \tag{4·26}$$

Comparing the coefficients of (η^*, η) of both the sides of Eq. (4·24), we have

$$(s-1) G_{rs}^{(\lambda_0)} + (s+1) G_{s+1,r-1}^{(\lambda_0)*} = -f_{rs} , \quad (r+s \geq 2) \tag{4·27}$$

where the right-hand side of Eq. (4·24) is symbolically written as

$$f = \sum_n f(n) \equiv \sum_n \cdot \sum_{\substack{r,s \\ (r+s=n)}} f_{rs} \cdot (\eta^*)^r (\eta)^s . \tag{4·28}$$

From Eq. (4·27) and its complex conjugate equation, we obtain

$$G_{rs}^{(\lambda_0)} = -\frac{1}{2(r+s-1)} \{(2-r) f_{rs} + (s+1) f_{s+1,r-1}^*\}_{(r+s\geq 2)} \tag{4·29a}$$

which is formally expressed as

$$G^{(\lambda_0)}(\eta^*\eta) = -\frac{1}{2}\left(\eta\frac{\partial}{\partial\eta} + \eta^*\frac{\partial}{\partial\eta^*} - 1\right)^{-1} \cdot \left\{\left(2 - \eta^*\frac{\partial}{\partial\eta^*}\right) \cdot f + \eta^* \frac{\partial}{\partial\eta} f^* \right\} . \tag{4·29b}$$

In the same sense, Eq. (4·23) can be formally expressed as

$$\begin{aligned}
G^{(\lambda\neq\lambda_0)}(\eta^*\eta) &= \left\{\omega_\lambda + \omega_{\lambda_0} \cdot \left(\eta\frac{\partial}{\partial\eta} - \eta^*\frac{\partial}{\partial\eta^*}\right)\right\}^{-1} \\
&\times \left(\left\{ \frac{\partial G^{(\lambda\neq\lambda_0)}}{\partial\eta^*} \cdot \frac{\partial \mathcal{H}_c{}^{(\text{int})}}{\partial\eta} - \frac{\partial G^{(\lambda\neq\lambda_0)}}{\partial\eta} \cdot \frac{\partial \mathcal{H}_c{}^{(\text{int})}}{\partial\eta^*} \right\} \right. \\
&+ \sum_{n\geq 2} \frac{1}{n!} \langle \phi_0 | [iX_{\lambda\neq\lambda_0}^\dagger, \{[\overbrace{\cdots [H, i\widehat{G}], \cdots], i\widehat{G}}^{n}]\}] | \phi_0 \rangle \\
&- \sum_{m\geq 1} \frac{1}{(2m+1)!} \langle \phi_0 | \Big[iX_{\lambda\neq\lambda_0}^\dagger, \Big\{ \Big[\cdots \Big[\Big(i\frac{\partial\widehat{G}}{\partial\eta} \cdot \frac{\partial\mathcal{H}_c}{\partial\eta^*} \\
&\left. - i\frac{\partial\widehat{G}}{\partial\eta^*} \cdot \frac{\partial\mathcal{H}_c}{\partial\eta} \Big), \overbrace{i\widehat{G}\Big], \cdots\Big], i\widehat{G}}^{2m}\Big]\Big\} \Big] | \phi_0 \rangle \right) .
\end{aligned} \tag{4·30}$$

The expressions (4·29b) and (4·30) of the basic equations are convenient for the (η^*, η)-expansion method. With these equations with the (η^*, η)-expansion we can easily determine the higher order terms $G^{(\lambda)}(n)$ (i.e., $G^{(\lambda)}_{r,s}$ with $r+s=n$) successively, starting with the lowest-order term $G^{(\lambda)}(1)$ given by Eq. (4·21). Thus, for instance, we obtain

$$G^{(\lambda_0)}(2)=0\,, \tag{4·31a}$$

$$G^{(\lambda\neq\lambda_0)}(2)=\left\{\omega_\lambda+\omega_{\lambda_0}\cdot\left(\eta\frac{\partial}{\partial\eta}-\eta^*\frac{\partial}{\partial\eta^*}\right)\right\}^{-1}$$
$$\times\left\{\frac{1}{2}\langle\phi_0|[iX_\lambda^\dagger,\ [[H, i\hat{G}(1)], i\hat{G}(1)]]|\phi_0\rangle\right\}, \tag{4·31b}$$

$$h(3)=\frac{1}{3!}\langle\phi_0|[[[H, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle\,, \tag{4·32}$$

and

$$G^{(\lambda_0)}(3)=-\frac{1}{2}\left(\eta\frac{\partial}{\partial\eta}+\eta^*\frac{\partial}{\partial\eta^*}-1\right)^{-1}$$
$$\times\left\{\left(2-\eta^*\frac{\partial}{\partial\eta^*}\right)f(3)+\eta^*\frac{\partial}{\partial\eta}f^*(3)\right\}, \tag{4·33a}$$

$$G^{(\lambda\neq\lambda_0)}(3)=\left\{\omega_\lambda+\omega_{\lambda_0}\cdot\left(\eta\frac{\partial}{\partial\eta}-\eta^*\frac{\partial}{\partial\eta^*}\right)\right\}^{-1}$$
$$\times\left(\left\{\frac{\partial G^{(\lambda)}(2)}{\partial\eta}\frac{\partial h(3)}{\partial\eta^*}-\frac{\partial G^{(\lambda)}(2)}{\partial\eta^*}\frac{\partial h(3)}{\partial\eta}\right.\right.$$
$$+\frac{1}{2!}\langle\phi_0|[iX_\lambda^\dagger,\ \{[[H, i\hat{G}(2)], i\hat{G}(1)]+[[H, i\hat{G}(1)], i\hat{G}(2)]\}]|\phi_0\rangle$$
$$+\frac{1}{3!}\langle\phi_0|[iX_\lambda^\dagger,\ \{[[[H, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]\}]|\phi_0\rangle$$
$$-\frac{1}{3!}\langle\phi_0|\left[iX_\lambda^\dagger,\ \left\{\left[\left[\left(i\frac{\partial\hat{G}(1)}{\partial\eta}\cdot\frac{\partial\mathcal{H}_c{}^{(0)}}{\partial\eta^*}\right.\right.\right.\right.\right.$$
$$\left.\left.\left.\left.\left.\left.-i\frac{\partial\hat{G}(1)}{\partial\eta^*}\cdot\frac{\partial\mathcal{H}_c{}^{(0)}}{\partial\eta}\right), i\hat{G}(1)\right], i\hat{G}(1)\right]\right\}\right]|\phi_0\rangle\right), \tag{4·33b}$$

$$h(4)=\omega_0\{iG^{(\lambda_0)*}(3)\eta^*-iG^{(\lambda_0)}(3)\eta\}+\sum_{\lambda\neq\lambda_0}\omega_\lambda G^{(\lambda)}(2)G^{(\lambda)*}(2)$$
$$+\frac{1}{4!}\langle\phi_0|[[[[H, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle$$
$$+\frac{1}{3!}\langle\phi_0|\{[[[H, i\hat{G}(2)], i\hat{G}(1)], i\hat{G}(1)]$$

$$+[[[H, i\widehat{G}(1)], i\widehat{G}(2)], i\widehat{G}(1)]+[[[H, i\widehat{G}(1)], i\widehat{G}(1)], i\widehat{G}(2)]\}|\phi_0\rangle, \tag{4·34}$$

where

$$\widehat{G}(n)\equiv\sum_{\lambda}\{G^{(\lambda)}(n)\cdot X_{\lambda}+G^{(\lambda)*}(n)\cdot X_{\lambda}^{\dagger}\}. \tag{4·35}$$

Acknowledgements

The authors express their thanks to Professor M. Yamamura, Professor S. Nishiyama, Dr. K. Matsuyanagi and the members of Theory Division of the Institute for Nuclear Study for their valuable discussions.

Appendix A

——Proof of Lemma 1——

Here we give a proof of Lemma 1 in a rather general form with k real parameters ξ_i $(i=1, 2, \cdots, k)$.

First of all, we notice the following important remark.

[Remark] Let us represent a one-body hermitian operator $\widehat{G}(g)$ as

$$\widehat{G}(g)\equiv\sum_{\alpha\beta} g_{\alpha\beta}c_{\alpha}^{\dagger}c_{\beta} \tag{A1·1}$$

and regard g as an $N\times N$ matrix with $(\alpha=1, 2, \cdots, N)$. We then have the relation

$$[\widehat{G}(g), \widehat{G}(g')]=\widehat{G}([g, g']) \tag{A1·2}$$

which shows an important correspondence

$$\widehat{G}(g) \leftrightarrow g\,. \tag{A1·3}$$

Now, (corresponding to Eqs. (2·13a) and (2·14) with (2·11b)) the infinitesimal generators in our general case are defined by

$$U(\xi)\frac{\partial}{\partial\xi_i}U^{-1}(\xi)=i\widehat{G}(g_i(\xi)), \quad (i=1, 2, \cdots k) \tag{A1·4}$$

with the condition

$$\left.\begin{aligned}&\widehat{G}(g_i)\in\mathfrak{z}\oplus\{\mathbf{1}\}, \quad \widehat{G}^{\dagger}(g_i)=\widehat{G}(g_i),\\ &U(\xi=0)=1\,.\end{aligned}\right\} \tag{A1·5}$$

Since the generators and so $g_i(\xi)$ satisfy the integrability condition, we can obtain the following unitary matrix $u(\xi)$ satisfying

$$u(\xi)\frac{\partial}{\partial\xi_i}u^{-1}(\xi)=ig_i(\xi). \quad (i=1, 2, \cdots, k) \tag{A1·6}$$

Thus, it is always possible to find such a hermitian matrix $g(\xi)$ that satisfies

$$u(\xi)=e^{ig(\xi)}, \quad u(0)=1\,, \tag{A1·7}$$

because $u(\xi)$ is an $N\times N$ matrix.

Corresponding to Eq. (A1·7), let us introduce a unitary operator

$$U_0(\xi)=e^{-i\hat{G}(g(\xi))}, \quad U_0(0)=1\,. \tag{A1·8}$$

Then, with the aid of Eq. (A1·6) and with the use of Eq. (A1·2), we obtain

$$U_0(\xi)\frac{\partial}{\partial\xi_i}U_0^{-1}(\xi)=i\hat{G}(g_i(\xi))\,. \quad (i=1,2,\cdots,k) \tag{A1·9}$$

Since

$$\frac{\partial}{\partial\xi_i}\{U_0^{-1}(\xi)U(\xi)\}=U_0^{-1}(\xi)\{i\hat{G}(g_i)-i\hat{G}(g_i)\}U(\xi)=0,$$

we have

$$U_0^{-1}(\xi)U(\xi)=U_0^{-1}(0)U(0)=1\,. \tag{A1·10}$$

Thus, we have the following lemma:

[*Lemma* 1] When we have Eq. (A1·4) with the condition (A1·5), there always exists such a hermitian operator $\hat{G}(g(\xi))\in z\oplus\{\mathbf{1}\}$ that satisfies

$$U(\xi)=e^{-i\hat{G}(g(\xi))}, \quad U(0)=1\,.$$

Appendix B

——*Proof of Lemma 2*——

Here we give an outline of a proof of Lemma 2.

[*Definition*] Consider an $N\times N$ matrix A with $A_{\alpha\beta}$ $(\alpha,\beta=1,2,\cdots,N)$. When $A_{\alpha\beta}=0$ for $(\alpha>n,\beta\leq n)$ and $(\alpha\leq n,\beta>n)$ with a fixed number n satisfying $n<N$, we call the matrix A an H-type matrix. In the case $A_{\alpha\beta}=0$ for $(\alpha\leq n,$ $\beta\leq n)$ and $(\alpha>n,\beta>n)$, the matrix A is called a K-type matrix.

[*Proposition* 1] For an arbitrary $N\times N$ unitary matrix u, we can choose such a hermitian K-type matrix K that makes $e^{-iK}u$ an H-type matrix, i.e.,

$$u=e^{iK}\cdot e^{iH}, \tag{A2·1}$$

where H is a hermitian H-type matrix.

Before we give a proof of Proposition 1, we here make a few remarks.

[*Remark* 1] For an arbitrary square matrix M with det $M\neq 0$, there exists a unitary matrix u_1 and a positive-definite diagonal matrix h which can be written as $MM^\dagger=u_1h^2u_1^\dagger$, because $MM^\dagger$ is hermitian and its eigenvalues are positive. If we define $u_2 \doteq h^{-1}u_1^\dagger M$, then u_2 becomes a unitary matrix. Thus we can write $M = u_1 h u_2$. For the sake of abbreviation, here we do not give a proof for the case det $M=0$, although we can generally show that there exist such unitary matrices u_1 and u_2 and a non-negative-definite diagonal matrix h that satisfy $M = u_1 h u_2$.

[*Remark* 2] Suppose a matrix $\Gamma_{\mu i}\,(\mu=1, 2, \cdots, n; i=1, 2, \cdots, m; n \geq m; m+n=N)$ and regards $[\gamma_i]_\mu \equiv (\Gamma_{\mu i})\ (i=1, 2, \cdots, m)$ as m vectors with the components $(\mu=1, 2, \cdots, n)$. Then, there always exist such m unitary matrices $u_i\,(i=1, 2, \cdots, m)$ that satisfy

$$\left.\begin{aligned} &[u_m \gamma_m]_\mu = 0 \quad \text{except } \mu=m\,, \\ &[u_{m-1} u_m \gamma_{m-1}]_\mu = 0 \quad \text{except } \mu=m,\ \mu=m-1\,, \\ &[u_{m-1} u_m \gamma_m]_\mu = [u_m \gamma_m]_\mu\,, \end{aligned}\right\} \tag{A2·2}$$

and so on. Thus, it is always possible to make the following matrix:

$$\left.\begin{aligned} &[u_1 u_2 \cdots u_m \gamma_i]_\mu \equiv (u_1 u_2 \cdots u_m \Gamma)_{\mu i} = 0 \\ &\qquad\qquad \text{for} \quad \mu > m\,. \end{aligned}\right\} \tag{A2·3}$$

Now, we can show, with the aid of Remark 1, that there exist such an $n \times n$ unitary matrix u_I and an $m \times m$ unitary matrix u_{II} that satisfy

$$(u_I \Gamma u_{II})_{\mu i} = h_i \delta_{\mu i}^{[m]}\,, \tag{A2·4a}$$

where

$$\delta_{\mu i}^{[m]} = \delta_{\mu i}, \quad (\mu \leq m) \qquad \delta_{\mu i}^{[m]} = 0\,. \quad (\mu > m) \tag{A2·4b}$$

[*Remark* 3] When we represent an $N \times N$ hermitian K-type matrix in a form

$$K = \begin{pmatrix} 0 & k \\ k^\dagger & 0 \end{pmatrix} \tag{A2·5a}$$

with

$$\begin{aligned} K_{\alpha\beta} &= k_{\alpha\beta}, \quad (\alpha \leq n, \beta > n) \\ K_{\alpha\beta} &= k_{\alpha\beta}^\dagger, \quad (\alpha > n, \beta \leq n) \end{aligned} \tag{A2·5b}$$

we obtain

$$e^{iK} = \begin{pmatrix} \cos\sqrt{kk^\dagger}\,, & i\dfrac{\sin\sqrt{kk^\dagger}}{\sqrt{kk^\dagger}} \cdot k \\ i\dfrac{\sin\sqrt{k^\dagger k}}{\sqrt{k^\dagger k}} \cdot k^\dagger, & \cos\sqrt{k^\dagger k} \end{pmatrix}. \tag{A2·6}$$

[*Outline of a Proof of Proposition* 1]

For any unitary matrix v with the condition $v_{\alpha\beta} = 0\,(\alpha \leq n$ and $\beta > n)$, we always obtain $v_{\alpha\beta} = 0\,(\alpha > n$ and $\beta \leq n)$ by definition. For a proof of Proposition 1, therefore, it is necessary and enough to show

$$(e^{-iK}u)_{\alpha\beta}=0, \quad (\alpha\leq n \text{ and } \beta>n) \tag{A2·7}$$

where K is the hermitian K-type matrix. With the use of Remark 3, the condition (A2·7) can be written as

$$\cos\sqrt{kk^\dagger}\cdot a=i\frac{\sin\sqrt{kk^\dagger}}{kk^\dagger}\cdot k\cdot b\,, \tag{A2·8}$$

where k, a and b are $n\times m, n\times m$ and $m\times m$ matrices with $m=N\text{-}n$, respectively, and are defined as

$$\left.\begin{array}{l} k_{\alpha\beta}=K_{\alpha\beta},\quad a_{\alpha\beta}=u_{\alpha\beta} \quad \text{for} \quad \alpha\leq n \text{ and } \beta>n\,, \\ b_{\alpha\beta}=u_{\alpha\beta} \quad \text{for} \quad \alpha>n \text{ and } \beta>n\,. \end{array}\right\} \tag{A2·9}$$

For the sake of abbreviation, here we show that there exists a solution k for Eq. (A2·8) in the case det $b\neq 0$. (An extension of this method to the case det $b=0$, however, is straightforward.) With the use of Remark 2, we can write the $n\times m$ matrix ab^{-1} as

$$(ab^{-1})_{\mu i}=\sum_{\nu=1}^{n}\cdot\sum_{j=1}^{m}(u_1)_{\mu\nu}\cdot[h_j\delta_{\nu j}^{[m]}]\cdot(u_2)_{ji}\,. \tag{A2·10}$$

The form of Eq. (2·8) shows that the matrix k can be put, with the same unitary matrices u_1 and u_2, in the following form:

$$k_{\mu i}=\sum_{\nu}\sum_{j}(u_1)_{\mu\nu}\cdot[\theta_j\delta_{\nu j}^{[m]}]\cdot(u_2)_{ji}\,. \tag{A2·11}$$

Then Eq. (2·8) can be written as

$$h_j\cdot\cos|\theta_j|=i\cdot\frac{\theta_j}{|\theta_j|}\cdot\sin|\theta_j|. \quad (j=1,2,\cdots,m) \tag{A2·12}$$

Thus, we may choose θ_j as that satisfying

$$\tan|\theta_j|=|h_j|, \quad \arg h_j=\frac{\pi}{2}+\arg\theta_j\,. \tag{A2·13}$$

(q.e.d.)

We are now at a position to give a proof of the following lemma:

[*Lemma* 2] When an $N\times N$ hermitian matrix g is given, there exist such hermitian H-type and K-type matrices, H and K, that satisfy

$$e^{i\hat{G}(g)}=e^{i\hat{G}(K)}\cdot e^{i\hat{G}(H)}\,, \tag{A2·14}$$

where

$$\hat{G}(A)=\sum_{\alpha\beta}A_{\alpha\beta}c_\alpha^\dagger c_\beta\,.$$

Proof According to Proposition 1, we choose the hermitian matrices K and H to satisfy $e^{ig}=e^{iK}\cdot e^{iH}$. Since we have

$$e^{i\hat{G}(g)}c_\alpha e^{-i\hat{G}(g)}=\sum_\beta (e^{-ig})_{\alpha\beta}c_\beta\,, \tag{A2·15}$$

we obtain the following relations:

$$[e^{-i\hat{G}(H)}\cdot e^{-i\hat{G}(K)}\cdot e^{i\hat{G}(g)},\ c_\alpha]=0\,,$$
$$[e^{-i\hat{G}(H)}\cdot e^{-i\hat{G}(K)}\cdot e^{i\hat{G}(g)},\ c_\alpha^\dagger]=0\,, \tag{A2·16}$$

which imply that $e^{-i\hat{G}(H)}\cdot e^{-i\hat{G}(K)}\cdot e^{i\hat{G}(g)}$ is a c-number. Since we have

$$\widehat{G}(g)\,|0\rangle=\widehat{G}(H)\,|0\rangle=\widehat{G}(K)\,|0\rangle=0 \tag{A2·17}$$

for the "vacuum" state $|0\rangle$ satisfying $c_\alpha|0\rangle=0$, this c-number is unity.

Appendix C

——*Canonical-Variables Condition*——

Here we show the possibility of choice of such collective parameters that satisfy the canonical-variables condition (2·10) in a rather general way with $2N$ real parameters ξ_i $(i=1, 2, \cdots, 2N)$.

To do this, it is convenient to use the following theorem of Frobenius and Darboux:

THEOREM When

$$\omega=\sum_{i=1}^{2N} f_i(\xi)\,d\xi_i \quad\text{and}\quad \det{}_{2N}\left\{\frac{\partial f_j}{\partial \xi_i}-\frac{\partial f_i}{\partial \xi_j}\right\}\neq 0\,, \tag{A3·1}$$

there exist such variables $(p_r(\xi), q_r(\xi))$ $(r=1, 2, \cdots, N)$ that satisfy

$$\omega=\sum_{r=1}^{N} p_r dq_r\,. \tag{A3·2}$$

Proof of the theorem For the sake of abbreviation, here we give a proof for the case $N=1$. (For the general case, see Ref. 8).) Consider an equation

$$f_1(\xi_1, \xi_2)\frac{d\xi_1}{d\xi_2}+f_2(\xi_1, \xi_2)=0 \tag{A3·3}$$

and represent its solution as

$$\xi_1=\xi_1(\xi_1^0, \xi_2)\,, \tag{A3·4}$$

where ξ_1^0 is the initial value at $\xi_2=0$. With the variables transformation from (ξ_1, ξ_2) to (ξ_1^0, ξ_2), we then obtain the following relation:

$$\omega = f_1 d\xi_1 + f_2 d\xi_2$$
$$= f_1\left(\frac{\partial\xi_1}{\partial\xi_1{}^0}d\xi_1{}^0 + \frac{\partial\xi_1}{\partial\xi_2}d\xi_2\right) + f_2 d\xi_2$$
$$= f_1\frac{\partial\xi_1}{\partial\xi_1{}^0}d\xi_1{}^0\,, \tag{A3·5}$$

where we have used Eq. (A3·3). Thus we can set up

$$p = f_1\frac{\partial\xi_1}{\partial\xi_1{}^0}, \quad q = \xi_1{}^0 \tag{A3·6}$$

so that $\omega = pdq$.

[*Corollary*] For any function $S(P,Q)$, we have

$$\omega = \sum_{i=1}^{2N} f_i(\xi)\,d\xi_i = \sum_{r=1}^{N} P_r dQ_r + dS(P,Q)\,. \tag{A3·7}$$

Proof There exist such variables (p_r, q_r) $(r=1,2,\cdots,N)$ that satisfy both $\sum_i f_i d\xi_i = \sum_r p_r dq_r$ and $\sum_r P_r dQ_r + dS(P,Q) = \sum_r p_r dq_r$. Thus we obtain $(P_r(\xi), Q_r(\xi))$ $(r=1,2,\cdots,N)$ from $(p_r(\xi), q_r(\xi))$ and $(P_r(p,q), Q_r(p,q))$.

We are now at a position to show the possibility of choice of the collective parameters which satisfy the canonical variables condition (2·10). Let us define the infinitesimal generators of a unitary operator $U(\xi)$ by

$$\mathring{G}_{\xi_i} = U(\xi)\frac{1}{i}\frac{\partial}{\partial\xi_i}U^{-1}(\xi), \quad (i=1,2,\cdots 2N) \tag{A3·8}$$

and represent their expectation value with respect to $|\phi_0\rangle$ by

$$\langle\phi_0|\mathring{G}_{\xi_i}|\phi_0\rangle \equiv F_{\xi_i}\,. \tag{A3·9}$$

With the use of the integrability condition $\partial^2 U^{-1}(\xi)/\partial\xi_i\cdot\partial\xi_j = \partial^2 U^{-1}(\xi)/\partial\xi_j\cdot\partial\xi_i$, we then obtain the following equation:

$$\frac{\partial}{\partial\xi_i}(F_{\xi_j}) - \frac{\partial}{\partial\xi_j}(F_{\xi_i}) = -i\langle\phi_0|[\mathring{G}_{\xi_i}, \mathring{G}_{\xi_j}]|\phi_0\rangle\,. \tag{A3·10}$$

According to the theorem of Frobenius and Darboux, it is possible to choose such variables (p_r, q_r) $(r=1,2,\cdots,N)$ for any $S(p,q)$, which satisfy

$$-\sum_{i=1}^{2N} F_{\xi_i} d\xi_i = \sum_{r=1}^{N} p_r dq_r + dS(p,q), \tag{A3·11}$$

so that we have

$$-\sum_i F_{\xi_i}\frac{\partial\xi_i}{\partial q_r} = p_r + \frac{\partial S}{\partial q_r}, \quad -\sum F_{\xi_i}\frac{\partial\xi_i}{\partial p_r} = \frac{\partial S}{\partial p_r}\,. \tag{A3·12}$$

We now introduce the following infinitesimal generators:

$$\left.\begin{aligned}\mathring{q}_r &\equiv U(\xi(pq))\frac{1}{i}\frac{\partial}{\partial p_r}U^{-1}(\xi(p,q)),\\ \mathring{p}_r &\equiv -U(\xi(pq))\frac{1}{i}\frac{\partial}{\partial q_r}U^{-1}(\xi(p,q)).\end{aligned}\right\} \quad \text{(A3·13)}$$

We then obtain

$$\left.\begin{aligned}\langle\phi_0|\mathring{q}_r|\phi_0\rangle &= \sum_i \frac{\partial\xi_i}{\partial p_r}\langle\phi_0|\mathring{G}_{\xi_i}|\phi_0\rangle = \sum_i F_{\xi_i}\cdot\frac{\partial\xi_i}{\partial p_r} = -\frac{\partial S}{\partial p_r},\\ \langle\phi_0|\mathring{p}_r|\phi_0\rangle &= -\sum_i \frac{\partial\xi_i}{\partial q_r}\langle\phi_0|\mathring{G}_{\xi_i}|\phi_0\rangle = -\sum_i F_{\xi_i}\cdot\frac{\partial\xi_i}{\partial q_r} = p_r + \frac{\partial S}{\partial q_r}.\end{aligned}\right\} \quad \text{(A3·14)}$$

Equation (A3·10) for the new variables (p_r, q_r) now becomes

$$\left.\begin{aligned}&\langle\phi_0|[\mathring{q}_r, \mathring{q}_s]|\phi_0\rangle = 0, \quad \langle\phi_0|[\mathring{p}_r, \mathring{p}_s]|\phi_0\rangle = 0,\\ &\langle\phi_0|[\mathring{q}_r, \mathring{p}_s]|\phi_0\rangle = i\delta_{rs}. \quad (r, s = 1, 2, \cdots, N)\end{aligned}\right\} \quad \text{(A3·15)}$$

In Eq. (A3·14), when we adopt

$$\left.\begin{aligned}&S = -\frac{1}{2}\sum_r p_r q_r,\\ &q_r \equiv \alpha_r = \frac{1}{\sqrt{2}}\{\eta_r^* + \eta_r\}, \quad p_r \equiv \pi_r = \frac{1}{\sqrt{2}}i\{\eta_r^* - \eta_r\},\end{aligned}\right\} \quad \text{(A3·16)}$$

we obtain Eq. (2·10) with (2·13a) in the general form.

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