Maximally-Decoupled Collective Submanifold in a Simple Solvable Model$^*$

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(Received March 28, 1983)

The self-consistent collective-coordinate method formulated within the framework of the time-dependent Hartree-Fock theory is illustrated by using a simple solvable model. A concept of "maximally-decoupled" collective submanifold obtained by this method turns out to be a so-called hypersurface in the $l_p$-$l_h$ phase space, on which the TDHF trajectory corresponding to the "classical" large-amplitude collective motion travels. Various roles of dynamical and kinematical anharmonicity effects neglected under the random phase approximation are also clarified.

§ 1. Introduction

The main objective for describing the large-amplitude collective motion is to develop a new microscopic theory capable by itself of determining a "maximally-decoupled" collective subspace out of a huge-dimensional many fermion state-space. Here the "maximally-decoupled" collective subspace must satisfy such a dynamical condition that there does not exist any serious coupling between the collective subspace and the rest of fermion state-space. Namely it must be an approximate invariant subspace of the Hamiltonian. In order to define such a collective subspace, we proposed a self-consistent collective coordinate (SCC) method$^{3,4}$ on the basis of a fundamental principle called the invariance principle of the (time-dependent) Schrödinger equation.$^{5,6,7}$ Our method is quite different from the local harmonic approximation$^8$ and the adiabatic time-dependent Hartree-Fock approach.$^9$

The first aim of this paper is to illustrate feasibility of the SCC method by the use of a simple solvable model, within the framework of the time-dependent Hartree-Fock (TDHF) theory. As is well known, the TDHF theory gives a "classical" equation of motion in a $2MN$-dimensional phase space. Here, $M(N)$ denotes a number of single-particle(hole) states under consideration. In order to get a TDHF trajectory corresponding to the "classical" large-amplitude collective motion within the $2MN$-dimensional phase space, one has to face a difficult problem of solving the equation of motion which consists of a huge $2MN$-dimensional coupled differential equations. However, we are only interested in a "maximally-decoupled" collective motion whose trajectory can be described by, in principle, a few set of "collective" variables. In order to find out such collective variables without having to solve the $2MN$-dimensional coupled differential equation directly, the SCC method (within the framework of the TDHF theory) intends to

$^*$ A preliminary version of this work has been reported in the INS International Symposium on "Dynamics of the Nuclear Collective Motion" held on July 6-10, 1982 at the foot of Mt. Fuji.$^1$

$^{**}$ A detailed and self-contained explanation on the self-consistent collective-coordinate method as well as the invariance principle of the (time-dependent) Schrödinger equation is given in Lecture$^9$ at the 1982 Brasov International Summer School.
dynamically extract the so-called hypersurface (i.e., collective submanifold characterized by a few collective variables), on which a "collective" trajectory is determined so as to reproduce the TDHF trajectory under consideration as precisely as possible. The basic equations of the SCC method consist of two types of equations: The equation of path and equation of motion. The former equation defines the collective hypersurface within the 2MN-dimensional phase space and the latter equation describes a time-evolution of the collective motion on the hypersurface extracted by the former.

The second aim of this paper is to clarify the properties of the collective motion obtained by the SCC method in connection with various anharmonicity effects neglected under the random phase approximation (RPA): The SCC method has been developed for the aim to go beyond the RPA, and the maximally-decoupled collective subspace has to be dynamically extracted so as to automatically incorporate the main parts of the anharmonicity effects. The anharmonicity effects can be classified into two characteristic types; 1) dynamical anharmonicity effects due to the residual interaction which has been omitted within the RPA framework and ii) kinematical anharmonicity effects due to the Pauli principle between the particles (and holes) belonging to the different particle-hole pair operators. These effects will play various roles in defining the hypersurface as well as the collective Hamiltonian which governs the time evolution of the "collective" trajectory on the hypersurface.

In § 2, a simple model will be introduced and the TDHF theory will be applied to it. The SCC method will be recapitulated in § 3 by using the simple model, within the framework of the TDHF theory. In order to examine the various anharmonicity effects, a perturbative treatment of the basic equations of the SCC method is applied to it, with a "boundary" condition that the collective motion under consideration is connected with the RPA-phonon mode (with lowest eigenvalue) in the "small-amplitude" limit. The numerical results will be discussed in § 5, and § 6 will be devoted to the conclusion.

§ 2. Model Hamiltonian and application of the TDHF theory

Let us start with a simple model Hamiltonian given by

$$
\hat{H} = \varepsilon_0 \hat{K}_{\alpha\alpha} + \varepsilon_1 \hat{K}_{11} + \varepsilon_2 \hat{K}_{22} + \frac{V_1}{2} \{ \hat{K}_{10} \hat{K}_{10} + \text{h.c.} \} + \frac{V_2}{2} \{ \hat{K}_{20} \hat{K}_{20} + \text{h.c.} \} + \frac{V_3}{2} [ (\hat{K}_{10} + \hat{K}_{20}) (\hat{K}_{11} + \hat{K}_{21}) + \text{h.c.} ].
$$

(2.1)

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

$$
\overline{K}_{\alpha\beta} = \sum_{m=1}^{N} c_{2m} c_{\beta m}, \quad (\alpha, \beta = 0, 1, 2)
$$

(2.2)

which satisfy the following commutation relations:

$$
[\overline{K}_{\alpha\beta}, \overline{K}_{\gamma\delta}] = \delta_{\beta\gamma} \overline{K}_{\alpha\delta} - \delta_{\alpha\delta} \overline{K}_{\gamma\beta}.
$$

(2.3)

Hereafter, we will consider a system with $N$ particles and the lowest energy state $|\phi_0\rangle$. * A three level model with $V_1 = 0$ has been investigated in detail by Li, Klein and Dreizler. (10)
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\[ |\phi_0\rangle = \prod_{m=1}^N c_{\alpha m}^* |0\rangle, \quad (2.4) \]

where \(|0\rangle\) denotes the vacuum of the fermion operators \(c_{\alpha m}^*\) and \(c_{\alpha m}\).

For latter convenience, we introduce the RPA modes

\[ \tilde{X}_a = \phi_a \tilde{K}_a + \phi_a^* \tilde{K}_a^*, \quad (a=1, 2) \quad (2.5) \]

whose correlation amplitudes \((\phi_a, \phi_a^*)\) and excitation energies \(\omega_a\) are determined by the usual RPA equation,

\[ [\tilde{H}, \tilde{X}_a] = \omega_a \tilde{X}_a^* \quad (2.6) \]

Now, let us apply the TDHF theory to the present system. In the TDHF theory we introduce a time-dependent single Slater determinant given by

\[ |F(t), F(t)\rangle = \exp(i\tilde{F}(t)) |\phi_0\rangle, \]

\[ \tilde{F}(t) = F_1(t) \tilde{K}_{10} + F_2(t) \tilde{K}_{20} + F_1^*(t) \tilde{K}_{01} + F_2^*(t) \tilde{K}_{02}, \]

where parameters \(F_1\) and \(F_2\) are supposed to be complex and have explicit time-dependence. Instead of the parameters \(F_1\) and \(F_2\), it is convenient to employ the other set of parameters \(f_1\) and \(f_2\) which are related to the original parameters through

\[ F_k = -i \frac{f_k}{\sqrt{f_1 f_1^* + f_2 f_2^*}} \sin^{-1} \left( \frac{f_1 f_1^* + f_2 f_2^*}{N} \right), \quad (2.8a) \]

\[ f_k - i \sqrt{N} \frac{F_k}{\sqrt{F_1 F_1^* + F_2 F_2^*}} \sin \sqrt{F_1 F_1^* + F_2 F_2^*}. \quad (2.8b) \]

From the TDHF equation, i.e.,

\[ \partial_t \langle \phi_0 | e^{-i\tilde{H}t} \phi_0 \rangle = 0, \quad (2.9) \]

we then have a canonical equation of motion consisting of

\[ i \dot{f}_k = -\frac{\partial \mathcal{H}}{\partial f_k^*}, \quad i \dot{f}_k^* = -\frac{\partial \mathcal{H}}{\partial f_k}, \quad (2.10a) \]

where

\[ \mathcal{H} = \langle \phi_0 | e^{-i\tilde{H}t} \phi_0 \rangle - \langle \phi_0 | \tilde{H} | \phi_0 \rangle. \quad (2.10b) \]

Thus the "classical" equation of motion (2.10a) determines a trajectory within the 4-dimensional phase space given by

\[ \{p_1, q_1, p_2, q_2\}; \quad p_1 = \frac{i}{\sqrt{2}} (f_1^* - f_2), \quad q_1 = -\frac{i}{\sqrt{2}} (f_1^* + f_2). \quad (2.11) \]

\(^*)\) Throughout this paper, we adopt the convention of using \(\hbar = 1\).
§ 3. Application of self-consistent collective coordinate method

In contrast with Eq. (2·7), the SCC method\(^2\) introduces a unitary transformation 
\( e^{i\bar{\mathcal{H}}(t)}|\phi_0\rangle \) whose time-dependence is supposed to be specified by a few time-dependent collective parameters, i.e., in the present case, by a single pair of parameters \( \{\eta, \eta^*\} \):

\[
|\eta(t)\rangle = e^{i\bar{\mathcal{G}}(t, \eta^*)}|\phi_0\rangle, \\
\bar{\mathcal{G}}(\eta, \eta^*) = \{G_1(\eta, \eta^*)\bar{K}_{10} + G_2(\eta, \eta^*)\bar{K}_{20}\} + \text{h.c.}
\] (3·1)

According to the SCC method, the time-dependence of the collective parameters \( \{\eta(t), \eta^*(t)\} \) as well as the hermitian operator \( \bar{\mathcal{G}}(t) \) must be determined in such a way that the time-dependent Schrödinger equation remains invariant under the unitary transformation \( \exp(i\bar{\mathcal{G}}) \). In the TDHF variational form, this is simply written as

\[
\delta \langle \phi_0 | e^{-i\bar{\mathcal{H}} \left\{ \frac{\partial}{\partial t} - \bar{\mathcal{H}} \right\}} e^{i\bar{\mathcal{G}}} | \phi_0 \rangle = 0, 
\] (3·2)

which is a manifestation of the invariance principle of the Schrödinger equation formulated within the framework of the TDHF theory. Since the time-dependence of the unitary transformation is supposed to be completely specified by the time-dependent "collective" parameters \( \{\eta(t), \eta^*(t)\} \) alone, Eq. (3·2) can be rewritten as

\[
\delta \langle \phi_0 | e^{-i\bar{\mathcal{H}} - i\bar{\mathcal{G}}(\eta, \eta^*) + i\eta^* \bar{O}_0(\eta, \eta^*)} e^{i\bar{\mathcal{G}}} | \phi_0 \rangle = 0, 
\] (3·3)

where operators \( \bar{O}_0'(\eta, \eta^*) \) and \( \bar{O}_0(\eta, \eta^*) \) are the local infinitesimal generators with respect to \( \eta \) and \( \eta^* \) defined by

\[
\bar{O}_0'(\eta, \eta^*) = -\left( \frac{\partial}{\partial \eta} e^{i\bar{\mathcal{G}}} \right) e^{-i\bar{\mathcal{G}}}, 
\bar{O}_0(\eta, \eta^*) = -\left( \frac{\partial}{\partial \eta^*} e^{i\bar{\mathcal{G}}} \right) e^{-i\bar{\mathcal{G}}}. 
\] (3·4)

The second basic ingredient of the SCC method is a requirement that the time-dependence of the collective parameters \( \{\eta(t), \eta^*(t)\} \) must be determined by a canonical equation of motion

\[
i\dot{\eta} = \frac{\partial \bar{\mathcal{K}}}{\partial \eta^*}, 
i\dot{\eta}^* = -\frac{\partial \bar{\mathcal{K}}}{\partial \eta},
\] (3·5)

where the "collective" Hamiltonian \( \bar{\mathcal{K}}(\eta, \eta^*) \) is defined by

\[
\bar{\mathcal{K}} = \langle \phi_0 | e^{-i\bar{\mathcal{H}} + i\bar{\mathcal{G}}} \bar{\mathcal{H}} e^{i\bar{\mathcal{G}}} | \phi_0 \rangle - \langle \phi_0 | \bar{\mathcal{H}} | \phi_0 \rangle.
\] (3·6)

As will be shown later, this requirement can be expressed as

\[
\langle \phi_0 | e^{-i\bar{\mathcal{G}}} \bar{O}_0'(\eta, \eta^*) e^{i\bar{\mathcal{G}}} | \phi_0 \rangle = \frac{1}{2} \eta^*, \\
\langle \phi_0 | e^{-i\bar{\mathcal{G}}} \bar{O}_0(\eta, \eta^*) e^{i\bar{\mathcal{G}}} | \phi_0 \rangle = \frac{1}{2} \eta
\] (3·7)

which are called the canonical-variables condition.\(^3\) Equation (3·7) certifies that the infinitesimal generators satisfy a "weak" boson-like commutation relation:
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\[ \langle \phi_0 | e^{-i\theta} [\hat{O}(\eta, \eta^*), \hat{O}(\eta, \eta^*)] \rangle \phi_0 = \langle \phi_0 | [\hat{O}(\eta, \eta^*), \hat{O}(\eta, \eta^*)] \rangle \phi_0 = 1, \quad (3.8) \]

where

\[ \hat{O}(\eta, \eta^*) = e^{-i\theta} \hat{O}(\eta, \eta^*) e^{i\theta}. \quad (3.9) \]

In deriving Eq. (3.8) from Eq. (3.7), we have used an assumption that the functions \( G_k(\eta, \eta^*) \) in Eq. (3.1) are analytic functions of \( \{\eta, \eta^*\}.^{23} \)

Equations (3.3) and (3.7) are basic equations of the SCC method. In order to clarify physical meaning of these equations, it is worth-while to see that they are alternatively expressed as two types of equations: \textit{equation of motion} and \textit{equation of path}. The former is obtained from Eq. (3.3) by taking variations with respect to collective directions \( \delta_\eta |\phi_0\rangle \),

\[ |\delta_\eta |\phi_0\rangle = : \hat{O}^*(\eta, \eta^*) : |\phi_0\rangle \quad \text{and} \quad : \hat{O}(\eta, \eta^*) : |\phi_0\rangle, \quad (3.10) \]

where

\[ : \hat{O}^*(\eta, \eta^*) : \equiv \hat{O}^*(\eta, \eta^*) - \langle \phi_0 | \hat{O}^*(\eta, \eta^*) |\phi_0\rangle. \quad (3.11) \]

Namely, with the aid of Eq. (3.8) derived from the canonical-variables condition (3.7), the variational equation

\[ \delta_\eta \langle \phi_0 | e^{-i\theta} \{ \hat{H} - i \eta \hat{O}_0^*(\eta, \eta^*) + i \eta^* \hat{O}_0(\eta, \eta^*) \} e^{i\theta} |\phi_0\rangle = 0, \quad (3.12) \]

is reduced to the canonical \textit{equation of motion} (3.5). In contrast with the TDHF theory which determines a trajectory within the 4-dimensional phase space \( \{p_1, p_2, q_1, q_2\} \) given by Eq. (2.11), Eq. (3.5) gives a trajectory within a 2-dimensional collective phase space:

\[ \{p, q\}; \quad p = \frac{i}{\sqrt{2}} (\eta^* - \eta), \quad q = \frac{1}{\sqrt{2}} (\eta^* + \eta). \quad (3.13) \]

The rest of the equation is derived from Eq. (3.3) by taking variations perpendicular to the collective directions, \( \delta_\perp |\phi_0\rangle \) defined by

\[ \langle \delta_\perp |\phi_0\rangle |\phi_0\rangle = 0, \quad (3.14) \]

and it is written as

\[ \delta_\perp |\phi_0\rangle e^{-i\theta} \hat{H} e^{i\theta} |\phi_0\rangle = 0. \quad (3.15) \]

Equations (3.15) and (3.7) provide a set of necessary and sufficient conditions to determine the functional forms of \( G_k(\eta, \eta^*) \) \( (k=1, 2) \) in Eq. (3.1).

Since we can obtain a hypersurface in the 4-dimensional phase space by substituting \( G_k(\eta, \eta^*) \) for \( F_k \) in Eq. (2.7), Eq. (3.15) is called an \textit{equation of path} for determining the collective submanifold within the TDHF phase space. In the same way, by substituting \( G_k(\eta, \eta^*) \) for \( F_k \) in Eq. (2.8b), the trajectory in the TDHF phase space governed by Eq. (2.10a) can be regarded as a trajectory on the hypersurface which is governed by Eq. (3.5).

From the above discussion, it becomes clear that the SCC method intends to define a collective hypersurface along the TDHF trajectory in such a way that the collective Hamiltonian (3.6) determines a trajectory on the hypersurface so as to realize the TDHF trajectory as precisely as possible (see Fig. 2). We call this collective hypersurface a
§ 4. Perturbative treatment of the self-consistent collective coordinate method

As it may be difficult to solve the basic equations analytically except for a very simple case, we have developed a perturbative treatment called an \((\eta, \eta^*)\)-expansion method\(^3\) which is suitable for clarifying various roles of the anharmonicity effects neglected under the RPA. In this treatment, we express \(\vec{F}(t)\) and \(\vec{G}(t)\) in Eqs. (2·7) and (3·1) in the forms, respectively,

\[
\vec{F}(t) = \sum_{r=1}^{2} \{ F_{r\nu} \vec{X}_{\nu} + F_{r\nu}^* \vec{X}_{\nu}^* \},
\]

\[
\vec{G}(t) = \sum_{r=1}^{2} \{ G_{2\nu}(\eta, \eta^*) \vec{X}_{\nu} + G_{2\nu}^*(\eta, \eta^*) \vec{X}_{\nu}^* \}, \tag{4·1}
\]

where the complete set of the RPA modes defined by Eq. (2·5) is employed instead of the particle-hole pair operators. Then, the coefficients \(G_{2\nu}(\eta, \eta^*)\) in Eq. (4·1) and the collective Hamiltonian in Eq. (3·6) are expanded as power series of \((\eta, \eta^*)\),

\[
G_{2\nu} = \sum_{n=1}^{\infty} G_{2\nu}(n); \quad G_{2\nu}(n) = \sum_{r, s=1}^{2} G_{2\nu}^s(\eta^*)^s(\eta)^r, \tag{4·2a}
\]

\[
\vec{R} = \sum_{n=2}^{\infty} \vec{R}(n); \quad \vec{R}(n) = \sum_{r, s=1}^{2} \eta_{rs}(n)^{r+s}. \tag{4·2b}
\]

We also use the following notations:

\[
\vec{G} = \sum_{n=1}^{\infty} \vec{G}(n); \quad \vec{G}(n) = \sum_{r=1}^{2} \{ G_{2\nu}(n) \vec{X}_{\nu} + G_{2\nu}^*(n) \vec{X}_{\nu}^* \}. \tag{4·3}
\]

In this perturbative method, it is convenient to express Eq. (3·15) in the form

\[
\delta \langle \phi_0 | e^{-\frac{i}{\hbar} \vec{H} e^{\frac{i}{\hbar} \vec{c}} - \frac{\partial \vec{R}}{\partial \eta} \vec{O}(\eta, \eta^*) - \frac{\partial \vec{R}}{\partial \eta^*} \vec{O}(\eta, \eta^*) } | \phi_0 \rangle = 0, \tag{4·4}
\]

where the second and third terms are retained so as to automatically cancel the non-zero components \(\delta \langle \phi_0 | e^{-\frac{i}{\hbar} \vec{H} e^{\frac{i}{\hbar} \vec{c}} } | \phi_0 \rangle\) with the aid of relations:

\[
\langle \phi_0 | [ \vec{O}(\eta, \eta^*), e^{-\frac{i}{\hbar} \vec{H} e^{\frac{i}{\hbar} \vec{c}} } ] | \phi_0 \rangle = \frac{\partial \vec{R}}{\partial \eta} \quad \text{and} \quad \text{h.c.} \tag{4·5}
\]

The advantage of Eq. (4·4) over Eq. (3·15) exists in the fact that we can evaluate
Eq. (3.15) without having to advance the knowledge of the variations $|\delta_1 \phi_0\rangle$.

Thus the set of basic equations are summarized as

\[ i \dot{\eta} = \frac{\partial \mathcal{R}}{\partial \eta^*}, \quad \dot{\eta} = -\frac{\partial \mathcal{R}}{\partial \eta} \quad \text{(I)} \]

with the definition of the collective Hamiltonian

\[ \mathcal{R} \equiv \langle \phi_0 | e^{-i \mathcal{H} t} \mathcal{H} e^{i \mathcal{H} t} | \phi_0 \rangle - \langle \phi_0 | \mathcal{H} | \phi_0 \rangle. \quad \text{(II)} \]

\[ \delta \langle \phi_0 | e^{-i \mathcal{H} t} \mathcal{H} e^{i \mathcal{H} t} \left( \frac{\partial \mathcal{R}}{\partial \eta^*} \dot{\eta}^* + \frac{\partial \mathcal{R}}{\partial \eta} \dot{\eta} \right) | \phi_0 \rangle = 0 \quad \text{(III)} \]

with the canonical variables condition

\[ \langle \phi_0 | e^{-i \mathcal{H} t} \frac{\partial}{\partial \eta^*} e^{i \mathcal{H} t} | \phi_0 \rangle = -\frac{\eta^*}{2}, \quad \langle \phi_0 | e^{-i \mathcal{H} t} \frac{\partial}{\partial \eta} e^{i \mathcal{H} t} | \phi_0 \rangle = -\frac{\eta}{2} \quad \text{(IV)} \]

By substituting Eq. (4.2) into Eqs. (II)~(IV), we get the basic equations expanded in the forms of the power series of $(\eta, \eta^*)$. Since these equations may be assumed to be valid for continuous ranges of $\eta$ and $\eta^*$, each power of them is supposed to be satisfied order by order. Thus, by starting with the lowest order coefficients $G_0(1)$ and proceeding to the higher order coefficients step by step, we can uniquely determine the functional forms of $G_k(\eta, \eta^*)$ as well as the collective Hamiltonian $\mathcal{H}(\eta^*, \eta)$ self-consistently.

An important task in this expansion method is to set up a "boundary" condition, which characterizes the collective motion under consideration in the "small-amplitude" (i.e., small-$\eta$) limit. Namely, we choose the functional forms of the lowest order coefficients $G_k(1)$ so as to specify the nature of the collective motion under consideration. Since we are interested in the solution which is connected with the lower-eigenvalue RPA-phonon mode\(^*\) in the "small-amplitude" limit, we make the following choice for $G_k(1)$ in Eq. (4.2a):

\[ G_{1b}^b = i, \quad G_{0a}^b = 0, \quad \text{(for the collective phonon mode)} \]
\[ G_{1b}^b = G_{0a}^b = 0, \quad \text{(for the non-collective RPA mode)} \quad \text{(4.6)} \]

where $\lambda_1$ and $\lambda_2$ denote the collective-phonon and the non-collective RPA modes, respectively. Equation (4.6) means that $\tilde{G}(1)$ in Eq. (4.3) is expressed as

\[ \tilde{G}(1) = i \{ \eta^* \tilde{X}_b^a - \eta \tilde{X}_a^b \}. \quad \text{(4.7)} \]

Due to the choice (4.7), the lowest-order collective Hamiltonian $\mathcal{H}(2)$ becomes the RPA-phonon (harmonic) Hamiltonian,

\[ \mathcal{H}(2) = \omega \eta \eta^*. \quad \text{(4.8)} \]

From the second order equation of (IV), we get

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*In the system under consideration, there are two RPA modes. In the following discussion, the RPA mode with lower energy eigenvalue $\omega_1$ and the other RPA mode with higher eigenvalue $\omega_2$ will be referred to as a "collective" phonon mode and a "non-collective" RPA mode, respectively.
and the second-order equation of (III) gives
\[
G_{a3}^{(2)} = 0
\]
(4.9a)

\[
\{\omega_{a3} + \omega_a \left( \eta \frac{\partial}{\partial \eta} - \eta^* \frac{\partial}{\partial \eta^*} \right)\} G_{a3}^{(2)} = \frac{1}{2} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)] | \phi_0 \rangle,
\]
which is formally rewritten as
\[
G_{a3}^{(2)} = \left( \omega_{a3} + \omega_a \left( \eta \frac{\partial}{\partial \eta} - \eta^* \frac{\partial}{\partial \eta^*} \right) \right)^{-1} \left\{ \frac{1}{2} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)] | \phi_0 \rangle \right\}.
\]
(4.9b)

The third-order collective Hamiltonian is derived from (II) and is given by
\[
\mathcal{H}(3) = \frac{1}{3!} \langle \phi_0 | [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1), i \tilde{G}(1) | \phi_0 \rangle.
\]
(4.10)

As is seen from Eq. (4.10), the dynamical anharmonicity effects, which originate from the interaction term with \( V_3 \) in Hamiltonian (2.1), firstly manifest themselves as the third-order collective Hamiltonian \( \mathcal{H}(3) \) displaying coupling among the collective-phonon modes. The other dynamical anharmonicity effects between the collective-phonon mode and the non-collective RPA-mode manifest themselves in the non-zero coefficients \( G_{a3}^{(2)} \) in Eq. (4.9b), and play a role to specify the maximally-decoupled collective submanifold involving a non-collective RPA-mode phase space defined by \( \{ F_{a4}, F_{a4}^* \} \). Namely, a part of the dynamical anharmonicity effects, which is not included in the third-order collective Hamiltonian \( \mathcal{H}(3) \), is incorporated in specifying the maximally-decoupled collective submanifold (in the second order) so that the collective submanifold is no more described in terms of a collective-phonon phase space \( \{ F_{a4}, F_{a4}^* \} \) alone.

From the third-order of our basic equation (IV), we get
\[
G_{a3}^{(3)} = -\frac{1}{2} \left\{ \eta \frac{\partial}{\partial \eta} + \eta^* \frac{\partial}{\partial \eta^*} \right\} \left\{ \frac{1}{2} \left\{ \frac{\partial G_{a3}^{(2)}}{\partial \eta} - \frac{\partial G_{a3}^{(2)}}{\partial \eta^*} \right\} \right\} + \frac{1}{4!} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)], i \tilde{G}(1) | \phi_0 \rangle
\]
(4.11a)

with
\[
f(3) = \frac{1}{2} \left\{ \frac{\partial G_{a3}^{(2)}}{\partial \eta} - \frac{\partial G_{a3}^{(2)}}{\partial \eta^*} \right\} \frac{1}{2} \left\{ \frac{\partial G_{a3}^{(2)}}{\partial \eta} - \frac{\partial G_{a3}^{(2)}}{\partial \eta^*} \right\} + \frac{1}{4!} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)], i \tilde{G}(1) | \phi_0 \rangle.
\]
(4.11b)

The third-order equation of (III) gives
\[
G_{a3}^{(3)} = \left\{ \omega_{a3} + \omega_a \left( \eta \frac{\partial}{\partial \eta} - \eta^* \frac{\partial}{\partial \eta^*} \right) \right\} \left\{ \frac{1}{2} \left\{ \frac{\partial G_{a3}^{(2)}}{\partial \eta} - \frac{\partial G_{a3}^{(2)}}{\partial \eta^*} \right\} \right\} + \frac{1}{3!} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)], i \tilde{G}(1) | \phi_0 \rangle
\]
\[
+ \frac{1}{3!} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)], i \tilde{G}(1) | \phi_0 \rangle
\]
\[
- \frac{1}{3!} \langle \phi_0 | [i \tilde{X}_{a3}, [\tilde{H}, i \tilde{G}(1)], i \tilde{G}(1)], i \tilde{G}(1) | \phi_0 \rangle.
\]
(4.12)
After obtaining the $G_4$ coefficients, we get the fourth-order collective Hamiltonian given as

$$\mathcal{H}(4)=\omega_4\{iG_4^*(3)\eta^* - iG_4(3)\eta\} + \omega_4 G_4^*(2)G_2(2)$$

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

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

$$+ \frac{1}{4!}\langle\phi_0|[[[\hat{H}, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle.$$  \hspace{1cm} (4.13)

As is easily seen from Eqs. (4.11)~(4.13), the third-order coefficients $G_4(3)$ and the fourth-order collective Hamiltonian $\mathcal{H}(4)$ contain both the dynamical and kinematical anharmonicity effects, so that a fairly large amount of the anharmonicity effects neglected under the RPA are well incorporated into the collective submanifold as well as the collective Hamiltonian $\mathcal{H}(\eta, \eta^*)$.

In addition, we can see an essential difference of our theory from the conventional boson-mapping theories: In sharp contrast with the conventional boson-mapping theories where the microscopic structure of the boson is assumed to be unchanged from the outset, our collective Hamiltonian automatically includes the effects due to the non-collective RPA mode, which become more and more important for the higher order terms of the collective Hamiltonian, displaying dynamical change of the internal structure of the boson-correspondents $\{\eta, \eta^*\}$ due to the maximal-decoupling condition of the collective submanifold.

Here it is interesting to examine a genuine effect coming from the kinematical anharmonicity effects. For this aim, we eliminate the dynamical anharmonicity effects from Eqs. (4.9)~(4.13) by putting $V_3=0$. We then obtain the following expressions:

$$G_4^{(\text{kin})}(2)=G_4^{(\text{kin})}(2)=0,$$  \hspace{1cm} (4.14a)

$$G_4^{(\text{kin})}(3)=-\frac{1}{2}\left\{\eta \frac{\partial}{\partial \eta} + \eta^* \frac{\partial}{\partial \eta^*}\right\}^{-1}\left\{\left(2 - \eta^* \frac{\partial}{\partial \eta^*}\right)f^{(\text{kin})}(3) + \eta \frac{\partial}{\partial \eta} f^{(\text{kin})}(3)\right\},$$  \hspace{1cm} (4.14b)

where

$$f^{(\text{kin})}(3)=-\frac{2}{4!}i\langle\phi_0|[\left[i\frac{\partial}{\partial \eta}, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle,$$  \hspace{1cm} (4.14c)

and

$$G_4^{(\text{kin})}(3)=0,$$  \hspace{1cm} (4.14d)

$$\mathcal{H}^{(\text{kin})}(4)=\omega_4\{iG_4^{(\text{kin})}(3)\eta^* - iG_4^{(\text{kin})}(3)\eta\}$$

$$+ \frac{1}{4!}\langle\phi_0|[\left[i\hat{H}, i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)], i\hat{G}(1)]|\phi_0\rangle.$$  \hspace{1cm} (4.14e)

Here, the superscript (kin) means the case where there are no dynamical anharmonicity effects originating from the $V_3$ interaction. From Eqs. (4.14), we can see that the kinematical anharmonicity effects appear for the first time in the third-order coefficients $G_4^{(\text{kin})}(3)$ and consequently in the fourth-order collective Hamiltonian $\mathcal{H}^{(\text{kin})}(4)$. Generally
the term $G^{(3)}_{4\nu}$ in Eq. (4.14d) may play a role to mix up the non-collective RPA mode phase space \( \{ F_{4\nu}, F_{4\nu}^* \} \) into the maximally-decoupled collective submanifold. In our present model, however, we have $G^{(3)}_{4\nu}=0$ owing to the special algebra among the basis operators $K_{ip}$. This implies that the maximally-decoupled collective submanifold in the case with $V_3=0$ is still described by the collective-phonon phase-space $\{ F_{4\nu}, F_{4\nu}^* \}$ alone.

§ 5. Numerical results

In the preceding sections, we have clarified that the SCC method intends to approximately describe the TDHF trajectory (corresponding to the "classical" collective motion) by introducing two kinds of new concepts: the maximally-decoupled collective submanifold and the collective motion in this submanifold, i.e., the collective hypersurface and the trajectory restricted on it. We are now in a position to make a numerical calculation and to discuss how well the trajectory on the collective hypersurface can reproduce the TDHF trajectory under consideration.

By using a fourth order collective Hamiltonian obtained in the previous section,

$$\mathcal{H}^{(4)} = \mathcal{H}(2) + \mathcal{H}(3) + \mathcal{H}(4),$$

(5.1)

Eq. (1) is reduced to the following set of coupled differential equations:

$$i\dot{\eta} = \frac{\partial \mathcal{H}^{(4)}}{\partial \eta^*}, \quad i\dot{\eta} = -\frac{\partial \mathcal{H}^{(4)}}{\partial \eta}.$$  

(5.2)

We have made a numerical calculation for Eq. (5.2) with the initial condition

$$\eta(t)\rvert_{t=0}^{t_1} = \nu; \quad \nu = 1, 2, 3, \ldots,$$

(5.3)

where $\nu$ can be regarded as a "classical" correspondent of the number of collective bosons. After obtaining a trajectory within the 2-dimensional collective phase space $\{p, q\}$, i.e., after obtaining the time dependent values of $\eta(t)$ and $\eta^*(t)$, we have calculated the values of coefficients $G^{(4)}_{4\nu}$:

$$G^{(4)}_{4\nu} = G_{4\nu}(1) + G_{4\nu}(2) + G_{4\nu}(3),$$

(5.4)

where $\{\eta, \eta^*\}$-dependence is given by Eqs. (4.6), (4.9), (4.11) and (4.12).

As discussed in § 3, these time-dependent values give a trajectory restricted on the collective hypersurface.

We have also made a numerical calculation for the TDHF equation (2.10). In order to treat the same time-dependent motion described by Eq. (5.2) with condition (5.3), the
initial condition for Eq. (2·10) has been taken in such a way that the following relations are satisfied:

\[ F_n(f_1, f_2, f_1^*, f_2^*)(t=0) = G_n^{(0)}(\eta, \eta^*)(t=0); \quad i = 1, 2, \]

(5·5)

where \( F_n \) is defined by Eq. (4·1) and is related to \( F_i \) in Eq. (2·7) through

\[ F_i = F_n^0 \phi_n + F_n \phi_n. \]

(5·6)

As the relation between \( F_i \) and \((f_1, f_2, f_1^*, f_2^*)\) is given by Eq. (2·8), the solution of the TDHF equation (2·10) gives a trajectory within a 4-dimensional phase space.

In order to clarify the relation between both trajectories, we have calculated the following quantities:

\[ F_{ni} = R_j e^{i \phi_j}, \quad G_n^{(0)} = R_j^{(0)} e^{i \phi_j^{(0)}}. \]

(5·7)

In Fig. 3, the numerical results for the case \( V_3 = 0 \) under various initial conditions are shown. As discussed in § 4, the genuine effects coming from the kinematical anharmonicity effects can be visualized in this case. Owing to the fact \( G_n^{(0)}(3) = 0 \), the non-collective mode does not play any role in the present \( V_3 = 0 \) case, and the TDHF trajectory under consideration is completely described within the 2-dimensional collective-phonon phase-space \( \{ F_n, F_n^0 \} \). From Fig. 3, we can see that the solutions starting from one and two phonon states, i.e., the solutions with initial conditions \( \nu = 1 \) and 2, give a fairly good agreement with those of the TDHF theory. As the boson number increases, i.e., the initial value of \( \nu \) becomes large, there come out small differences between the trajectories given by the SCC method and TDHF theory, indicating that we need the higher order terms of \( G_n \) and \( \mathcal{R} \) than \( G_n^{(0)} \) and \( \mathcal{R}^{(0)} \). Here, it is worth-while to compare our results with those obtained under the RPA. If we employ

\[ \mathcal{R}^{(0)} = \mathcal{R}(2), \quad G_n^{(0)} = G_n(1) \]

(5·8)

instead of \( \mathcal{R}^{(0)} \) and \( G_n^{(0)} \) in Eqs. (5·1) and (5·4), we get the RPA solution given by

\[ G_n^{(0)} = i \nu e^{i \omega_{\nu}} \delta_{j,1}. \]

(5·9)

By comparing with the trajectory under the RPA, our next order calculation gives a remarkable improvement in reproducing the TDHF trajectory. Namely, the fourth order Hamiltonian \( \mathcal{R}^{(4)} \) as well as the third order coefficients \( G_n^{(0)} \) in the SCC method can include a major part of kinematical anharmonicity effects neglected under the RPA.

In order to see the main effects originated from the dynamical anharmonicity effects, in Fig. 4 the numerical results for the case with \( V_3 \neq 0 \) are shown with the initial condition \( \nu = 1 \). Owing to the effects, the non-collective degree of freedom is inevitably introduced in constructing the maximally-decoupled collective submanifold (surface) and the trajectory on it. As is seen from Fig. 4(a) where the case for a small value of \( V_3 \) is shown, the SCC method gives a good agreement with the TDHF theory for both the collective and non-collective degrees of freedom. From the above result, we can see that the concepts of the collective submanifold (surface) and the trajectory on it are actually realized in the present case and the SCC method can well reproduce a TDHF trajectory. In Fig. 4(b), the numerical results for the case with a much larger value of \( V_3 \) are shown. Even in such
Fig. 4. Numerical results for the case $N=10, (N-1)V_i=(N-1)V_2=0.6$ with the initial value $\psi=1$.
Figure (a) is for $V_3=0.0067$ and (b) for $V_3=0.010$. See also the caption of Fig. 3.

case, the fourth order perturbative solution of the SCC method gives a fairly good agreement with the TDHF trajectory.

§ 6. Conclusion

By the use of a simple solvable model, we have illustrated the essential ingredients of the SCC method formulated within a framework of the TDHF theory. It introduces the maximally-decoupled collective submanifold (or collective path) and the collective Hamiltonian describing a collective motion within the submanifold.

The collective submanifold has turned out to be a hypersurface, on which the TDHF trajectory corresponding to the collective motion is described. This conclusion is in agreement with a transparent interpretation of the invariance principle of the (time-dependent) Schrödinger equation\textsuperscript{29} by da Providencia and Urbano.\textsuperscript{13} It is also clarified that the major parts of the anharmonicity effects neglected under the RPA are well
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incorporated into specifying the collective submanifold as well as the collective Hamiltonian. As our perturbative fourth-order calculation based on the SCC method gives a remarkable improvement over the RPA, we are convinced of the applicability of our SCC method for more complex and realistic system.

An important condition of the SCC method is whether the collective trajectory on the hypersurface is really stable or not. The problem for clarifying this condition in connection with the stability\textsuperscript{13} of the hypersurface is now in progress.\textsuperscript{12}

Acknowledgements

The authors wish to express their gratitude to Professor J. da Providencia for stimulating discussions on the occasion of the INS International Symposium held on July 6~10, 1982 at the foot of Mt. Fuji. The numerical calculations were carried out with M 180 II-AD at INS, University of Tokyo.

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