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Optimum Collective Submanifold in Resonant Cases by the Self-Consistent Collective-Coordinate Method for Large-Amplitude Collective Motion*)

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With the purpose of clarifying characteristic difference of the optimum collective submanifolds between in *nonresonant* and *resonant* cases, we propose an improved method of solving the basic equations of the self-consistent collective-coordinate (SCC) method, which describes optimum ("maximally-decoupled") large-amplitude collective motion within the time-dependent Hartree-Fock theory. It is shown that, in the resonant cases, there inevitably arise *essential coupling terms* which break the maximal-decoupling property of the collective motion, so that we have to extend the optimum collective submanifold so as to properly treat the degrees of freedom bringing about the resonances. An illustrative example is given with a simple model Hamiltonian.

§ 1. Introduction and summary

The self-consistent collective-coordinate (SCC) method[1),**)] has been proposed as a microscopic theory to properly define *global* collective coordinates which specify an "optimum" collective submanifold in the huge-dimensional time-dependent Hartree-Fock (TDHF) manifold. The basic principle of the SCC method is to define the optimum collective submanifold (surface) in such a way that the expectation value of the Hamiltonian with the TDHF wave function is *stationary* at each point on the surface with respect to variations perpendicular to the surface. This principle is called the *maximal-decoupling condition* and has been formulated in the form named the *invariance principle of the time-dependent Schrödinger equation.*[1)~3)] The global collective coordinates are thus defined as canonical variables to specify the optimum surface, and the collective Hamiltonian is simply given by the expectation value of the Hamiltonian *on the surface.*

The basic equations of the SCC method have been proved to be of the very simple form, and self-consistent solutions of the set of the basic equations have been easily obtained in terms of the power series expansion of the basic equations with respect to the collective variables.[1),2)] In this expansion method, it is necessary to set up a specific "boundary condition" characterizing the collective motion under consideration. Supposing the large-amplitude collective vibration in soft nuclei, for example, we may set up the boundary condition in such a way that the large-amplitude

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**) The detailed and self-contained explanation of the basic idea of the SCC method and its recent development are given in Refs. 2) and 3), respectively.

collective motion is connected with the lowest-energy RPA ("phonon") mode in the "small-amplitude" (harmonic) limit. With this boundary condition, it has been shown that the set of the basic equations can be uniquely solved, provided that the frequency of the RPA phonon mode is in a *nonresonant case.* In this nonresonant case, the frequency of the RPA phonon mode *does not* satisfy the *resonance condition*

$$\omega_{\lambda\neq0}-n_0\omega_{\lambda=0}\simeq 0\,, \qquad n_0=2, 3, \cdots, \tag{1·1}$$

$\omega_{\lambda=0}$ and $\omega_\lambda(\lambda=1, 2, \cdots)$ being the frequencies of the RPA phonon mode and the other RPA normal modes, respectively.

In the realistic large-amplitude collective motion of soft nuclei, however, we may often encounter the *resonant cases* satisfying Eq. (1·1).[4] In such resonant cases, the power-series expansion method with respect to the collective variables has the well-known difficulty of small denominator in the expansion series, and we have to properly take into account the degrees of freedom which bring about the resonance difficulty in the power series expansion.

With the purpose of investigating behaviour of the optimum collective submanifold in the resonant cases, in this paper we propose an improved method of solving the basic equations of the SCC method. In § 2, the SCC method is recapitulated in a form suitable for our purpose. The basic idea of the improved method is to employ a specific representation of the collective (canonical) variables, in which the collective Hamiltonian in the nonresonant cases is brought into a normal (diagonal) form in the collective variables. This representation is just the c-number version of the "physical boson" representation[5),6)] where the optimum collective Hamiltonian has a diagonal form with respect to the number of physical bosons. It is shown in § 3 that we can easily obtain the normal (diagonal) collective Hamiltonian in the nonresonant cases, by positively making use of the degrees of freedom in the canonical-variable condition for collective variables. In the resonant case, the initially chosen collective submanifold has to be extended so as to include a new set of canonical variables responsible for the resonance. This is formulated in § 4, and it is shown that the optimum collective Hamiltonian in the extended submanifold can never be expressed in the normal (diagonal) form within the representation of the collective variables which have the boundary condition to be connected with RPA modes in the small-amplitude limit. Then, the collective Hamiltonian inevitably has to have *off-diagonal coupling terms* originating from the resonances. An illustrative example is given in § 5 with a simple model Hamiltonian.

§ 2. Basic equations of the SCC method

We start with the basic equation of the TDHF theory,

$$\delta\langle\phi(t)|\left[i\frac{\partial}{\partial t}-\hat{H}\right]|\phi(t)\rangle=0\,,^{*)} \tag{2·1}$$

where the time-dependent Slater determinant $|\phi(t)\rangle$ is given by

*) Throughout this paper, we adopt the convention of using $\hbar=1$.

$$|\phi(t)\rangle = e^{i\hat{F}(t)}|\phi_0\rangle \cdot e^{-iE_0 t},$$
$$\hat{F}(t) = \sum_{\mu i}\{f_{\mu i}(t)a_\mu{}^\dagger b_i{}^\dagger + f_{\mu i}^*(t)b_i a_\mu\}. \tag{2·2}$$

Here $|\phi_0\rangle$ denotes the Hartree-Fock ground state with energy $E_0 = \langle\phi_0|\hat{H}|\phi_0\rangle$, and $a_\mu{}^\dagger$ and $b_i{}^\dagger$ represent the particle- and hole-creation operators with respect to $|\phi_0\rangle$:

$$a_\mu|\phi_0\rangle = 0, \qquad \mu = 1, 2, \cdots, M,$$
$$b_i|\phi_0\rangle = 0, \qquad i = 1, 2, \cdots, N. \tag{2·3}$$

$M(N)$ being a number of single-particle (hole) states under consideration.

Through a variable transformation $f_{\mu i} = f_{\mu i}(C^*, C)$, it is always possible[7] to introduce a set of canonical variables $\{C_{\mu i}^*, C_{\mu i}\}$, by which the TDHF equation (2·1) can be expressed as the canonical equations of motion in classical mechanics:

$$i\dot{C}_{\mu i} = \partial H/\partial C_{\mu i}^*, \qquad i\dot{C}_{\mu i}^* = -\partial H/\partial C_{\mu i},$$
$$H \equiv \langle\phi_0|e^{-i\hat{F}}\hat{H}e^{i\hat{F}}|\phi_0\rangle. \tag{2·4}$$

The condition for the variables $\{C_{\mu i}^*, C_{\mu i}\}$ to be *canonical* is that their local infinitesimal generators

$$\hat{O}_{\mu i}^\dagger \equiv e^{-i\hat{F}}\frac{\partial}{\partial C_{\mu i}}e^{i\hat{F}}, \qquad \hat{O}_{\mu i} \equiv -e^{-i\hat{F}}\frac{\partial}{\partial C_{\mu i}^*}e^{i\hat{F}} \tag{2·5}$$

have to satisfy the "weak" boson-like commutation relations

$$\langle\phi_0|[\hat{O}_{\mu i}, \hat{O}_{\nu j}^\dagger]|\phi_0\rangle = \delta_{\mu\nu}\delta_{ij}, \qquad \langle\phi_0|[\hat{O}_{\mu i}, \hat{O}_{\nu j}]|\phi_0\rangle = 0. \tag{2·6}$$

Since the TDHF equation (2·1) can be written as

$$\delta\langle\phi_0|i\sum_{\mu i}(\dot{C}_{\mu i}\hat{O}_{\mu i}^\dagger - \dot{C}_{\mu i}^*\hat{O}_{\mu i}) - e^{-i\hat{F}}\hat{H}e^{i\hat{F}}|\phi_0\rangle = 0, \tag{2·7}$$

we can easily see that, with the use of Eq. (2·6), the canonical equations of motion (2·4) are derived from the TDHF equation (2·7), by taking $|\delta\phi_0\rangle \propto :\hat{O}_{\mu i}:|\phi_0\rangle$ and $:\hat{O}_{\mu i}^\dagger:|\phi_0\rangle$.

One of the simplest choices of the canonical variables $\{C_{\mu i}^*, C_{\mu i}\}$ satisfying Eq. (2·6) is[7]

$$C_{\mu i} = \sum_\nu\left[\frac{\sin\sqrt{FF^\dagger}}{\sqrt{FF^\dagger}}\right]_{\mu\nu}\cdot F_{\nu i}, \qquad C_{\mu i}^* = \sum_\nu F_{\nu i}^*\cdot\left[\frac{\sin\sqrt{FF^\dagger}}{\sqrt{FF^\dagger}}\right]_{\nu\mu},$$
$$(F)_{\mu i} = F_{\mu i}, \qquad (F^\dagger)_{i\mu} = F_{\mu i}^*, \tag{2·8}$$

which is derived by the so-called "canonical-variable condition"[1),2)]

$$\langle\phi_0|\hat{O}_{\mu i}^\dagger|\phi_0\rangle = \frac{1}{2}C_{\mu i}^*, \qquad \langle\phi_0|\hat{O}_{\mu i}|\phi_0\rangle = \frac{1}{2}C_{\mu i}. \tag{2·9}$$

The set of canonical variables $\{C_{\mu i}^*, C_{\mu i}\}$ thus determined is known[7] to be the c-number correspondent of the set of Holstein-Primakoff-type bosons $\{B_{\mu i}^\dagger, B_{\mu i}\}$ employed in the nuclear boson-expansion theory.[8]

The SCC method intends to extract an optimum collective surface (submanifold) out of the TDHF phase space (manifold) characterized by $\{C^*_{\mu i}, C_{\mu i}\}$, in such a way that the Hamiltonian H is *stationary at each point on the surface* with respect to variations perpendicular to the surface. Supposing the dimension of the surface to be $2L$ which is much smaller than the dimension $2MN$ of the TDHF phase space, we may introduce L-pairs of global collective variables $\{\eta_\alpha^*, \eta_\alpha; \alpha=1, 2, \cdots L\}$ to specify the surface. The canonical variables $\{C^*_{\mu i}, C_{\mu i}\}$ *on the surface* are then regarded as functions of the collective variables $\{\eta_\alpha^*, \eta_\alpha\}$:

$$[C_{\mu i}] \equiv c_{\mu i}(\eta^*, \eta)\,, \qquad [C^*_{\mu i}] \equiv c^*_{\mu i}(\eta^*, \eta)\,. \tag{2·10}$$

For any function K of the canonical variables $\{C^*_{\mu i}, C_{\mu i}\}$, hereafter, we use a symbol $[K]$ to denote the function *on the surface*:

$$[K] = k(\eta^*, \eta)\,. \tag{2·11}$$

In the neighborhood of the surface , thus, the TDHF equation (2·7) is reduced to

$$\delta\langle\phi_0|i\sum_\alpha(\dot\eta_\alpha\hat{O}_\alpha{}^\dagger - \dot\eta_\alpha{}^*\hat{O}_\alpha) - e^{-i[\hat F]}\hat{H}e^{i[\hat F]}|\phi_0\rangle = 0\,, \tag{2·12}$$

where $\hat{O}_\alpha{}^\dagger$ and $\hat{O}_\alpha$ are the local infinitesimal generators with respect to the collective variables, defined by

$$\begin{aligned}
\hat{O}_\alpha{}^\dagger &= e^{-i[\hat F]}\frac{\partial}{\partial\eta_\alpha}e^{i[\hat F]} \\
&= \sum_{\mu i}\left\{\frac{\partial[C_{\mu i}]}{\partial\eta_\alpha}[\hat{O}^\dagger_{\mu i}] - \frac{\partial[C^*_{\mu i}]}{\partial\eta_\alpha}[\hat{O}_{\mu i}]\right\}, \\
\hat{O}_\alpha &= -e^{-i[\hat F]}\frac{\partial}{\partial\eta_\alpha{}^*}e^{i[\hat F]} \\
&= -\sum_{\mu i}\left\{\frac{\partial[C_{\mu i}]}{\partial\eta_\alpha{}^*}[\hat{O}^\dagger_{\mu i}] - \frac{\partial[C^*_{\mu i}]}{\partial\eta_\alpha{}^*}[\hat{O}_{\mu i}]\right\}.
\end{aligned} \tag{2·13}$$

Equation (2·12) is just the starting basic equation of the SCC method, which is called the *invariance principle of the time-dependent Schrödinger equation.*[1),2),9)]

The condition for the global collective variables $\{\eta_\alpha^*, \eta_\alpha\}$ to be *canonical* is that the weak boson-like commutation relations

$$\langle\phi_0|[\hat{O}_\alpha, \hat{O}_\beta{}^\dagger]|\phi_0\rangle = \delta_{\alpha\beta}\,, \qquad \langle\phi_0|[\hat{O}_\alpha, \hat{O}_\beta]|\phi_0\rangle = 0 \tag{2·14}$$

have to be satisfied: By taking the variation $|\delta\phi_0\rangle$ in Eq. (2·12) to be collective directions $|\delta_\parallel\phi_0\rangle \propto :\hat{O}_\alpha:|\phi_0\rangle$ and $:\hat{O}_\alpha{}^\dagger:|\phi_0\rangle$, with the use of Eq. (2·14), we obtain the *canonical equations of collective motion*

$$\begin{aligned}
&i\dot\eta_\alpha = \partial[H]/\partial\eta_\alpha{}^*\,, \qquad i\dot\eta_\alpha{}^* = -\partial[H]/\partial\eta_\alpha\,, \\
&[H] = \langle\phi_0|e^{-i[\hat F]}\hat{H}e^{i[\hat F]}|\phi_0\rangle\,,
\end{aligned} \tag{2·15a}$$

i.e.,

$$\begin{aligned}
&\dot q_\alpha = \partial[H]/\partial p_\alpha\,, \qquad \dot p_\alpha = -\partial[H]/\partial q_\alpha\,, \\
&q_\alpha = (\eta_\alpha{}^* + \eta_\alpha)/\sqrt{2}\,, \qquad p_\alpha = i(\eta_\alpha{}^* - \eta_\alpha)/\sqrt{2}\,.
\end{aligned} \tag{2·15b}$$

By taking the variation $|\delta\phi_0\rangle$ in Eq. (2·12) to be perpendicular to the collective directions, i.e., $|\delta_\perp\phi_0\rangle$ satisfying $\langle\delta_\perp\phi_0|\delta_\parallel\phi_0\rangle=0$, we also obtain from Eq. (2·12)

$$\delta_\perp\langle\phi_0|e^{-i[\hat{F}]}\hat{H}e^{i[\hat{F}]}|\phi_0\rangle=0\,, \tag{2·16}$$

which explicitly demonstrates that the Hamiltonian H on the surface, i.e., $[H]$, has to be stationary with respect to the variations perpendicular to the surface. With the aid of the equations of collective motion (2·15a), Eq. (2·16) can be written as

$$\text{[I]}\quad \begin{aligned}&\delta\langle\phi_0|e^{-i[\hat{F}]}\hat{H}e^{i[\hat{F}]}-\sum_\alpha\left(\frac{\partial[H]}{\partial\eta_\alpha{}^*}\right)\hat{O}_\alpha{}^\dagger-\sum_\alpha\left(\frac{\partial[H]}{\partial\eta_\alpha}\right)\hat{O}_\alpha|\phi_0\rangle\\ &\equiv\delta\langle\phi_0|e^{-i[\hat{F}]}\left\{\hat{H}-\sum_\alpha\left(\frac{\partial[H]}{\partial\eta_\alpha{}^*}\right)\frac{\partial}{\partial\eta_\alpha}+\sum_\alpha\left(\frac{\partial[H]}{\partial\eta_\alpha}\right)\frac{\partial}{\partial\eta_\alpha{}^*}\right\}e^{i[\hat{F}]}|\phi_0\rangle=0\,,\end{aligned} \tag{2·17}$$

which is called the *equation of collective submanifold* and is denoted by [I] hereafter.

So far we have seen that the condition (2·14) for the generators $\{\hat{O}_\alpha{}^\dagger, \hat{O}_\alpha\}$ enables us to decompose the basic equation (2·12) into a) the canonical equations of collective motion (2·15) and b) the equation of collective submanifold [I]. It has been proved[1),2)] that the generators $\{\hat{O}_\alpha{}^\dagger, \hat{O}_\alpha\}$ which have to satisfy the condition (2·14) are generally determined through the relations:

$$\text{[II]}\quad \begin{aligned}&\langle\phi_0|\hat{O}_\alpha{}^\dagger|\phi_0\rangle=\frac{1}{2}\eta_\alpha{}^*+i\frac{\partial}{\partial\eta_\alpha}S(\eta^*,\eta)\,,\\ &\langle\phi_0|\hat{O}_\alpha|\phi_0\rangle=\frac{1}{2}\eta_\alpha-i\frac{\partial}{\partial\eta_\alpha{}^*}S(\eta^*,\eta)\,,\end{aligned} \tag{2·18}$$

where $S(\eta^*, \eta)$ is an arbitrary real function of the collective variables $\{\eta_\alpha{}^*, \eta_\alpha\}$. From Eq. (2·18), we can easily obtain the condition (2·14) through

$$\begin{aligned}&i\left\{\frac{\partial}{\partial\eta_\alpha{}^*}\left(\frac{\partial}{\partial\eta_\beta}S\right)-\frac{\partial}{\partial\eta_\beta}\left(\frac{\partial}{\partial\eta_\alpha{}^*}S\right)\right\}=\frac{\partial}{\partial\eta_\alpha{}^*}\left\{\langle\phi_0|\hat{O}_\beta{}^\dagger|\phi_0\rangle-\frac{1}{2}\eta_\beta{}^*\right\}\\ &\quad+\frac{\partial}{\partial\eta_\beta}\left\{\langle\phi_0|\hat{O}_\alpha|\phi_0\rangle-\frac{1}{2}\eta_\alpha\right\}=\langle\phi_0|[\hat{O}_\alpha, \hat{O}_\beta{}^\dagger]|\phi_0\rangle-\delta_{\alpha\beta}=0\,,\\ &i\left\{\frac{\partial}{\partial\eta_\beta}\left(\frac{\partial}{\partial\eta_\alpha}S\right)-\frac{\partial}{\partial\eta_\alpha}\left(\frac{\partial}{\partial\eta_\beta}S\right)\right\}=\frac{\partial}{\partial\eta_\beta}\left\{\langle\phi_0|\hat{O}_\alpha{}^\dagger|\phi_0\rangle-\frac{1}{2}\eta_\alpha{}^*\right\}\\ &\quad-\frac{\partial}{\partial\eta_\alpha}\left\{\langle\phi_0|\hat{O}_\beta{}^\dagger|\phi_0\rangle-\frac{1}{2}\eta_\beta{}^*\right\}=\langle\phi_0|[\hat{O}_\alpha{}^\dagger, \hat{O}_\beta{}^\dagger]\phi_0\rangle=0\,.\end{aligned} \tag{2·19}$$

We may thus express the condition (2·14) in the following form:

$$\begin{aligned}&\frac{\partial T_\alpha{}^*}{\partial\eta_\beta}+\frac{\partial T_\beta}{\partial\eta_\alpha{}^*}=0\,,\qquad \frac{\partial T_\alpha}{\partial\eta_\beta}-\frac{\partial T_\beta}{\partial\eta_\alpha}=0\,,\\ &i\frac{\partial}{\partial\eta_\alpha}S=T_\alpha\equiv\langle\phi_0|e^{-i[\hat{F}]}\frac{\partial}{\partial\eta_\alpha}e^{i[\hat{F}]}|\phi_0\rangle-\frac{1}{2}\eta_\alpha{}^*\,.\end{aligned} \tag{2·20}$$

Equation (2·18) is the second of the basic equations of the SCC method, which is hereafter called the *canonical-variable condition* and is denoted by [II]. (In the previous expansion method,[1),2)] we have fixed the special canonical variables $\{\eta_\alpha^*, \eta_\alpha\}$ *from the outset* so as to satisfy the simplest case with $S(\eta^*, \eta)=0$ in [II].) The canonical-variable condition [II] means that we can generally keep the degrees of freedom to choose canonical collective variables $\{\eta_\alpha^*, \eta_\alpha\}$ through the arbitrary real function $S(\eta^*, \eta)$.[10)]

§ 3. Self-consistent solutions of the SCC equations (I) —— *Nonresonant Cases* ——

An essential idea of the present improved method of solving the basic equations of the SCC method is to choose the canonical collective variables $\{\eta_\alpha^*, \eta_\alpha\}$ so as to put the collective Hamiltonian into the normal (diagonal) form

$$\text{[III]}\quad \begin{aligned}\mathcal{H}(\eta^*, \eta)&\equiv[H]-E_0=\langle\phi_0|e^{-i[\hat{F}]}\hat{H}e^{i[\hat{F}]}|\phi_0\rangle-E_0\\ &=\mathcal{H}(n_1, n_2, \cdots, n_L)\,, \qquad n_\alpha\equiv\eta_\alpha{}^*\eta_\alpha\,,\end{aligned} \tag{3·1}$$

by adopting an appropriate function $S(\eta^*, \eta)$ *in* [*II*].*) According to the Birkhoff-Gustavson normal-form expansion method,[11)] it is always possible to choose such canonical collective variables $\{\eta_\alpha^*, \eta_\alpha\}$, provided that the frequencies of the RPA normal modes are *in the nonresonant case.* The requirement (3·1) is called [III] hereafter.

It is easily seen that the problem of solving the set of basic equations [I]~[III] self-consistently can be reduced to finding the hermitian operator $[\hat{F}]$ (in the unitary operator $\exp(i[\hat{F}])$ satisfying the set of equations. In order to simplify the presentation, hereafter, we restrict ourselves to the simplest case $L=1$ corresponding to a single pair of collective variables $\{\eta^*, \eta\}$.

Since the hermitian operator $[\hat{F}]$ is a one-body operator by definition, we can express it in the form

$$i[\hat{F}]\equiv i\hat{G}(\eta^*, \eta)=\sum_\lambda\{g_\lambda(\eta^*, \eta)\hat{X}_\lambda{}^\dagger-g_\lambda{}^*(\eta^*, \eta)\hat{X}_\lambda\}\,, \tag{3·2}$$

where $\{\hat{X}_\lambda{}^\dagger, \hat{X}_\lambda\,; \lambda=0, 1, 2, \cdots, MN-1\}$ is the complete set of creation and annihilation operators of the RPA normal modes:

$$\hat{X}_\lambda{}^\dagger=\sum_{\mu i}\{\psi_\lambda(\mu i)a_\mu{}^\dagger b_i{}^\dagger-\phi_\lambda(\mu i)b_i a_\mu\}\,, \tag{3·3}$$

satisfying the RPA equation

$$\begin{aligned}&\delta\langle\phi_0|[\hat{H}, \hat{X}_\lambda{}^\dagger]-\omega_\lambda\hat{X}_\lambda{}^\dagger|\phi_0\rangle=0\,, \qquad \omega_\lambda>0\,,\\ &\langle\phi_0|[\hat{X}_\lambda, \hat{X}_{\lambda'}^\dagger]|\phi_0\rangle=\delta_{\lambda\lambda'}\,, \qquad \langle\phi_0|[\hat{X}_\lambda, \hat{X}_{\lambda'}]|\phi_0\rangle=0\,.\end{aligned} \tag{3·4}$$

We then expand the coefficient $g_\lambda(\eta^*, \eta)$ in Eq. (3·2) as a power series of $\{\eta^*, \eta\}$:

$$g_\lambda(\eta^*, \eta)=\sum_{n\geq1}g_\lambda(n)\,, \qquad g_\lambda(n)=\sum_{r,s}g_{rs}^{[\lambda]}\cdot(\eta^*)^r(\eta)^s\,, \qquad r+s=n\,, \tag{3·5}$$

*) It is notable that the requirement (3·1) has been just what employed in realizing the original idea[9)] of the invariance principle of the time-dependent Schrödinger equation.

so that the operator $i\hat{G}(\eta^*, \eta)$ in Eq. (3·2) is expressed as

$$i\hat{G}(\eta^*, \eta)=\sum_{n\geq 1} i\hat{G}(n), \qquad i\hat{G}(n)=\sum_\lambda \{g_\lambda(n)\hat{X}_\lambda{}^\dagger - g_\lambda{}^*(n)\hat{X}_\lambda\}. \tag{3·6}$$

The important input of this power-series expansion is to set up a specific boundary condition appropriate for the collective motion under consideration. Here we set up the following boundary condition:

$$g_\lambda(n=1)=\eta\cdot\delta_{\lambda 0}, \qquad \text{i.e., } i\hat{G}(n=1)=\eta\hat{X}_0{}^\dagger-\eta^*\hat{X}_0, \tag{3·7}$$

where $\hat{X}^\dagger_{\lambda=0}$ is the creation operator of the RPA phonon mode. The condition (3·7) means that the large-amplitude collective vibration under consideration is connected with RPA phonon mode in its small-amplitude harmonic limit.

The basic equations [I]~[III] in the present case are

(i) $$\langle\phi_0|\left[\hat{X}_\lambda, e^{-i\hat{G}}\left\{\hat{H}-\left(\frac{\partial\mathcal{H}}{\partial\eta^*}\right)\frac{\partial}{\partial\eta}+\left(\frac{\partial\mathcal{H}}{\partial\eta}\right)\frac{\partial}{\partial\eta^*}\right\}e^{i\hat{G}}\right]|\phi_0\rangle=0, \qquad \lambda\neq 0, ^{*)} \tag{3·8}$$

(ii) $$i\frac{\partial}{\partial\eta}S(\eta^*, \eta)=T(\eta^*, \eta), \qquad \text{i.e., } i\frac{\partial}{\partial\eta}S(n+1)=T(n),$$

$$T(\eta^*, \eta)\equiv\langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}|\phi_0\rangle-\frac{1}{2}\eta^*=\sum_n T(n),$$

$$S(\eta^*, \eta)=\sum_n S(n), \quad S(n)=S^*(n)=\sum_{\substack{r,s\\(r+s=n)}} S_{rs}\cdot(\eta^*)^r(\eta)^s, \tag{3·9}$$

(iii) $$\mathcal{H}(\eta^*, \eta)=\langle\phi_0|e^{-i\hat{G}}\hat{H}e^{i\hat{G}}|\phi_0\rangle-E_0=\sum_n\mathcal{H}(n)$$

$$=\omega_0\eta^*\eta+\sum_{r\geq 2}h_r\cdot(\eta^*\eta)^r, \tag{3·10}$$

($\omega_{\lambda=0}$: the frequency of the RPA phonon mode),

where we use the relations

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

$$\equiv\frac{\partial i\hat{G}}{\partial\eta}+\sum_{m\geq 2}\frac{1}{m!}\Bigg[\cdot\cdot\Bigg[\frac{\partial i\hat{G}}{\partial\eta}, \overbrace{i\hat{G}\Bigg], \cdots\Bigg], i\hat{G}}^{(m-1)}\Bigg], \tag{3·11}$$

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*) The equation of collective submanifold [I] is decomposed into Eq. (3·8) and an identical equation

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

Because the generator $\hat{O}^\dagger$ is a one-body operator by definition and the set $\{\hat{X}_\lambda{}^\dagger, \hat{X}_\lambda; \lambda=0, 1, \cdots, MN-1\}$ is the complete set, the identical equation becomes equivalent to

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

provided that Eq. (3·8) is satisfied.

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

$$=\hat{H}+\sum_{m\geq 1}\frac{1}{m!}[\cdot\cdot[\hat{H}, \overbrace{i\hat{G}], \cdots], i\hat{G}]}^{(m)} . \tag{3·12}$$

In the following, we show how to determine $i\hat{G}(\eta^*, \eta)$ in Eq. (3·6) as well as the normal collective Hamiltonian $\mathcal{H}(\eta^*, \eta)$ in Eq. (3·10) by choosing an appropriate real function $S(\eta^*, \eta)$ in Eq. (3·9).

The boundary condition (3·7) leads us to

$$T(n=1)=0 , \qquad S(n=1)=S(n=2)=0 ,$$
$$\mathcal{H}(n=2)=\omega_0\eta^*\eta . \tag{3·13}$$

The equation of submanifold (3·8) directly determines $g_\lambda(n=2)$ with $\lambda\neq 0$ in Eq. (3·6):

$$\left\{\omega_\lambda-\omega_0\left(\eta\frac{\partial}{\partial\eta}-\eta^*\frac{\partial}{\partial\eta^*}\right)\right\}g_\lambda(2)$$

$$=-\frac{1}{2}\langle\phi_0|[\hat{X}_\lambda, [[\hat{H}, i\hat{G}(1)], i\hat{G}(1)]]|\phi_0\rangle , \qquad \lambda\neq 0 , \tag{3·14a}$$

i.e.,

$$g_{\lambda\neq 0}(2)=\sum_{r,s}g_{rs}^{[\lambda\neq 0]}\cdot(\eta^*)^r(\eta)^s , \qquad r+s=2 ,$$

$$g_{rs}^{[\lambda\neq 0]}=-\frac{1}{2}\{\omega_\lambda-(s-r)\omega_0\}^{-1}[\langle\phi_0|[\hat{X}_\lambda, [[\hat{H}, i\hat{G}(1)], i\hat{G}(1)]]|\phi_0\rangle]_{rs} , \tag{3·14b}$$

where the symbol $[A]_{rs}$ for an arbitrary function $A(\eta^*, \eta)$ represents the coefficient of the power-series expansion:

$$A(\eta^*, \eta)=\sum_{r,s}A_{rs}\cdot(\eta^*)^r(\eta)^s , \qquad A_{rs}\equiv[A]_{rs} . \tag{3·15}$$

To determine $g_{\lambda=0}(2)$, we employ Eqs. (3·9) and (3·10).

With the use of Eq. (3·11), we easily obtain

$$T(2)=\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(1)}{\partial\eta}, i\hat{G}(2)\right]|\phi_0\rangle+\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(2)}{\partial\eta}, i\hat{G}(1)\right]|\phi_0\rangle$$

$$=\frac{1}{2}g_0^*(2)+\frac{1}{2}\left\{\eta^*\frac{\partial}{\partial\eta}g_0(2)-\eta\frac{\partial}{\partial\eta}g_0^*(2)\right\} . \tag{3·16}$$

Integrating $T(2)$ with respect to η, we thus have

$$S(3)=-i\left\{\frac{1}{2}(g_{02}^{[0]*}+g_{11}^{[0]})(\eta^*)^2\eta+\frac{1}{2}g_{02}^{[0]}\cdot\eta^*\eta^2-\frac{1}{6}g_{20}^{[0]*}\cdot\eta^3+\frac{1}{6}g_{20}^{[0]}\cdot(\eta^*)^3\right\} \tag{3·17}$$

with

$$2g_{02}^{[0]}+g_{11}^{[0]*}=0 , \tag{3·18}$$

where we have used the condition $S(3)=S^*(3)$ by definition.

With the use of Eq. (3·12), the third-order part of the collective Hamiltonian $\mathscr{H}(n=3)$ is written as

$$\mathscr{H}(3)=\omega_0\{\eta^*\cdot g_0(2)+\eta\cdot g_0^*(2)\}+\Delta\mathscr{H}(3)\,,$$

$$\Delta\mathscr{H}(3)\equiv\frac{1}{3!}\langle\phi_0|[[[\hat{H},\, i\hat{G}(1)],\, i\hat{G}(1)],\, i\hat{G}(1)]|\phi_0\rangle\,. \tag{3·19}$$

The condition (3·10) for $\mathscr{H}(\eta^*, \eta)$ to be normal demands $\mathscr{H}(3)=0$, by which we obtain

$$\omega_0 g_{20}^{[0]}+[\Delta\mathscr{H}(3)]_{30}=0\,,$$

$$\omega_0(g_{11}^{[0]}+g_{02}^{[0]*})+[\Delta\mathscr{H}(3)]_{21}=0\,. \tag{3·20}$$

The set of Eqs. (3·18) and (3·20) is enough to determine $g_0(2)$ specifying the optimum choice of $S(3)$ in Eq. (3·17).

We now go on to determine $g_\lambda(3)$. The fourth-order part of the collective Hamiltonian $\mathscr{H}(n=4)$ is written as

$$\mathscr{H}(4)=\omega_0\{\eta^*\cdot g_0(3)+\eta\cdot g_0^*(3)\}+\Delta\mathscr{H}(4)\,, \tag{3·21}$$

where $\Delta\mathscr{H}(4)$ is a known function, defined by

$$\begin{aligned}\Delta\mathscr{H}(4)\equiv&\frac{1}{2}\langle\phi_0|[[\hat{H},\, i\hat{G}(2)],\, i\hat{G}(2)]|\phi_0\rangle\\ &+\frac{1}{3!}\langle\phi_0|[[[\hat{H},\, i\hat{G}(1)],\, i\hat{G}(1)],\, i\hat{G}(2)]+[[[\hat{H},\, i\hat{G}(1)],\, i\hat{G}(2)],\, i\hat{G}(1)]\\ &+[[[\hat{H},\, i\hat{G}(2)],\, i\hat{G}(1)],\, i\hat{G}(1)]|\phi_0\rangle\\ &+\frac{1}{4!}\langle\phi_0|[[[[\hat{H},\, i\hat{G}(1)],\, i\hat{G}(1)],\, i\hat{G}(1)],\, i\hat{G}(1)]|\phi_0\rangle\,.\end{aligned} \tag{3·22}$$

For $T(n=3)$ in Eq. (3·9), we also have

$$T(n=3)=\frac{1}{2}g_0^*(3)+\frac{1}{2}\left\{\eta^*\frac{\partial}{\partial\eta}g_0(3)-\eta\frac{\partial}{\partial\eta}g_0^*(3)\right\}+\Delta T(3)\,, \tag{3·23}$$

where $\Delta T(3)$ is a known function, defined by

$$\begin{aligned}\Delta T(3)\equiv&\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(2)}{\partial\eta},\, i\hat{G}(2)\right]|\phi_0\rangle\\ &+\frac{1}{4!}\langle\phi_0|\left[\left[\left[\frac{\partial i\hat{G}(1)}{\partial\eta},\, i\hat{G}(1)\right],\, i\hat{G}(1)\right],\, i\hat{G}(1)\right]|\phi_0\rangle\,.\end{aligned} \tag{3·24}$$

Now, in the analogous way to the case of $g_\lambda(2)$, the equation of submanifold (3·8) directly determines $g_{\lambda\neq0}(3)$:

$$g_{\lambda\neq0}(3)=\sum_{rs}g_{rs}^{[\lambda\neq0]}\cdot(\eta^*)^r(\eta)^s\,,\qquad r+s=3\,,$$

$$\begin{aligned}g_{rs}^{[\lambda\neq0]}=&\{\omega_\lambda-(s-r)\omega_0\}^{-1}\\ &\times[-\frac{1}{2!}\langle\phi_0|[\hat{X}_\lambda,\, ([[\hat{H},\, i\hat{G}(1)],\, i\hat{G}(2)]+[[\hat{H},\, i\hat{G}(2)],\, i\hat{G}(1)])]|\phi_0\rangle\end{aligned}$$

$$+\frac{1}{3!}\langle\phi_0|[\hat{X}_\lambda, [[[\hat{H}, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]]|\phi_0\rangle$$

$$+\frac{1}{3!}\langle\phi_0|\Big[\hat{X}_\lambda, \Big[\Big[\Big\{\omega_0\Big(\eta\frac{\partial}{\partial\eta}-\eta^*\frac{\partial}{\partial\eta^*}\Big)i\hat{G}(1)\Big\}, i\hat{G}(1)\Big], i\hat{G}(1)\Big]\Big]|\phi_0\rangle]_{rs}\,. \tag{3·25}$$

To determine $g_{\lambda=0}(3)$ by choosing an appropriate function $S(4)$, we use Eqs. (3·9) and (3·10) together with the expressions (3·21) and (3·23).

By integrating $T(3)$ in Eq. (3·23) with respect to η and then by setting the condition $S(4)=S^*(4)$, we obtain

$$\begin{aligned}S(4)=-i\Big\{&-\frac{1}{4}(-g_{30}^{[0]}+[\varDelta T(3)]_{03}^*)(\eta^*)^4+\frac{1}{4}(-g_{30}^{[0]*}+[\varDelta T(3)]_{03})\eta^4\\&+\Big(\frac{1}{2}g_{03}^{[0]*}+\frac{1}{2}g_{21}^{[0]}+[\varDelta T(3)]_{30}\Big)(\eta^*)^3\eta+\frac{1}{3}\Big(-\frac{1}{2}g_{21}^{[0]*}+\frac{3}{2}g_{03}^{[0]}\\&+[\varDelta T(3)]_{12}\Big)\eta^*\eta^3+\frac{1}{2}(g_{12}^{[0]}+[\varDelta T(3)]_{21})(\eta^*\eta)^2\Big\}\end{aligned} \tag{3·26}$$

with

$$3g_{03}^{[0]}+g_{21}^{[0]*}=-[\varDelta T(3)]_{12}-3[\varDelta T(3)]_{30}^*\,, \tag{3·27a}$$

$$g_{12}^{[0]}+g_{12}^{[0]*}=-[\varDelta T(3)]_{21}-[\varDelta T(3)]_{21}^*\,. \tag{3·27b}$$

Demanding $\mathcal{H}(4)$ in Eq. (3·21) to be normal according to Eq. (3·10), i.e., demanding $[\mathcal{H}(4)]_{rs}=0$ for $r\neq s$, we have the relations

$$\begin{aligned}&\omega_0 g_{30}^{[0]}+[\varDelta\mathcal{H}(4)]_{40}=0\,,\\&\omega_0(g_{21}^{[0]}+g_{03}^{[0]*})+[\varDelta\mathcal{H}(4)]_{31}=0\,.\end{aligned} \tag{3·28}$$

It is clear that Eqs. (3·27a) and (3·28) are enough to determine $g_{30}^{[0]}$, $g_{03}^{[0]}$ and $g_{21}^{[0]}$.

The coefficient $h_{r=2}$ of the diagonal term in $\mathcal{H}(4)$ in Eq. (3·10) is given as

$$\begin{aligned}h_{r=2}&\equiv[\mathcal{H}(4)]_{22}\\&=\omega_0(g_{12}^{[0]}+g_{12}^{[0]*})+[\varDelta\mathcal{H}(4)]_{22}\\&=[\varDelta\mathcal{H}(4)]_{22}-\omega_0\{[\varDelta T(3)]_{21}+[\varDelta T(3)]_{21}^*\}\,,\end{aligned} \tag{3·29}$$

where we have used Eq. (3·27b).

Thus, we have obtained the fourth-order Hamiltonian in diagonal form. In order to determine $g_{12}^{[0]}$ which is not specified yet, we make use of the fact that the function $S(\eta^*, \eta)$ is a generating function of canonical transformation and the choice of the functional form of $S(\eta^*, \eta)$ just corresponds to fixing the degree of freedom of canonical transformation. Therefore, here, we choose a simple functional form of $S(\eta^*, \eta)$ so that it has no terms with the diagonal forms of η^* and η, such as $(\eta^*\eta)^r$, by which the collective Hamiltonian (3·10) is expressed. According to this choice, we obtain the following relation to determine $g_{12}^{[0]}$,

$$g_{12}^{[0]}+[\varDelta T(3)]_{21}=0\,. \tag{3·30}$$

Thus, starting with the boundary condition (3·7) and evaluating each power of $\{\eta^*, \eta\}$ in the basic equations (3·8)~(3·10) step by step, we can determine the higher order terms $g_\lambda(n)$ in Eq. (3·5) as well as the collective Hamiltonian $\mathcal{H}(n)$ in Eq. (3·10), provided that the frequency of the RPA-phonon mode ω_0 is in a nonresonant case.

§ 4. Self-consistent solutions of the SCC equations (II)
—— *Resonant Cases* ——

When there exists a resonance condition (1·1), i.e., $\omega_1 - n_0\omega_0 \simeq 0$, with an integer $n_0(\geq 2)$, the power-series expansion in § 3 encounters the well-known problems of the appearance of "zero-denominator", $1/(\omega_1 - n_0\omega_0)$, in the coefficients of the power series expansion with the collective variables $\{\eta^*, \eta\}$. In such a resonant case, therefore, we have to properly take into account a set of degrees of freedom $\{\eta_1^*, \eta_1\}$, which is connected with the RPA normal mode with the frequency ω_1 in the small-amplitude harmonic limit, by extending the collective submanifold to $\{\eta^*, \eta; \eta_1^*, \eta_1\}$.

In this case the basic equations [I] and [II] are

$$\text{(i)}\quad \langle\phi_0|\Big[\hat{X}_\lambda, e^{-i\hat{G}}\Big\{\hat{H} - \Big(\frac{\partial\mathcal{H}}{\partial\eta^*}\Big)\frac{\partial}{\partial\eta} + \Big(\frac{\partial\mathcal{H}}{\partial\eta}\Big)\frac{\partial}{\partial\eta^*} - \Big(\frac{\partial\mathcal{H}}{\partial\eta_1^*}\Big)\frac{\partial}{\partial\eta_1} + \Big(\frac{\partial\mathcal{H}}{\partial\eta_1}\Big)\frac{\partial}{\partial\eta_1^*}\Big\}e^{i\hat{G}}\Big]|\phi_0\rangle = 0\,, \quad \lambda \neq 0, 1\,, \tag{4·1}$$

$$\text{(ii)}\quad i\frac{\partial}{\partial\eta}S(\eta^*, \eta; \eta_1^*, \eta_1) = T_0(\eta^*, \eta; \eta_1^*, \eta_1)\,,$$

$$i\frac{\partial}{\partial\eta_1}S(\eta^*, \eta; \eta_1^*, \eta_1) = T_1(\eta^*, \eta; \eta_1^*, \eta_1)\,,$$

$$T_0(\eta^*, \eta; \eta_1^*, \eta_1) \equiv \langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}|\phi_0\rangle - \frac{1}{2}\eta^*\,,$$

$$T_1(\eta^*, \eta; \eta_1^*, \eta_1) \equiv \langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta_1}e^{i\hat{G}}|\phi_0\rangle - \frac{1}{2}\eta_1^*\,, \tag{4·2}$$

where

$$i\hat{G}(\eta^*, \eta; \eta_1^*, \eta_1) = \sum_\lambda\{g_\lambda(\eta^*, \eta; \eta_1^*, \eta_1)\hat{X}_\lambda^\dagger - g_\lambda^*(\eta^*, \eta; \eta_1^*, \eta_1)\hat{X}_\lambda\}\,. \tag{4·3}$$

In the resonant case, it is *impossible* to demand the condition [III], which puts the collective Hamiltonian into the *complete* normal (diagonal) form. By choosing an appropriate function $S(\eta^*, \eta; \eta_1^*, \eta_1)$ in Eq. (4·2), however, we can put the collective Hamiltonian into a form being as normal (diagonal) as possible. (The detail is given in the Appendix.) Thus, the "maximally" normal (diagonal) Hamiltonian finally has the following form:

$$\text{[III]}'\quad \mathcal{H}(\eta^*, \eta; \eta_1^*, \eta_1) = \langle\phi_0|e^{-i\hat{G}}\hat{H}e^{i\hat{G}}|\phi_0\rangle - E_0$$

$$= \mathcal{H}^{(0)} + \mathcal{H}^{(1)} + \mathcal{H}^{(0-1)} + \mathcal{H}^{(\mathrm{res})}\,, \tag{4·4a}$$

$$\mathcal{H}^{(0)} \equiv \omega_0\eta^*\eta + \sum_{r\geq 2}h_r^{(0)}(\eta^*\eta)^r\,, \tag{4·4b}$$

$$\mathcal{H}^{(1)} \equiv \omega_1 \eta_1{}^* \eta_1 + \sum_{r\geq 2} h_r{}^{(1)} (\eta_1{}^* \eta_1)^r , \tag{4·4c}$$

$$\mathcal{H}^{(0-1)} \equiv \sum_{r,s\geq 1} h_{rs}^{(0-1)} \cdot (\eta^* \eta)^r (\eta_1{}^* \eta_1)^s , \tag{4·4d}$$

$$\mathcal{H}^{(\text{res})} \equiv \sum_{l\geqq 1} \sum_{r,s\geqq 0} h_{lrs}^{(\text{res})} \{(\eta_1{}^*(\eta)^{n_0})^l + ((\eta^*)^{n_0}\eta_1)^l\} (\eta^*\eta)^r (\eta_1{}^*\eta_1)^s , \tag{4·4e}$$

where the term $\mathcal{H}^{(\text{res})}$ can never be expressed in the normal (diagonal) form and displays an *essential coupling* between the $\{\eta^*, \eta\}$-mode and the $\{\eta_1{}^*, \eta_1\}$-mode through the resonance condition $\omega_1 - n_0\omega_0 \simeq 0$.

With the boundary condition in the small-amplitude harmonic limit,

$$\begin{aligned} &g_{\lambda=0}(\eta^*, \eta; \eta_1{}^*, \eta_1) \to \eta , \qquad g_{\lambda=1}(\eta^*, \eta; \eta_1{}^*, \eta_1) \to \eta_1 , \\ &g_{\lambda\neq 0,1}(\eta^*, \eta; \eta_1{}^*, \eta_1) \to 0 , \end{aligned} \tag{4·5}$$

the set of the basic equations, (4·1)~(4·3), enables us to determine $g_\lambda(\eta^*, \eta; \eta_1{}^*, \eta_1)$ in the power-series expansion form,

$$\begin{aligned} &g_\lambda(\eta^*, \eta; \eta_1{}^*, \eta_1) = \sum_{n\geq 1} g_\lambda(n) , \\ &g_\lambda(n) = \sum_{(rs, r_1 s_1)} g^{[\lambda]}(rs, r_1 s_1) (\eta^*)^r (\eta)^s (\eta_1{}^*)^{r_1} (\eta_1)^{s_1} , \quad r + s + r_1 + s_1 = n , \end{aligned} \tag{4·6}$$

as well as the coefficients $h_r{}^{(0)}$, $h_r{}^{(1)}$, $h_{rs}^{(0-1)}$ and $h_{lrs}^{(\text{res})}$ in the collective Hamiltonian (4·4). It turns out that the optimum function $S(\eta^*, \eta; \eta_1{}^*, \eta_1)$ in this case has the following form: It contains *no terms* with the forms of η^*, η, $\eta_1{}^*$ and η_1 like $(\eta^*\eta)^r(\eta_1{}^*\eta_1)^s$ $(r, s \geq 0)$, $(\eta_1{}^*(\eta)^{n_0})^l$ and $((\eta^*)^{n_0}\eta_1)^l (l \geq 1)$, by which the maximally normal Hamiltonian (4·4) is expressed. A full detail of the method is given in the Appendix.

§ 5. Illustrative example of solutions

In order to illustrate the solutions in the resonant and non-resonant cases, let us consider a simple model Hamiltonian

$$\begin{aligned} &\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} , \\ &\hat{H}_0 = \varepsilon_0 \hat{K}_{00} + \varepsilon_1 \hat{K}_{11} + \varepsilon_2 \hat{K}_{22} + \varepsilon_3 \hat{K}_{33} , \\ &\hat{H}_{\text{int}} = V_{12} \cdot \{\hat{K}_{12}\hat{K}_{10} + \hat{K}_{01}\hat{K}_{21}\} + V_{13} \cdot \{\hat{K}_{13}\hat{K}_{10} + \hat{K}_{01}\hat{K}_{31}\} . \end{aligned} \tag{5·1}$$

There are four levels with energies $\varepsilon_0 < \varepsilon_1 < \varepsilon_2 < \varepsilon_3$ and each level has N-fold degeneracy. The fermion pair operators are defined as

$$\hat{K}_{ij} = \sum_{m=1}^{N} c_{im}^\dagger c_{jm} , \qquad i, j = 0, 1, 2, 3 . \tag{5·2}$$

The lowest energy state without the interaction, i.e., $V_{12} = V_{13} = 0$, is

$$|\phi_0\rangle = \prod_{m=1}^{N} c_{0m}^\dagger |0\rangle , \qquad c_{im}|0\rangle = 0 . \tag{5·3}$$

The time-dependent single Slater determinant is given as

$$|\phi(t)\rangle = e^{i\hat{F}(t)}|\phi_0\rangle\,,$$

$$i\hat{F}(t) = \frac{1}{\sqrt{N}}\{f_1(t)\hat{K}_{10} + f_2(t)\hat{K}_{20} + f_3(t)\hat{K}_{30}\} - \text{h.c.}\,, \tag{5·4}$$

where the basic excitation modes are $\hat{K}_{10}$, $\hat{K}_{20}$ and $\hat{K}_{30}$. The excitation energies corresponding to $\{\omega_\lambda;\ \lambda=0, 1, 2, \cdots\}$ in the previous sections are $\varepsilon_{10} \equiv \varepsilon_1 - \varepsilon_0$, $\varepsilon_{20} \equiv \varepsilon_2 - \varepsilon_0$ and $\varepsilon_{30} \equiv \varepsilon_3 - \varepsilon_0$.

Instead of the variables $\{f_i^*, f_i;\ i=1, 2, 3\}$, it is convenient to use the following canonical variables:

$$C_i = -\frac{f_i}{\sqrt{\Omega}}\sin\sqrt{\Omega}\,, \qquad \Omega \equiv \frac{1}{N}\sum_{k=1}^{3} f_k^* f_k\,. \tag{5·5}$$

Then, the TDHF equation

$$\delta\langle\phi_0|e^{-i\hat{F}}\left(i\frac{\partial}{\partial t} - \hat{H}\right)e^{i\hat{F}}|\phi_0\rangle = 0 \tag{5·6}$$

is simply reduced to a set of classical equations of motion

$$i\dot{C}_k = \partial H/\partial C_k^*\,, \qquad i\dot{C}_k^* = -\partial H/\partial C_k\,, \qquad k=1, 2, 3\,,$$

$$H \equiv \langle\phi_0|e^{-i\hat{F}}\hat{H}e^{i\hat{F}}|\phi_0\rangle - \langle\phi_0|\hat{H}|\phi_0\rangle\,. \tag{5·7}$$

A solution of the canonical equations of motion (5·7) gives a TDHF-trajectory in a 6-dimensional phase space $\{q_k, p_k;\ k=1, 2, 3\}$ with

$$q_k = \frac{1}{\sqrt{2}}(C_k^* + C_k)\,, \qquad p_k = \frac{i}{\sqrt{2}}(C_k^* - C_k)\,. \tag{5·8}$$

In the nonresonant case, the boundary condition in the small-amplitude (harmonic) limit is given by

$$[f_i] \to \eta \cdot \delta_{i,1}\,, \tag{5·9}$$

where the symbol $[f_i]$ is defined by Eq. (2·11) and a function of the collective variables η^* and η. Following the method given in § 3 by reading $\hat{X}_0^\dagger$ as $\hat{K}_{10}$ and $\{\hat{X}_{\lambda\neq0}^\dagger\}$ as $\{\hat{K}_{20}, \hat{K}_{30}\}$, we then can obtain the solution satisfying the basic equations (3·8)~(3·10). The normal-form Hamiltonian thus obtained is written (up to the fourth order) as

$$\mathcal{H}(\eta^*, \eta) = \varepsilon_{10}\eta^*\eta - \frac{1}{N}\left[\frac{\{(N-1)V_{12}\}^2}{\varepsilon_{20} - 2\cdot\varepsilon_{10}} + \frac{\{(N-1)V_{13}\}^2}{\varepsilon_{30} - 2\cdot\varepsilon_{10}}\right](\eta^*\eta)^2\,, \tag{5·10}$$

and the SCC trajectories are obtained by the equations of collective motion

$$i\dot{\eta} = \partial\mathcal{H}/\partial\eta^*\,, \qquad i\dot{\eta}^* = -\partial\mathcal{H}/\partial\eta\,. \tag{5·11}$$

In Fig. 1, we show the TDHF trajectory from Eq. (5·7) and the SCC trajectory from Eq. (5·11) in the nonresonant case by making use of the Lissajous figures. We can see that the SCC trajectory obtained by our power-series expansion method reproduces the gross property of the TDHF trajectory very well. In the nonresonant case it is seen that the time-dependence of the amplitude $f_i(t)$ is regular and energy exchange among the f_i's is quite small.

When the resonance condition $\varepsilon_{20}-2\varepsilon_{10}=0$ is satisfied, according to the method in § 4, we have to introduce a new set of variables $\{\eta_1^*, \eta_1\}$ which corresponds to the degree of freedom of $\hat{K}_{20}$. The boundary condition in the small-amplitude (harmonic) limit is given in this case as

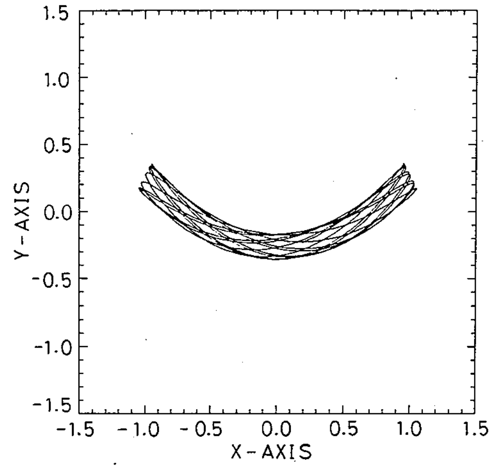
$$[f_1]\to\eta\,,\qquad [f_2]\to\eta_1\,,\qquad [f_3]\to 0\,, \tag{5·12}$$

and $\hat{X}_\lambda$ in Eq. (4·1) should be read as $\hat{K}_{03}$. Solving the basic equations (4·1), (4·2) and (4·4), we obtain the maximally normal Hamiltonian (up to the fourth order)

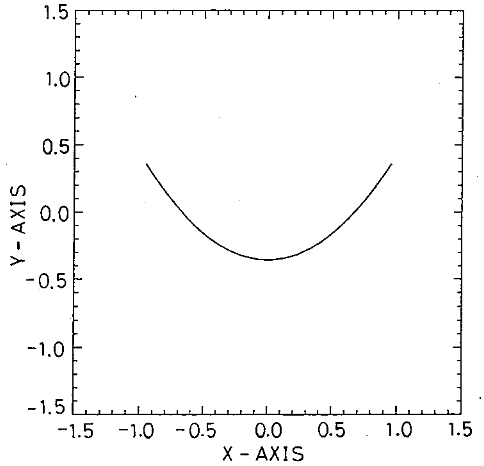
$$\mathscr{H}(\eta^*, \eta;\eta_1^*, \eta_1)=\varepsilon_{10}\eta^*\eta+\varepsilon_{20}\eta_1^*\eta_1 - \frac{\{(N-1)V_{13}\}^2}{N(\varepsilon_{30}-2\varepsilon_{10})}(\eta^*\eta)^2+\mathscr{H}^{(\text{res})}\,, \tag{5·13a}$$

$$\mathscr{H}^{(\text{res})}=\frac{1}{\sqrt{N}}(N-1)V_{12}\cdot\{\eta_1^*(\eta)^2+(\eta^*)^2\eta_1\}\,. \tag{5·13b}$$

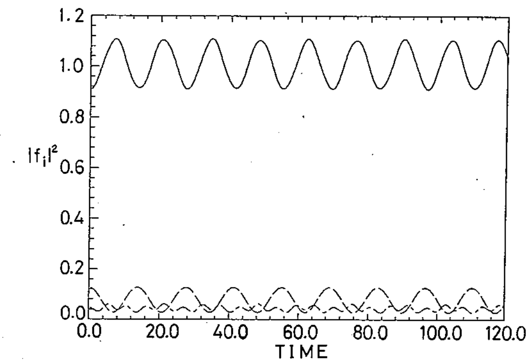
The SCC trajectory in this resonant case is then obtained by solving the equations of



(a)



(b)



(c)

Fig. 1.(a) A TDHF trajectory projected on the plane spanned by Re(f_1) (X-axis) and Re(f_2) (Y-axis) in the nonresonant case.
The parameters are: $\varepsilon_{10}=1.$, $\varepsilon_{20}=1.7$, $\varepsilon_{30}=3.2$, $V_{12}=0.033$ and $V_{13}=0.033$.

(b) An SCC-method trajectory corresponding to Fig. 1 (a).

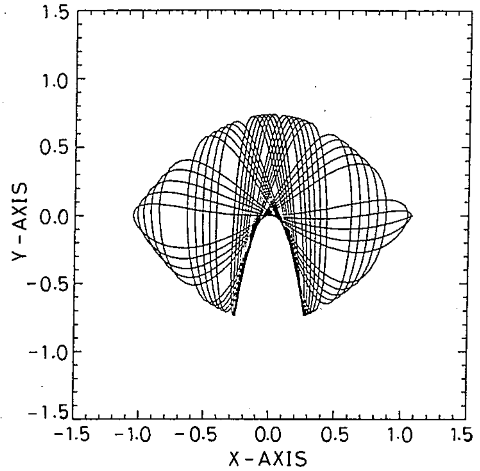
(c) Time dependence of $|f_i|^2$ ($i=1, 2, 3$) for the trajectory in Fig. 1(a), denoted by solid curve ($i=1$), broken curve ($i=2$) and dash-dotted curve ($i=3$), respectively. The curve for $i=3$ is magnified by ten times. The unit of time is 0.1.

motion

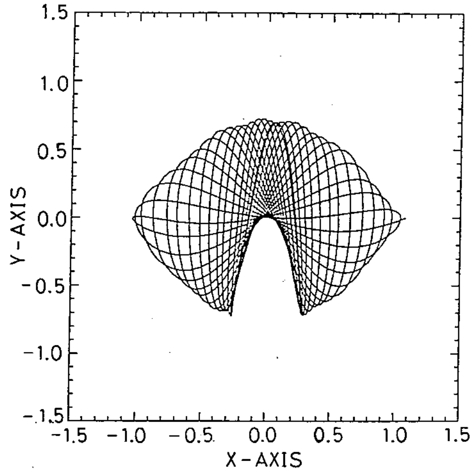
$$i\dot{\eta}=\partial\mathcal{H}/\partial\eta^*\,,\qquad i\dot{\eta}^*=-\partial\mathcal{H}/\partial\eta\,,$$

$$i\dot{\eta}_1=\partial\mathcal{H}/\partial\eta_1^*\,,\qquad i\dot{\eta}_1^*=-\partial\mathcal{H}/\partial\eta_1\,. \tag{5·14}$$

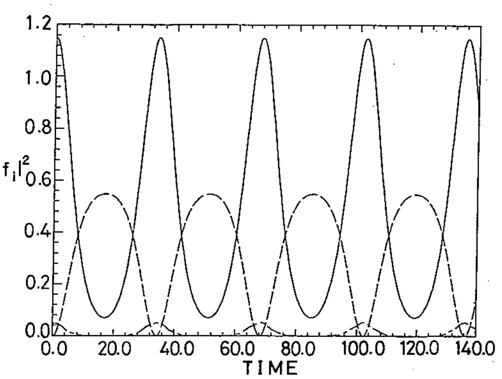
In Fig. 2, we show a TDHF trajectory from Eq. (5·7) and an SCC trajectory from Eq. (5·14) in the resonant case. As is seen from the figure, the TDHF trajectory is drastically different from those in the nonresonant cases. Demonstrating the effects of the resonance condition, the trajectory goes around on the plane spanned by f_1 and f_2, and it is essentially necessary to introduce a pair of new dynamical variables to describe such a motion. The SCC trajectory obtained from Eq. (5·14) approximates the TDHF trajectory very well, thus showing that the method given in § 4 enables us to clarify *dynamical structure* of the effects of resonance: In this resonant case it is seen that the time-dependence of the amplitude $f_i(t)$ (i=1, 2) is large, indicating appreciable energy exchange between f_1 and f_2. In our method, the source of the energy exchange is simply visualized as the essential coupling terms $\mathcal{H}^{(\mathrm{res})}$ in the maximally normal collective Hamiltonian (5·13).



(a)



(b)



(c)

Fig. 2.(a) A TDHF trajectory in the resonant case with the parameters given by ε_{10}=1., ε_{20}=2., ε_{30}=3.2, V_{12}=0.033 and V_{13}=0.033.

(b) An SCC-method trajectory corresponding to Fig. 2(a).

(c) Time dependence of $|f_i|^2$ (i=1, 2, 3) for the trajectory in Fig. 2(a). The solid curve, broken curve and dash-dotted curve correspond to i=1, 2, 3, respectively. The curve for i=3 is magnified by ten times. The unit of time is 0.1.

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Appendix

In this appendix, we show how to determine $i\hat{G}(\eta^*, \eta; \eta_1^*, \eta_1)$ in Eq. (4·3) and the maximally-normal collective Hamiltonian $\mathcal{H}(\eta^*, \eta; \eta_1^*, \eta_1)$ in Eq. (4·4), by choosing an optimum real function $S(\eta^*, \eta; \eta_1^*, \eta_1)$ in Eq. (4·2) in the power-series expansion forms with respect to η^*, η, η_1^* and η_1. For the sake of simplicity, here we adopt the resonant case with $n_0=2$; i.e.,

$$\omega_1 - 2\omega_0 \simeq 0\,. \tag{A·1}$$

With the use of Eq. (4·6), the expansion form of $i\hat{G}(\eta^*, \eta; \eta_1^*, \eta_1)$ is written as

$$i\hat{G}(\eta^*, \eta; \eta_1^*, \eta_1) = \sum_{n\geq 1} i\hat{G}(n)\,, \quad i\hat{G}(n) = \sum_{\lambda}\{g_\lambda(n)\hat{X}_\lambda{}^\dagger - g_\lambda{}^*(n)\hat{X}_\lambda\}\,, \tag{A·2}$$

where $i\hat{G}(n=1)$ is given from the outset by the boundary condition (4·5) as

$$i\hat{G}(1) = (\eta\hat{X}_0{}^\dagger - \eta^*\hat{X}_0) + (\eta_1\hat{X}_1{}^\dagger - \eta_1{}^*\hat{X}_1)\,. \tag{A·3}$$

In the similar way, we expand the quantities $S(\eta^*, \eta; \eta_1^*, \eta_1)$ and $T_k(\eta^*, \eta; \eta_1^*, \eta_1)$ $(k=0, 1)$ in Eq. (4·2) as

$$S(\eta^*, \eta; \eta_1^*, \eta_1) = \sum_{n\geq 1} S(n)\,,$$

$$S(n) = \sum_{(rs, r_1 s_1)} S(rs, r_1 s_1)(\eta^*)^r(\eta)^s(\eta_1{}^*)^{r_1}(\eta_1)^{s_1}\,, \quad r+s+r_1+s_1=n\,, \tag{A·4}$$

$$T_k(\eta^*, \eta; \eta_1^*, \eta_1) = \sum_{n\geq 1} T_k(n)\,, \qquad k=0, 1\,,$$

$$T_k(n) \equiv \left[\langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta_k}e^{i\hat{G}}|\phi_0\rangle\right]^{(n)} - \frac{1}{2}\eta_k{}^*\cdot\delta_{n,1}\,, \qquad \eta_{k=0}\equiv\eta\,, \tag{A·5}$$

where the symbol $[\cdots]^{(n)}$ denotes the n-th order part of the quantity $[\cdots]$ with respect to the power series expansion. From Eq. (A·3) we have

$$T_k(1)=0\,, \qquad S(1)=S(2)=0\,. \tag{A·6}$$

[I] *Determination of* $i\hat{G}(n=2)$

The equation of submanifold (4·1) directly determines $g_\lambda(n=2)$ with $\lambda\neq 0$ and 1 as

$$\left\{\omega_\lambda - \sum_{k=0,1}\omega_k\left(\eta_k\frac{\partial}{\partial\eta_k} - \eta_k{}^*\frac{\partial}{\partial\eta_k{}^*}\right)\right\}g_\lambda(2)$$

$$=-\frac{1}{2}\langle\phi_0|[\hat{X}_\lambda, [[\hat{H}, i\hat{G}(1)], i\hat{G}(1)]]|\phi_0\rangle\,, \quad \lambda\neq 0, 1 \quad (\eta_{k=0}\equiv\eta)\,. \tag{A·7}$$

To determine $g_{\lambda=0}(2)$ and $g_{\lambda=1}(2)$, we employ the generalized canonical-variable condition (4·2). With this purpose, we divide $g_\lambda(2)$ in Eq. (4·6) with $\lambda=0$ and 1 into

$$g_\lambda(2)=g_\lambda(2\|\eta^*\eta)+g_\lambda^{[\mathrm{I}]}(2\|\eta^*\eta;\, \eta_1^*\eta_1)+g_\lambda(2\|\eta_1^*\eta_1)\,, \quad \lambda=0, 1\,,$$

$$g_\lambda(2\|\eta^*\eta)\equiv\sum_{\substack{rs\\(r+s=2)}} g^{[\lambda]}(rs, 00)(\eta^*)^r(\eta)^s\,,$$

$$g_\lambda(2\|\eta_1^*\eta_1)\equiv\sum_{\substack{rs\\(r+s=2)}} g^{[\lambda]}(00, rs)(\eta_1^*)^r(\eta_1)^s\,,$$

$$\begin{aligned}g_\lambda^{[\mathrm{I}]}(2\|\eta^*\eta;\, \eta_1^*\eta_1)\equiv\eta_1^*\{&\sum_{\substack{pq\\(p+q=1)}} g^{[\lambda]}(pq, 10)(\eta^*)^p(\eta)^q\}\\ &+\eta_1\{\sum_{\substack{pq\\(p+q=1)}} g^{[\lambda]}(pq, 01)(\eta^*)^p(\eta)^q\}\,, \quad \lambda=0, 1\,.\end{aligned} \tag{A·8}$$

Similarly we divide $S(n=3)$ in Eq. (A·4) into

$$S(3)=S(3\|\eta^*\eta)+S^{[\mathrm{I}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)+S^{[\mathrm{II}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)+S(3\|\eta_1^*\eta_1)\,,$$

$$S(3\|\eta^*\eta)\equiv\sum_{\substack{rs\\(r+s=3)}} S(rs, 00)(\eta^*)^r(\eta)^s\,,$$

$$S(3\|\eta_1^*\eta_1)\equiv\sum_{\substack{rs\\(r+s=3)}} S(00, rs)(\eta_1^*)^r(\eta_1)^s\,, \tag{A·9}$$

where $S^{[\mathrm{I}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)$ and $S^{[\mathrm{II}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)$ denote terms being *linear* and *quadratic* with respect to η_1^* and η_1, respectively. The third-order part of the collective Hamiltonian is also classified by the powers of η_1^* and η_1:

$$\begin{aligned}\mathcal{H}(n=3)&\equiv[\langle\phi_0|e^{-i\hat{G}}\hat{H}e^{i\hat{G}}|\phi_0\rangle]^{(n=3)}\\ &=\mathcal{H}(3\|\eta^*\eta)+\mathcal{H}^{[\mathrm{I}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)+\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\, \eta_1^*\eta_1)+\mathcal{H}(3\|\eta_1^*\eta_1)\,.\end{aligned} \tag{A·10}$$

Now, with use of Eq. (3·11), we easily obtain

$$\begin{aligned}T_0(2)&\equiv\left[\langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}|\phi_0\rangle\right]^{(n=2)}\\ &=\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(1)}{\partial\eta}, i\hat{G}(2)\right]|\phi_0\rangle+\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(2)}{\partial\eta}, i\hat{G}(1)\right]|\phi_0\rangle\\ &=\frac{1}{2}g_0^*(2)+\frac{1}{2}\left\{\eta^*\frac{\partial}{\partial\eta}g_0(2)-\eta\frac{\partial}{\partial\eta}g_0^*(2)+\eta_1^*\frac{\partial}{\partial\eta}g_1(2)-\eta_1\frac{\partial}{\partial\eta}g_1^*(2)\right\},\end{aligned} \tag{A·11a}$$

$$T_1(2)=\frac{1}{2}g_1^*(2)+\frac{1}{2}\left\{\eta_1^*\frac{\partial}{\partial\eta_1}g_1(2)-\eta_1\frac{\partial}{\partial\eta}g_1^*(2)+\eta^*\frac{\partial}{\partial\eta_1}g_0(2)-\eta\frac{\partial}{\partial\eta_1}g_0^*(2)\right\}. \tag{A·11b}$$

(I-1) *Choice of* $S(3\|\eta^*\eta)$ *and of* $S(3\|\eta_1^*\eta_1)$

Substituting (A·8) into (A·11a) and integrating $T_0(2)$ with respect to η, and then setting the condition $S(3)=S^*(3)$ by definition, for $S(3\|\eta^*\eta)$ we obtain

$$S(3\|\eta^*\eta)=-i\Big[\frac{1}{2}\{g^{[0]*}(02,00)+g^{[0]}(11,00)\}(\eta^*)^2\eta$$
$$+\frac{1}{2}g^{[0]}(02,00)\eta^*\eta^2-\frac{1}{6}g^{[0]*}(20,00)\eta^3+\frac{1}{6}g^{[0]}(20,00)(\eta^*)^3\Big] \quad (\mathrm{A}\cdot12)$$

with

$$2\cdot g^{[0]}(02,00)+g^{[0]*}(11,00)=0\,. \quad (\mathrm{A}\cdot13)$$

The way of determination of the optimum function $S(3\|\eta^*\eta)$ is thus completely the same as one given in § 3.

With the use of Eq. (3·2), the third-order part of the collective Hamiltonian $\mathcal{H}(n=3)$ in (A·10) is written as

$$\mathcal{H}(3)=\omega_0\{\eta^*\cdot g_0(2)+\eta\cdot g_0^*(2)\}+\omega_1\{\eta_1^*\cdot g_1(2)+\eta_1\cdot g_1^*(2)\}+\varDelta\mathcal{H}(3)\,, \quad (\mathrm{A}\cdot14)$$

$$\varDelta\mathcal{H}(3)\equiv\frac{1}{3!}\langle\phi_0|[[[\hat{H},i\hat{G}(1)],i\hat{G}(1)],i\hat{G}(1)]|\phi_0\rangle\,. \quad (\mathrm{A}\cdot15)$$

We thus have

$$\mathcal{H}(3\|\eta^*\eta)=\omega_0\{\eta^*\cdot g_0(2\|\eta^*\eta)+\eta\cdot g_0^*(2\|\eta^*\eta)\}+\varDelta\mathcal{H}(3\|\eta^*\eta)\,, \quad (\mathrm{A}\cdot16)$$

where we have classified $\varDelta\mathcal{H}(3)$ according to the powers with respect to η_1^* and η_1:

$$\varDelta\mathcal{H}(3)=\varDelta\mathcal{H}(3\|\eta^*\eta)+\varDelta\mathcal{H}^{[\mathrm{I}]}(3\|\eta^*\eta;\,\eta_1^*\eta_1)$$
$$+\varDelta\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\,\eta_1^*\eta_1)+\varDelta\mathcal{H}(3\|\eta_1^*\eta_1)\,. \quad (\mathrm{A}\cdot17)$$

The condition for $\mathcal{H}^{(0)}(\eta^*,\eta)$ in Eq. (4·4b) to be *normal* demands $\mathcal{H}(3\|\eta^*\eta)=0$, by which we obtain the relations

$$\omega_0 g^{[0]}(20,00)+[\varDelta\mathcal{H}(3\|\eta^*\eta)]_{30}=0\,, \quad (\mathrm{A}\cdot18)$$

$$\omega_0\{g^{[0]}(11,00)+g^{[0]*}(02,00)\}+[\varDelta\mathcal{H}(3\|\eta^*\eta)]_{21}=0\,, \quad (\mathrm{A}\cdot19)$$

where the symbol $[\cdots]_{rs}$ is defined in Eq. (3·15). It is now clear that the set of (A·13), (A·18) and (A·19) determines $g_0(2\|\eta^*\eta)$ in (A·8), which specifies the optimum choice of $S(3\|\eta^*\eta)$ in (A·9).

In the same manner, we can also determine $g_1(2\|\eta_1^*\eta_1)$ in (A·8) specifying the optimum choice of $S(3\|\eta_1^*\eta_1)$ in (A·9).

(I-2) *Appearance of Essential Coupling $\mathcal{H}^{(res)}$ and Choice of $S^{[I]}(3\|\eta^*\eta;\,\boldsymbol{\eta}_1^*\boldsymbol{\eta}_1)$*

Substituting (A·8) into (A·11a) and integrating $T_0(2)$ with respect to η, for $S^{[\mathrm{I}]}(3\|\eta^*\eta;\,\eta_1^*\eta_1)$ we obtain

$${}_0S^{[\mathrm{I}]}(3\|\eta^*\eta;\,\eta_1^*\eta_1)\equiv-i\frac{1}{2}\eta_1^*\cdot[\{g^{[0]*}(01,01)+g^{[0]}(01,10)$$
$$+g^{[1]}(11,00)\}\eta^*\eta+g^{[1]}(02,00)\eta^2+g^{[1]}(20,00)(\eta^*)^2]$$
$$-i\frac{1}{2}\eta_1\cdot[\{g^{[0]}(01,01)+g^{[0]*}(01,10)-g^{[1]*}(11,00)\}\eta^*\eta$$

$$-g^{[1]*}(20,00)\eta^2-g^{[1]*}(02,00)(\eta^*)^2] \tag{A·20}$$

with

$$g^{[0]}(01,01)+g^{[0]*}(01,10)=0\,, \tag{A·21}$$

where we have used the condition for $S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ to be a real function by definition.

Similarly, substituting (A·8) into (A·11b) and integrating $T_1(2)$ with respect to η_1, for $S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ we obtain

$$\begin{aligned}
{}_1S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)&\equiv i\frac{1}{2}\eta_1{}^*\cdot[\{g^{[1]}(20,00)-g^{[0]}(10,10)\}(\eta^*)^2\\
&+\{g^{[1]}(11,00)+g^{[0]*}(01,01)-g^{[0]}(01,10)\}\eta^*\eta\\
&+\{g^{[1]}(02,00)+g^{[0]*}(10,01)\}\eta^2]-i\frac{1}{2}\eta_1\cdot[\{g^{[1]*}(02,00)\\
&+g^{[0]}(10,01)\}(\eta^*)^2+\{g^{[1]*}(11,00)+g^{[0]}(01,01)\\
&-g^{[0]*}(01,10)\}\eta^*\eta+\{g^{[1]*}(20,00)-g^{[0]*}(10,10)\}\eta^2]\,.
\end{aligned} \tag{A·22}$$

By the definition of S in Eq. (4·2), we have to have the condition

$$S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)\equiv{}_0S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)={}_1S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)\,, \tag{A·23}$$

from which we obtain the following relations:

$$2g^{[1]}(20,00)-g^{[0]}(10,10)=0\,, \tag{A·24a}$$

$$g^{[1]}(11,00)+g^{[0]*}(01,01)=0\,, \tag{A·24b}$$

$$2g^{[1]}(02,00)+g^{[0]*}(10,01)=0\,. \tag{A·24c}$$

Now, with the use of (A·14) and (A·17), the part $\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ in (A·10) is written as

$$\begin{aligned}
\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)&=\omega_0\{\eta^*\cdot g_0{}^{[1]}(2\|\eta^*\eta;\,\eta_1{}^*\eta_1)\\
&+\eta\cdot g_0{}^{[1]*}(2\|\eta^*\eta;\,\eta_1{}^*\eta_1)\}+\omega_1\{\eta_1{}^*\cdot g_1(2\|\eta^*\eta)\\
&+\eta_1\cdot g_1{}^*(2\|\eta^*\eta)\}+\Delta\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)\,.
\end{aligned} \tag{A·25}$$

In the *nonresonant case* where the resonance condition (A·1) is not satisfied, the requirement $\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)=0$ (implying the collective Hamiltonian to be *normal*) always enables us to determine $g_0{}^{[1]}(2\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ and $g_1(2\|\eta^*\eta)$ in (A·8), together with the relations (A·21) and (A·24). We can thus specify the appropriate choice for $S^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ in the nonresonant case.

In the *resonant case* with (A·1) under consideration, however, it is *impossible* to demand $\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)=0$, because $\mathcal{H}^{[1]}(3\|\eta^*\eta;\,\eta_1{}^*\eta_1)$ includes the following term:

$$\begin{aligned}
&\{\omega_0\eta^2\eta_1{}^*\cdot g^{[0]*}(10,01)+\omega_1\eta_1{}^*\eta^2\cdot g^{[1]}(02,00)+\eta_1{}^*\eta^2[\Delta\mathcal{H}_{[1]}(3\|\eta^*\eta)]_{02}\}+\text{c.c.}\\
&=\eta_1{}^*\eta^2\{\omega_0 g^{[0]*}(10,01)+\omega_1 g^{[1]}(02,00)+[\Delta\mathcal{H}_{[1]}(3\|\eta^*\eta)]_{02}\}+\text{c.c.}\,,
\end{aligned} \tag{A·26}$$

where we have used the notation

$$\varDelta\mathcal{H}^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)\equiv\eta_1^*\cdot\varDelta\mathcal{H}_{[1]}(3\|\eta^*\eta)+\eta_1\cdot\varDelta\mathcal{H}^*_{[1]}(3\|\eta^*\eta) \tag{A·27}$$

and the symbol$[\cdots\cdots]_{rs}$ is defined in Eq. (3·15). In the resonant case with the relation $\omega_1=2\omega_0$ given in (A·1), Eq. (A·26) is simply reduced to

$$\eta_1^*\eta^2\cdot[\omega_0\{g^{[0]*}(10,01)+2g^{[1]}(02,00)\}+[\varDelta\mathcal{H}_{[1]}(3\|\eta^*\eta)_{02}]]+\text{c.c.} \tag{A·28}$$

Because of the existence of the relation (A·24c), this term never vanishes within any choice of $S^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ and there inevitably appears the essential coupling term in the third order:

$$\mathcal{H}^{(\mathrm{res})}(n=3)\equiv[\varDelta\mathcal{H}_{[1]}(3\|\eta^*\eta)]_{02}\cdot\eta_1^*\eta^2+\text{c.c.} \tag{A·29}$$

By using the fact that the choice of the functional form of $S(\eta^*\eta;\ \eta_1^*\eta_1)$ just corresponds to fixing the degree of freedom of canonical transformation, in this case, an optimum function $S^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ in this resonant case is determined by choosing the following form of it: Both ${}_0S^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ in (A·20) and ${}_1S^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ in (A·22) have no terms with the forms, $\eta_1^*\eta^2$ and $\eta_1(\eta^*)^2$, by which $\mathcal{H}^{(\mathrm{res})}(3)$ is expressed. This is satisfied by setting

$$g^{[1]}(02,00)=g^{[0]}(10,01)=0\,. \tag{A·30}$$

The other terms in $\mathcal{H}^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ except for $\mathcal{H}^{(\mathrm{res})}(n=3)$ can be made to vanish by setting

$$\omega_0\{g^{[0]}(01,10)+g^{[0]*}(01,01)\}+\omega_1g^{[1]}(11,00)+[\varDelta\mathcal{H}_{[1]}(3\|\eta^*\eta)]_{11}=0\,, \tag{A·31}$$

$$\omega_0g^{[0]}(10,10)+\omega_1g^{[1]}(20,00)+[\varDelta\mathcal{H}_{[1]}(3\|\eta^*\eta)]_{20}=0\,. \tag{A·32}$$

It is now clear that the set of (A·21), (A·24), (A·30), (A·31) and (A·32) is enough to determine $g_0^{[0]}(2\|\eta^*\eta;\ \eta_1^*\eta_1)$ and $g_1(2\|\eta^*\eta)$ in the resonant case, which specify the optimum choice of $S^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$.

(I-3) *Choice of* $S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$

Substituting (A·8) into (A·11a) and integrating $T_0(2)$ with respect to η, and then using the condition $S(3)=S^*(3)$, for $S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ we obtain

$$\begin{aligned}
&{}_0S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)\\
&\quad\equiv-i\frac{1}{2}(\eta_1^*)^2\cdot[\{g^{[1]}(01,10)+g^{[0]*}(00,02)\}\eta-\{g^{[0]}(00,20)-g^{[1]}(10,10)\}\eta^*]\\
&\quad-i\frac{1}{2}(\eta_1^*\eta_1)\cdot[\{g^{[1]}(01,01)-g^{[1]*}(10,01)+g^{[0]*}(00,11)\}\eta\\
&\qquad\qquad-\{g^{[1]*}(01,01)-g^{[1]}(10,01)+g^{[0]}(00,11)\}\eta^*]\\
&\quad-i\frac{1}{2}(\eta_1^2)\cdot[\{g^{[0]*}(00,20)-g^{[1]*}(10,10)\}\eta\\
&\qquad\qquad-\{g^{[1]*}(01,10)+g^{[0]}(00,02)\}\eta^*]\,.
\end{aligned} \tag{A·33}$$

Similarly, from $T_1(2)$ in (A·11b), we obtain

$$
\begin{aligned}
&{}_1S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1) \\
&\quad \equiv -i\frac{1}{2}(\eta_1^*)^2\cdot[g^{[0]}(00,20)\eta^* - g^{[0]*}(00,02)\eta] \\
&\qquad -i\frac{1}{2}(\eta_1^*\eta_1)\cdot[\{g^{[1]*}(01,01)+g^{[1]}(10,01)+g^{[0]}(00,11)\}\eta^* \\
&\qquad\qquad +\{g^{[1]*}(10,01)+g^{[1]}(01,01)-g^{[0]*}(00,11)\}\eta] \\
&\qquad -i\frac{1}{2}(\eta_1)^2\cdot[g^{[0]}(00,02)\eta^* - g^{[0]*}(00,20)\eta]\,. \qquad (\mathrm{A}\cdot 34)
\end{aligned}
$$

The condition

$$
S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)\equiv{}_0S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)={}_1S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1) \qquad (\mathrm{A}\cdot 35)
$$

leads to the relations

$$
\begin{aligned}
&2g^{[0]}(00,20)-g^{[1]}(10,10)=0\,, \\
&2g^{[0]*}(00,02)+g^{[1]}(01,10)=0\,, \\
&g^{[0]}(00,11)+g^{[1]*}(01,01)=0\,, \\
&g^{[0]*}(00,11)-g^{[1]*}(10,01)=0\,. \qquad (\mathrm{A}\cdot 36)
\end{aligned}
$$

With the use of (A·14) and (A·17), the part $\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ of the collective Hamiltonian (A·10) can be written as

$$
\begin{aligned}
\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)&=\omega_0\{\eta^*\cdot g_0(2\|\eta_1^*\eta_1)+\eta\cdot g_0^*(2\|\eta_1^*\eta_1)\} \\
&\quad +\omega_1\{\eta_1^*\cdot g_1^{[1]}(2\|\eta^*\eta;\ \eta_1^*\ \eta_1)+\eta_1\cdot g_1^{[1]*}(2\|\eta^*\eta;\ \eta_1^*\eta_1)\} \\
&\quad +\Delta\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)\,. \qquad (\mathrm{A}\cdot 37)
\end{aligned}
$$

By the definition in (A·17), $\Delta\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ is a known function obtained from (A·15), and we express it as

$$
\begin{aligned}
\Delta\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)&\equiv\Delta\mathcal{H}^{(20)}_{[\mathrm{II}]}(3\|\eta^*\eta)\cdot(\eta_1^*)^2 \\
&\quad +\Delta\mathcal{H}^{(11)}_{[\mathrm{II}]}(3\|\eta^*\eta)\cdot(\eta_1^*\eta_1)+\Delta\mathcal{H}^{(02)}_{[\mathrm{II}]}(3\|\eta^*\eta)\cdot(\eta_1)^2\,. \qquad (\mathrm{A}\cdot 38)
\end{aligned}
$$

Demanding $\mathcal{H}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)=0$, we thus have

$$
\begin{aligned}
&\omega_0\cdot g^{[0]}(00,20)+\omega_0\cdot g^{[1]}(10,10)+[\Delta\mathcal{H}^{(20)}_{[\mathrm{II}]}(3\|\eta^*\eta)]_{10}=0\,, \\
&\omega_0\cdot g^{[0]*}(00,02)+\omega_1\cdot g^{[1]}(01,10)+[\Delta\mathcal{H}^{(20)}_{[\mathrm{II}]}(3\|\eta^*\eta)]_{01}=0\,, \\
&\omega_0\cdot g^{[0]}(00,11)+\omega_1\{g^{[1]}(10,01)+g^{[1]*}(01,01)\}+[\Delta\mathcal{H}^{(11)}_{[\mathrm{II}]}(3\|\eta^*\eta)]_{10}=0\,, \qquad (\mathrm{A}\cdot 39)
\end{aligned}
$$

where the symbol $[\cdots\cdots]_{rs}$ is defined in Eq. (3·15).

It is clear that the set of (A·36) and (A·39) is enough to determine $g_0(2\|\eta_1^*\eta_1^*)$ and $g_1^{[1]}(2\|\eta^*\eta;\ \eta_1^*\eta_1)$, which specify the optimum choice of $S^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$.

[II] *Determination of* $i\hat{G}(n=3)$

We go on to determine $i\hat{G}(n=3)$ in (A·2):

$$i\hat{G}(3)=\sum_{\lambda}\{g_\lambda(3)\hat{X}_\lambda{}^\dagger-g_\lambda{}^*(3)\hat{X}_\lambda\}\,,$$

$$g_\lambda(3)=\sum_{(rs,pq)}g^{[\lambda]}(rs,pq)(\eta^*)^r(\eta)^s(\eta_1{}^*)^p(\eta_1)^q\,,\quad r+s+p+q=3\,, \tag{A·40}$$

provided that $i\hat{G}(1)$ and $i\hat{G}(2)$ are known.

In the analogous way to the case of $i\hat{G}(2)$, the equation of submanifold (4·1) directly determines $g_\lambda(3)$ with $\lambda\neq 0$ and 1. We use the canonical-variable condition (4·2), in order to determine $g_{\lambda=0}(3)$ and $g_{\lambda=1}(3)$ by choosing an optimum function $S(4)$ in (A·4).

With the use of Eq. (3·11), for $T_0(3)$ and $T_1(3)$ in (A·5) we have

$$T_0(3)\equiv\left[\langle\phi_0|e^{-i\hat{G}}\frac{\partial}{\partial\eta}e^{i\hat{G}}|\phi_0\rangle\right]^{(n=3)}$$

$$=\frac{1}{2}g_0{}^*(3)+\frac{1}{2}\left\{\eta^*\frac{\partial}{\partial\eta}g_0(3)-\eta\frac{\partial}{\partial\eta}g_0{}^*(3)\right.$$

$$\left.+\eta_1{}^*\frac{\partial}{\partial\eta}g_1(3)-\eta_1\frac{\partial}{\partial\eta}g_1{}^*(3)\right\}+\varDelta T_0(3)\,, \tag{A·41a}$$

$$T_1(3)=\frac{1}{2}g_1{}^*(3)+\frac{1}{2}\left\{\eta^*\frac{\partial}{\partial\eta_1}g_0(3)-\eta\frac{\partial}{\partial\eta_1}g_0{}^*(3)\right.$$

$$\left.+\eta_1{}^*\frac{\partial}{\partial\eta_1}g_1(3)-\eta_1\frac{\partial}{\partial\eta_1}g_1{}^*(3)\right\}+\varDelta T_1(3)\,, \tag{A·41b}$$

where $\varDelta T_k(3)$ $(k=0,1)$ are known functions, defined by

$$\varDelta T_k(3)\equiv\frac{1}{2}\langle\phi_0|\left[\frac{\partial i\hat{G}(2)}{\partial\eta_k},\,i\hat{G}(2)\right]|\phi_0\rangle$$

$$+\frac{1}{4!}\langle\phi_0|\left[\left[\left[\frac{\partial i\hat{G}(1)}{\partial\eta_k},\,i\hat{G}(1)\right],\,i\hat{G}(1)\right],\,i\hat{G}(1)\right]|\phi_0\rangle\,,$$

$$k=0,1\,,\quad \eta_{k=0}\equiv\eta\,. \tag{A·42}$$

With the use of Eq. (3·12), for the fourth-order part of the collective Hamiltonian we have

$$\mathcal{H}(n=4)\equiv[\langle\phi_0|e^{-i\hat{G}}\hat{H}e^{i\hat{G}}|\phi_0\rangle]^{(n=4)}$$

$$=\omega_0\{\eta^*\cdot g_0(3)+\eta\cdot g_0{}^*(3)\}+\omega_1\{\eta_1{}^*\cdot g_1(3)+\eta_1\cdot g_1{}^*(3)\}+\varDelta\mathcal{H}(4)\,, \tag{A·43}$$

where $\varDelta\mathcal{H}(4)$ is a known function, defined by

$$\varDelta\mathcal{H}(4)\equiv\frac{1}{2}\langle\phi_0|[[\hat{H},\,i\hat{G}(2)],\,i\hat{G}(2)]|\phi_0\rangle$$

$$+\frac{1}{3!}\langle\phi_0|[[[\hat{H},\,i\hat{G}(1)],\,i\hat{G}(1)],\,i\hat{G}(2)]+[[[\hat{H},\,i\hat{G}(1)],\,i\hat{G}(2)],\,i\hat{G}(1)]$$

$$+[[[\hat{H}, i\hat{G}(2)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle$$

$$+\frac{1}{4!}\langle\phi_0|[[[[\hat{H}, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle . \tag{A·44}$$

In the similar way to the case of $i\hat{G}(2)$, we classify $g_0(3)$, $g_1(3)$, $S(4)$ and $\mathcal{H}(4)$ according to the powers of $\eta_1{}^*$ and η_1:

$$g_\lambda(3)=g_\lambda(3\|\eta^*\eta)+g_\lambda{}^{[\mathrm{I}]}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)$$
$$+g_\lambda{}^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)+g_\lambda(3\|\eta_1{}^*\eta_1)\ ,\quad \lambda=0,1\ , \tag{A·45}$$

$$S(4)=S(4\|\eta^*\eta)+\sum_{N=\mathrm{I}}^{\mathrm{III}}S^{[N]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)+S(4\|\eta_1{}^*\eta_1)\ , \tag{A·46}$$

$$\mathcal{H}(4)=\mathcal{H}(4\|\eta^*\eta)+\sum_{N=\mathrm{I}}^{\mathrm{III}}\mathcal{H}^{(N)}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)+\mathcal{H}(4\|\eta_1{}^*\eta_1)\ . \tag{A·47}$$

The known quantity $\Delta\mathcal{H}(4)$ is also classified and is expressed as

$$\Delta\mathcal{H}(4)=\Delta\mathcal{H}(4\|\eta^*\eta)+\sum_{N=\mathrm{I}}^{\mathrm{III}}\Delta\mathcal{H}^{[N]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)+\Delta\mathcal{H}(4\|\eta_1{}^*\eta_1)\ ,$$

$$\Delta\mathcal{H}^{[\mathrm{I}]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)=\Delta\mathcal{H}^{(10)}_{[\mathrm{I}]}(4\|\eta^*\eta)\cdot\eta_1{}^*+\Delta\mathcal{H}^{(01)}_{[\mathrm{I}]}(4\|\eta^*\eta)\cdot\eta_1\ ,$$

$$\Delta\mathcal{H}^{[\mathrm{II}]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)=\sum_{p,q}\Delta\mathcal{H}^{(pq)}_{[\mathrm{II}]}(4\|\eta^*\eta)\cdot(\eta_1{}^*)^p(\eta_1)^q\ ,\quad p+q=2\ ,$$

$$\Delta\mathcal{H}^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)=\sum_{p,q}\Delta\mathcal{H}^{(pq)}_{[\mathrm{III}]}(4\|\eta^*\eta)\cdot(\eta_1{}^*)^p(\eta_1)^q\ ,\quad p+q=3\ . \tag{A·48}$$

(II-1) *Choice of* $S(4\|\eta^*\eta)$ *and of* $S(4|\eta_1{}^*\eta_1)$

Substituting (A·45) into (A·41a) and integrating $T_0(3)$ with respect to η, we obtain an expression for $S(4\|\eta^*\eta)$ similar to Eq. (3·26) in § 3. The condition $S(4\|\eta^*\eta)=S^*(4\|\eta^*\eta)$ leads us to the relation

$$3g^{[0]}(03,00)+g^{[0]*}(21,00)=-[\Delta T_0(3\|\eta^*\eta)]_{12}-3[\Delta T_0(3\|\eta^*\eta)]^*_{30}\ , \tag{A·49}$$

where $\Delta T_{k=0,1}(3)$ is classified according to the powers of $\eta_1{}^*$ and η_1:

$$\Delta T_k(3)=\Delta T_k(3\|\eta^*\eta)+\sum_{N=\mathrm{I}}^{\mathrm{II}}\Delta T_k{}^{[N]}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)+\Delta T_k(3\|\eta_1{}^*\eta_1)\ ,$$
$$k=0,1\ , \tag{A·50}$$

and the symbol $[\cdots\cdots]_{rs}$ is defined in Eq. (3·15). Demanding $\mathcal{H}(4\|\eta^*\eta)$ to be normal, i.e., $[\mathcal{H}(4\|\eta^*\eta)]_{rs}=0$ for $r\neq s$, from (A·43) we obtain the relations

$$\omega_0 g^{[0]}(30,00)+[\Delta\mathcal{H}(4\|\eta^*\eta)]_{40}=0\ ,$$
$$\omega_0\{g^{[0]}(21,00)+g^{[0]*}(03,00)\}+[\Delta\mathcal{H}(4\|\eta^*\eta)]_{31}=0\ , \tag{A·51}$$

which is similar to Eq. (3·28). An optimum functional form of $S(4\|\eta^*\eta)$ is so chosen that it contains no terms with the diagonal form $(\eta^*\eta)^2$. This leads to

$$g^{[0]}(12,00)+[\Delta T_0(3\|\eta^*\eta)]_{21}=0\ , \tag{A·52}$$

which is similar to Eq. (3·30).

The relations (A·49), (A·51) and (A·52) are enough to determine the function $g_0(3\|\eta^*\eta)$, specifying the optimum choice of $S(4\|\eta^*\eta)$. The coefficient $h^{(0)}_{r=2}$ of $\mathscr{H}^{(0)}(\eta^*, \eta)$ in Eq. (4·4b) is now given by

$$h^{(0)}_{r=2}\equiv[\mathscr{H}(4\|\eta^*\eta)]_{22}=\omega_0\{g^{[0]}(12,00)+g^{[0]*}(12,00)\}+[\Delta\mathscr{H}(4\|\eta^*\eta)]_{22}$$
$$=[\Delta\mathscr{H}(4\|\eta^*\eta)]_{22}-\omega_0\{[\Delta T_0(3\|\eta^*\eta)]_{21}+[\Delta T_0(3\|\eta^*\eta)]^*_{21}\}\,, \tag{A·53}$$

where we have used (A·52).

In the same manner, we can also determine $g_1(3\|\eta_1{}^*\eta_1)$, as well as the coefficient $h^{(1)}_{r=2}$ of $\mathscr{H}^{(1)}(\eta_1{}^*, \eta_1)$ in Eq. (4·4c).

(II-2) *Choice of* $S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$

By substituting (A·45) into (A·41a) and integrating $T_0(3)$ with respect to η, and then by setting the condition $S(4)=S^*(4)$, we obtain an explicit expression for $S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$ which is denoted by ${}_0S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$. The condition ${}_0S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)={}_0S^{[I]*}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$ leads us to the relations

$$g^{[0]}(02,01)+\frac{1}{2}g^{[0]*}(11,10)=-[\Delta T^{(10)}_{0,[I]}(\eta^*\eta)]^*_{20}-\frac{1}{2}[\Delta T^{(01)}_{0,[I]}(\eta^*\eta)]_{11}\,,$$
$$g^{[0]*}(02,10)+\frac{1}{2}g^{[0]}(11,01)=-[\Delta T^{(01)}_{0,[I]}(\eta^*\eta)]_{20}-\frac{1}{2}[\Delta T^{(10)}_{0,[I]}(\eta^*\eta)]^*_{11}\,, \tag{A·54}$$

where we have used for $\Delta T^{[N]}_{k=0,1}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)$ in Eq. (A·50) the expression

$$\Delta T_k{}^{[N]}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)\equiv\sum_{\substack{p,q\\(p+q=N)}}\Delta T^{(pq)}_{k,[N]}(3\|\eta^*\eta)\cdot(\eta_1{}^*)^p(\eta_1)^q\,,\quad k=0,1\,, \tag{A·55}$$

and the symbol $[\cdots\cdots]_{rs}$ is defined in Eq. (3·15).

Similarly, by integrating $T_1(3)$ in Eq. (A·41b) with respect to η_1 and setting $S(4)=S^*(4)$, for $S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$ we have an explicit expression denoted by ${}_1S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$. The condition, $S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)\equiv{}_0S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)={}_1S^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$, leads us to the relations

$$-\frac{1}{3}g^{[0]}(20,10)+g^{[1]}(30,00)=-[\Delta T_1(3\|\eta^*\eta)]^*_{03}+\frac{1}{3}[\Delta T^{(01)}_{0,[I]}(3\|\eta^*\eta)]_{02}\,,$$
$$g^{[0]*}(02,01)+g^{[1]}(21,00)=-[\Delta T_1(3\|\eta^*\eta)]^*_{12}-[\Delta T^{(10)}_{0,[I]}(3\|\eta^*\eta)]_{20}\,,$$
$$\frac{1}{2}g^{[0]*}(11,01)+g^{[1]}(12,00)=-[\Delta T_1(3\|\eta^*\eta)]^*_{30}-\frac{1}{2}[\Delta T^{(10)}_{0,[I]}(3\|\eta^*\eta)]_{11}\,,$$
$$\frac{1}{3}g^{[0]*}(20,01)+g^{[1]}(03,00)=-[\Delta T_1(3\|\eta^*\eta)]^*_{30}-\frac{1}{3}[\Delta T^{(10)}_{0,[I]}(3\|\eta^*\eta)]_{02}\,. \tag{A·56}$$

The part $\mathscr{H}^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)$ of the fourth-order Hamiltonian $\mathscr{H}(4)$ in (A·47) is written as

$$\mathscr{H}^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)=\omega_0\{\eta^*\cdot g_0{}^{[I]}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)+\eta\cdot g_0{}^{[I]*}(3\|\eta^*\eta;\ \eta_1{}^*\eta_1)\}$$
$$+\omega_1\{\eta_1{}^*\cdot g_1(3\|\eta^*\eta)+\eta_1\cdot g_1{}^*(3\|\eta^*\eta)\}+\Delta\mathscr{H}^{[I]}(4\|\eta^*\eta;\ \eta_1{}^*\eta_1)\,. \tag{A·57}$$

Demanding $\mathscr{H}^{[\mathrm{I}]}(4\|\eta^*\eta;\eta_1^*\eta_1)=0$, we obtain

$$\omega_0 g^{[0]}(20,10)+\omega_1 g^{[1]}(30,00)+[\Delta\mathscr{H}^{(10)}_{[\mathrm{I}]}(4\|\eta^*\eta)]_{30}=0\,,$$

$$\omega_0\{g^{[0]}(11,10)+g^{[0]*}(02,01)\}+\omega_1 g^{[1]}(21,00)+[\Delta\mathscr{H}^{(10)}_{[\mathrm{I}]}(4\|\eta^*\eta)]_{21}=0\,,$$

$$\omega_0\{g^{[0]}(02,10)+g^{[0]*}(11,01)\}+\omega_1 g^{[1]}(12,00)+[\Delta\mathscr{H}^{(10)}_{[\mathrm{I}]}(4\|\eta^*\eta)]_{12}=0\,,$$

$$\omega_0 g^{[0]*}(20,01)+\omega_1 g^{[1]}(03,00)+[\Delta\mathscr{H}^{(10)}_{[\mathrm{I}]}(4\|\eta^*\eta)]_{03}=0\,. \tag{A·58}$$

The set of the relations (A·54), (A·56) and (A·58) is enough to determine the functions $g_0^{[\mathrm{I}]}(3\|\eta^*\eta;\eta_1^*\eta_1)$ and $g_1(3\|\eta^*,\eta)$ in (A·45), which specify the optimum choice of $S^{[\mathrm{I}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$.

(II-3) *Choice of* $S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$

By integrating $T_0(3)$ with respect to η and setting $S(4)=S^*(4)$, for $S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ we obtain an explicit expression denoted by ${}_0S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$. The condition ${}_0S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)={}_0S^{[\mathrm{II}]*}(4\|\eta^*\eta;\eta_1^*\eta_1)$ leads us to the relations

$$g^{[0]}(01,02)+g^{[0]*}(01,20)=-[\Delta T^{(20)}_{0,[\mathrm{II}]}(\eta^*\eta)]^*_{10}-[\Delta T^{(02)}_{0,[\mathrm{II}]}(\eta^*\eta)]_{10}\,. \tag{A·59}$$

Similarly, by integrating $T_1(3)$ with respect to η_1, we have an explicit expression for $S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$. The optimum functional form of $S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ is so chosen that *both* ${}_0S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ *and* ${}_1S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ *have no terms with the normal form such as* $(\eta^*\eta)(\eta_1^*\eta_1)$, in terms of which the fourth-order part $\mathscr{H}^{(0-1)}(\eta^*,\eta;\eta_1^*,\eta_1)$ in Eq. (4·4 d) is expressed. Imposing this condition on ${}_0S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ and ${}_1S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$, respectively, we obtain

$$g^{[0]*}(01,11)+g^{[0]}(01,11)+g^{[1]}(11,01)-g^{[1]*}(11,01)+2[\Delta T^{(11)}_{0,[\mathrm{II}]}(\eta^*\eta)]_{10}=0\,, \tag{A·60a}$$

$$g^{[0]}(01,11)-g^{[0]*}(01,11)+g^{[1]}(11,01)+g^{[1]*}(11,01)+2[\Delta T^{(10)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{11}=0\,. \tag{A·60b}$$

The equivalence condition, $S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)\equiv{}_0S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)={}_1S^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$, leads us to the relations

$$g^{[0]}(10,02)+g^{[1]*}(02,10)=-[\Delta T^{(01)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{20}-[\Delta T^{(20)}_{0,[\mathrm{II}]}(\eta^*\eta)]^*_{01}\,,$$

$$2g^{[0]*}(01,20)-g^{[1]*}(11,10)=[\Delta T^{(01)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{11}-2[\Delta T^{(02)}_{0,[\mathrm{II}]}(\eta^*\eta)]_{10}\,,$$

$$g^{[0]*}(10,20)-g^{[1]*}(20,10)=[\Delta T^{(01)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{02}-[\Delta T^{(02)}_{0,[\mathrm{II}]}(\eta^*\eta)]_{01}\,,$$

$$2g^{[1]*}(02,01)+g^{[0]}(10,11)=-2[\Delta T^{(10)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{20}-[\Delta T^{(11)}_{0,[\mathrm{II}]}(\eta^*\eta)]^*_{01}\,,$$

$$2g^{[1]*}(20,01)-g^{[0]*}(10,11)=-2[\Delta T^{(10)}_{1,[\mathrm{I}]}(\eta^*\eta)]_{02}+[\Delta T^{(11)}_{0,[\mathrm{II}]}(\eta^*\eta)]_{01}\,. \tag{A·61}$$

The part $\mathscr{H}^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)$ in (A·47) is written as

$$\begin{aligned}&\mathscr{H}^{[\mathrm{II}]}(4\|\eta^*\eta;\eta_1^*\eta_1)\\&\quad=\omega_0\{\eta^*\cdot g_0^{[\mathrm{II}]}(3\|\eta^*\eta;\eta_1^*\eta_1)+\eta\cdot g_0^{[\mathrm{II}]*}(3\|\eta^*\eta;\eta_1^*\eta_1)\}\\&\qquad+\omega_1\{\eta_1^*\cdot g_1^{[\mathrm{I}]}(3\|\eta^*\eta;\eta_1^*\eta_1)+\eta_1\cdot g_1^{[\mathrm{I}]*}(3\|\eta^*\eta;\eta_1^*\eta_1)\}\end{aligned}$$

$$+\Delta\mathcal{H}^{[II]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)\,. \tag{A·62}$$

Demanding the off-diagonal terms of $\mathcal{H}^{[II]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$ to vanish, we obtain the relations

$$\begin{aligned}
&\omega_0 g^{[0]}(10,02)+\omega_1 g^{[1]*}(02,10)=-[\Delta\mathcal{H}^{(02)}_{[II]}(4\|\eta^*\eta)]_{20}\,,\\
&\omega_0\{g^{[0]}(01,02)+g^{[0]*}(01,20)\}+\omega_1 g^{[1]*}(11,10)=-[\Delta\mathcal{H}^{(02)}_{[II]}(4\|\eta^*\eta)]_{11}\,,\\
&\omega_0 g^{[0]*}(10,20)+\omega_1 g^{[1]*}(20,10)=-[\Delta\mathcal{H}^{(02)}_{[II]}(4\|\eta^*\eta)]_{02}\,,\\
&\omega_0 g^{[0]}(10,11)+\omega_1\{g^{[1]}(20,01)+g^{[1]*}(02,01)\}=-[\Delta\mathcal{H}^{(11)}_{[II]}(4\|\eta^*\eta)]_{20}\,.
\end{aligned} \tag{A·63}$$

The set of the relations (A·59), (A·60), (A·61) and (A·63) is enough to determine the function $g_1^{[I]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ and $g_0^{[II]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ specifying the optimum choice of $S^{[II]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$. The diagonal part of $\mathcal{H}^{[II]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$, i.e., the coefficient $h^{(0-1)}_{11}$ in $\mathcal{H}^{(0-1)}(\eta^*\eta;\ \eta_1^*\eta_1)$ of Eq. (4·4d) is given by

$$\begin{aligned}
h^{(0-1)}_{11}&\equiv\omega_0\{g^{[0]}(01,11)+g^{[0]*}(01,11)\}+\omega_1\{g^{[1]}(11,01)+g^{[1]*}(11,01)\}\\
&\quad+[\Delta\mathcal{H}^{(11)}_{[II]}(\eta^*\eta)]_{11}\\
&=-\omega_0\{[\Delta T^{(11)}_{0,[II]}(\eta^*\eta)]_{10}+[\Delta T^{(11)}_{0,[II]}(\eta^*\eta)]^*_{10}\}\\
&\quad-\omega_1\{[\Delta T^{(10)}_{1,[I]}(\eta^*\eta)]_{11}+[\Delta T^{(10)}_{1,[I]}(\eta^*\eta)]^*_{11}\}+[\Delta\mathcal{H}^{(11)}_{[II]}(\eta^*\eta)]_{11}\,,
\end{aligned} \tag{A·64}$$

where we have used the relations (A·60a) and (A·60b).

(II-4) *Choice of* $S^{[III]}$ $(4\|\eta^*\eta;\ \eta_1^*\eta_1)$

From $T_0(3)$ and $T_1(3)$, for $S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$ we obtain two expressions ${}_0S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$ and ${}_1S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$. The condition $S(4)=S^*(4)$ then leads us to the relations

$$\begin{aligned}
&2\cdot g^{[1]}(01,02)+g^{[1]*}(10,11)\\
&\quad=-2\cdot[\Delta T^{(20)}_{1,[II]}(3\|\eta^*\eta)]^*_{10}-[\Delta T^{(11)}_{1,[II]}(3\|\eta^*\eta)]_{01}\,,\\
&2\cdot g^{[1]}(10,02)+g^{[1]*}(01,11)\\
&\quad=-2\cdot[\Delta T^{(20)}_{1,[II]}(3\|\eta^*\eta)]^*_{01}-[\Delta T^{(11)}_{1,[II]}(3\|\eta^*\eta)]_{10}\,.
\end{aligned} \tag{A·65}$$

From the equivalence condition, $S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)\equiv{}_0S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)={}_1S^{[III]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$, we obtain

$$\begin{aligned}
&-g^{[1]}(10,20)+3g^{[0]}(00,30)=[\Delta T^{(02)}_{1,[II]}(3\|\eta^*\eta)]^*_{01}-3([\Delta T_0(3\|\eta_1^*\eta_1)]^{03})^*\,,\\
&g^{[1]}(01,20)+3g^{[0]*}(00,03)=[\Delta T^{(02)}_{1,[II]}(3\|\eta^*\eta)]^*_{10}+3\cdot[\Delta T_0(3\|\eta_1^*\eta_1)]^{30}\,,\\
&g^{[1]*}(01,02)+g^{[0]}(00,21)=-[\Delta T^{(20)}_{1,[II]}(3\|\eta^*\eta)]_{10}-([\Delta T_0(3\|\eta_1^*\eta_1)]^{12})^*\,,\\
&g^{[1]*}(10,02)-g^{[0]*}(00,12)=-[\Delta T^{(20)}_{1,[II]}(3\|\eta^*\eta)]_{01}+[\Delta T_0(3\|\eta_1^*\eta_1)]^{21}\,,
\end{aligned} \tag{A·66}$$

where the symbol $[B(\eta_1^*,\eta_1)]^{rs}$ for an arbitrary function $B(\eta_1^*,\eta_1)$ represents the coefficient of the power-series expansion with respect to η_1^* and η_1:

$$B(\eta_1^*,\eta_1)=\sum_{r,s}B^{rs}\cdot(\eta_1^*)^r(\eta_1)^s\,,\qquad B^{rs}\equiv[B(\eta_1^*,\eta_1)]^{rs}\,. \tag{A·67}$$

The part $\mathscr{H}^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$ in (A·47) is written as

$$\begin{aligned}\mathscr{H}^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)&=\omega_0\{\eta^*\cdot g_0(3\|\eta_1^*\eta_1)+\eta\cdot g_0^*(3\|\eta_1^*\eta_1)\}\\&+\omega_1\{\eta_1^*\cdot g_1^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)+\eta_1\cdot g_1^{[\mathrm{II}]*}(3\|\eta^*\eta;\ \eta_1^*\eta_1)\}\\&+\varDelta\mathscr{H}^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)\,.\end{aligned}\tag{A·68}$$

Demanding $\mathscr{H}^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)=0$, we have

$$\begin{aligned}&\omega_0 g^{[0]}(00,30)+\omega_1 g^{[1]}(10,20)=-[\varDelta\mathscr{H}^{(30)}_{[\mathrm{III}]}(4\|\eta^*\eta)]_{10}\,,\\&\omega_0 g^{[0]*}(00,03)+\omega_1 g^{[1]}(01,20)=-[\varDelta\mathscr{H}^{(30)}_{[\mathrm{III}]}(4\|\eta^*\eta)]_{01}\,,\\&\omega_0 g^{[0]}(00,21)+\omega_1\{g^{[1]}(10,11)+g^{[1]*}(01,02)\}=-[\varDelta\mathscr{H}^{(21)}_{[\mathrm{III}]}(4\|\eta^*\eta)]_{10}\,,\\&\omega_0 g^{[0]*}(00,12)+\omega_1\{g^{[1]}(01,11)+g^{[1]*}(10,02)\}=-[\varDelta\mathscr{H}^{(21)}_{[\mathrm{III}]}(4\|\eta^*\eta)]_{01}\,.\end{aligned}\tag{A·69}$$

The set of the relations (A·65), (A·66) and (A·69) is enough to determine the functions $g_1^{[\mathrm{II}]}(3\|\eta^*\eta;\ \eta_1^*\eta_1)$ and $g_0(3\|\eta_1^*\eta_1)$, which specify the optimum choice of $S^{[\mathrm{III}]}(4\|\eta^*\eta;\ \eta_1^*\eta_1)$.

[III] *Rules for the Optimum Choice of* $S(\eta^*,\eta;\eta_1^*,\eta_1)$

From the above discussion it turns out that, starting with the boundary condition (A·3) and evaluating each power of η^*, η, η_1^* and η_1, we can determine the higher order terms $g_\lambda(n)$ in (A·2) as well as the maximally normal Hamiltonian (4·4) step by step, by choosing an optimum function $S(n+1)$ in (A·4).

The rules for choosing the optimum function $S(\eta^*,\eta;\eta_1^*,\eta_1)$ (in (A·4)) are the following:

i) By integrating $T_0(\eta^*,\eta;\eta_1^*,\eta_1)$ and $T_1(\eta^*,\eta;\eta_1^*,\eta_1)$ (in (A·5)) with respect to η and η_1, respectively, we obtain two expressions for $S(\eta^*,\eta;\eta_1^*,\eta_1)$. Demanding these two expressions to be real and to be completely equivalent to each other, a set of conditions to determine $i\widehat{G}(\eta^*,\eta;\eta_1^*,\eta_1)$ (in (A·2)) is obtained.

ii) The rest of the conditions is given by choosing the functional form of $S(\eta^*,\eta;\eta_1^*,\eta_1)$ so that it contains no terms with the forms of η^*, η, η_1^* and η_1, such as $(\eta^*\eta)^r(\eta_1^*\eta_1)^s(r,s\geq 0)$, $(\eta_1^*(\eta)^{n_0})^l$ and $((\eta^*)^{n_0}\eta_1)^l(l\geqq 1)$, in terms of which the maximally normal Hamiltonian (4·4) is expressed.

References

1) T. Marumori, T. Maskawa, F. Sakata and A. Kuriyama, Prog. Theor. Phys. **64** (1980), 1294.
2) T. Marumori, F. Sakata, T. Maskawa, T. Une and Y. Hashimoto, *Nuclear Collective Dynamics (Lecture of the 1982 International Summer School of Nuclear Physics, Brasov, Romania),* ed. D. Bucurescu, V. Ceausescu and N. V. Zamfir (World Scientific, 1985), p. 1.
3) T. Marumori and F. Sakata, *Particles and Nuclei*, ed. H. Terazawa (World Scientific, 1986), p. 207.
4) M. Matsuo and K. Matsuyanagi, Kyoto Univ. Preprint KUNS 861.
5) A. Klein, *Dynamical Structure of Nuclear States*, ed. D. J. Rowe (University of Toront Press, 1972), p. 38.
6) T. Marumori, A. Hayashi, T. Tomoda, A. Kuriyama and T. Maskawa, Prog. Theor. Phys. **63** (1980), 1576.
7) A. Kuriyama and M. Yamamura, Prog. Theor. Phys. **66** (1981), 2130, 2147.
F. Sakata, T. Marumori, Y. Hashimoto and T. Une, Prog. Theor. Phys. **70** (1983), 424.
8) S. T. Beliaev and V. G. Zelevinsky, Nucl. Phys. **39** (1962), 582.

T. Marumori, M. Yamamura and A. Tokunaga, Prog. Theor. Phys. **31** (1964), 1009.
E. R. Marshalek, Nucl. Phys. **A347** (1980), 253.
P. Ring and P. Shuck, *The Nuclear Many-Body Problem* (Springer-Verlag, 1980), Chap. 9.
T. Marumori, K. Takada and F. Sakata, Prog. Theor. Phys. Suppl. No. 71 (1981), 1.
T. Marumori, K. Takada and F. Sakata, *Proceedings of the Winter College on Fundamental Nuclear Physics,* ed. K. Dietrich, M. Di Toro and H. J. Mang (World Scientific, 1985), p. 897.
9) T. Marumori, Prog. Theor. Phys. **57** (1977), 112.
10) A. Kuriyama and M. Yamamura, Prog. Theor. Phys. **70** (1983), 1675.
11) G. D. Birkhoff, *Dynamical Systems* (Am. Math. Soc. New York, 1927), vol. IX.
F. G. Gustavson, Astron. J. **71** (1966), 670.