

## Adiabatic Selfconsistent Collective Coordinate Method for Large Amplitude Collective Motion in Nuclei with Pairing Correlations

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(Received December 27, 1999)

An adiabatic approximation to the selfconsistent collective coordinate method is formulated in order to describe large amplitude collective motions in nuclei with pairing correlations on the basis of the time-dependent Hartree-Fock-Bogoliubov equations of motion. The basic equations are presented in a local harmonic form which can be solved in a manner similar to that of the quasiparticle RPA equations. The formalism guarantees the conservation of nucleon number expectation values. An extension to the multi-dimensional case is also discussed.

### §1. Introduction

Large amplitude collective motion (LACM), such as fission, shape transitions, anharmonic vibrations and low energy heavy ion reactions, are often encountered in studies of nuclear structure and dynamics. To go beyond the phenomenological models assuming some macroscopic or collective degrees of freedom motivated by the experimental facts and intuition, many attempts have been made to construct theories that are able to describe the LACM on the microscopic basis of the nuclear many-body Hamiltonian. In particular, theories based on the time-dependent Hartree-Fock (TDHF) approximation have been investigated extensively.<sup>1)-16)</sup> The TDHF is a general framework for describing low-energy nuclear dynamics accompanying evolution of the nuclear selfconsistent mean field.<sup>17),18)</sup> A LACM corresponds to a specific solution of the TDHF equation of motion. Since such a solution forms only a subset of the all TDHF states (Slater determinants), it is often called a collective path, a collective subspace, or a collective submanifold. The collective coordinates are then a set of a small number of variables that parameterize the collective subspace, and the collective Hamiltonian is a function governing the time evolution of the collective coordinates. One of the main purposes of the LACM theories is to provide a scheme to determine the collective subspace and the collective Hamiltonian on the basis of the microscopic many-body Hamiltonian. Although studies of LACM theories form a vast field of research with many recent developments in different directions, realistic applications to nuclear structure problems are rather limited. In this paper, we would like to propose a new practical method to calculate

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the collective subspace.

The adiabatic approximation has been often utilized for formulating the theory of the collective subspace. Indeed, some class of LACM, such as nuclear fission, can be regarded as slow motion, thus justifying the adiabatic approximation. The adiabatic TDHF (ATDHF) theory<sup>1)-3)</sup> is one of the best known adiabatic theories and has been applied in some cases to realistic descriptions of heavy ion reactions.<sup>3)</sup> The ATDHF theory, however, had the problem of the non-uniqueness of the solution.<sup>4),5)</sup> Efforts to settle the non-uniqueness problem were made from different viewpoints. Reference 6) emphasizes the importance of the canonical variable condition and the analyticity as a function of a collective coordinate for finding a unique solution. The proposed procedure relying on the Taylor expansion method has not been applied to realistic calculations. Another work<sup>7)</sup> points out that the collective subspace can be uniquely determined by using the next order equation of the ATDHF theory. It has been found also that the adiabatic collective path of LACM becomes the valley line of the potential function in the multi-dimensional space associated with the TDHF states.<sup>7)-9)</sup> Further, the adiabatic collective path can be defined by equations for a local harmonic mode at each point of the collective path. These developments are summarized in a consistent way in the formalism of Ref. 8). Note, however, that the adiabatic theory of Ref. 8) relies on a multi-dimensional classical phase space representation of the TDHF determinantal states.<sup>17),18)</sup> A realistic application of this theory has not been made, except in the case of a light nucleus.<sup>19)</sup> Furthermore, a problem of particle number conservation arises when applied to superconducting nuclei (i.e. nuclei with pairing correlations).<sup>10)</sup>

Theories without the adiabatic approximation have also been developed within the TDHF framework. The early works in this direction are called local harmonic approximations.<sup>12),13)</sup> Later, a set of general equations that can determine the collective subspace and the collective Hamiltonian were found and formulated in a consistent form known as the selfconsistent collective coordinate method (SCC or SCCM).<sup>14)</sup> The theory is purely based on the TDHF with no further approximation. The method also provides a concrete and practical scheme to solve the basic equations using a power series expansion with respect to the boson-like variables defined as a linear combination of the collective coordinates and momenta. The pairing correlation in superconducting nuclei is easily incorporated within the SCCM by adopting the time-dependent Hartree-Fock-Bogoliubov (TDHFB) equation in place of the TDHF, and the conservation law for the particle number is consistently introduced in the basic framework of the SCCM.<sup>15)</sup> Thanks to these features, the SCCM has been applied to many realistic descriptions of anharmonic vibrations in medium and heavy nuclei.<sup>16)</sup> However, the expansion method may not be suitable for large amplitude motion of an adiabatic nature, for which change of the nuclear mean-field is so large that the power series expansion of the collective coordinates may not be justified.

In the present paper, we attempt to combine the merits of the two approaches mentioned above, the SCCM and the adiabatic theory, in order to formulate a theory that provides a consistent and practical method easily applicable to realistic descriptions of the adiabatic LACM in superconducting nuclei. We achieve this aim by

introducing an adiabatic approximation into the general framework of the SCCM. Here we treat superconducting nuclei since the pairing correlations play essential roles in many cases, like spontaneous fission, tunneling between superdeformed and normally deformed configurations, and coupling between coexisting states with different nuclear shapes (shape coexistence phenomena). Although the use of the superconducting mean field requires us to respect particle number conservation, the SCCM allows a simple and consistent treatment of the conservation law. We also avoid the non-uniqueness problem by utilizing principles similar to those of Refs. 7)–9). Furthermore, we show that the equations of the adiabatic SCCM thus formulated can be transformed into another set of equations that have a similar structure as the local harmonic approach in the adiabatic theories.<sup>8)</sup> Therefore, the present formalism also inherits some aspects of the recent adiabatic theories such as Ref. 8).

In addition to the general formulation (§2), we present a practical scheme to solve the basic equations given in the local harmonic form for general classes of the many-body nuclear Hamiltonian (§3 and the Appendix). These equations are given in terms of the matrix elements of the many-body Hamiltonian written in terms of the quasiparticle operators, thus enabling us to develop a straightforward coding of a numerical program to solve the equations. In this way, we provide a concrete procedure to extract the collective subspace and the collective Hamiltonian. We also discuss a possible prescription to extend the formalism to cases of multi-dimensional collective motion (§4). Conclusions are outlined in §5.

## §2. Basic equations

### 2.1. The SCC method for superconducting nuclei

In this subsection, we recapitulate the basic equations of the SCC method<sup>14)</sup> in a manner suitable for treating superconducting nuclei.

We introduce the TDHFB approximation to describe LACM in superconducting many-fermion systems. Here the time-dependent many-body state vector  $|\phi(t)\rangle$  is constrained to a generalized Slater determinant, which is chosen as a variational wave function. The time evolution of  $|\phi(t)\rangle$  is then determined by the time-dependent variational principle

$$\delta \langle \phi(t) | i \frac{\partial}{\partial t} - \hat{H} | \phi(t) \rangle = 0, \quad (2.1)$$

where the variation is given by  $\delta |\phi(t)\rangle = a_\alpha^\dagger a_\beta^\dagger |\phi(t)\rangle$  in terms of the quasiparticle operators  $\{a_\alpha^\dagger, a_\alpha\}$ , which satisfy the vacuum condition  $a_\alpha |\phi(t)\rangle = 0$ .

We assume that the LACM can be described in terms of the collective variables, i.e. the collective coordinate and momentum  $\{q, p\}$  that are variables parameterizing the TDHFB state vector.<sup>\*)</sup> The whole space of the TDHFB state vectors can be parameterized by  $M \times (M - 1)$  variables ( $M$  being the number of the single particle states), as shown by the generalized Thouless theorem.<sup>17), 18)</sup> The set of the TDHFB state vectors  $|\phi(q, p)\rangle$  forms the collective subspace in which the LACM can be

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<sup>\*)</sup> We focus our discussion on the case of a single collective coordinate. A multi-dimensional case is discussed in §4.

properly described. One of the main problems with which we are concerned is how to determine the collective subspace on the basis of the TDHFB equations of motion. At the same time, we need to determine the collective Hamiltonian  $\mathcal{H}(q, p)$  that governs the equation of motion for the collective variables  $\{q, p\}$ . This is the general purpose of theories of LACM.

When we apply the LACM theories to nuclei in the superconducting phase, special attention has to be paid to particle number conservation. Since the TDHFB state vector is not an eigenstate of the particle number operator  $\hat{N}$ , one would like to formulate the LACM theory so that the particle number expectation value is conserved during the course of collective motion. This is a problem which is specific to the TDHFB, and does not exist for the TDHF for which the state vector is a number eigenstate.

It is well known<sup>17)</sup> that the expectation value of a conserved observable remains constant during the time-evolution of  $|\phi(t)\rangle$  governed by the TDHF(B) equations of motion. In the case of the pairing problem, the TDHFB state vector spontaneously violates the symmetry with respect to the gauge rotation  $e^{-i\varphi\hat{N}}$ , but rotational motion related to the gauge rotation (often called the ‘‘pairing rotation’’) emerges automatically to restore the gauge symmetry. Therefore, the LACM of superconducting nuclei, described by the TDHFB theory, necessarily accompany the pairing rotation, and we have to introduce<sup>15)</sup> the collective coordinate,  $\varphi$ , the gauge angle, and the conjugate collective momenta,  $N$ , which represents the particle number. Thus, we are obliged to consider a collective subspace that is parameterized by the set of four collective variables  $\{q, p, \varphi, N\}$ .\*)

Let us now present the basic equations of the SCCM that determine the collective subspace  $|\phi(q, p, \varphi, N)\rangle$  and the collective Hamiltonian  $\mathcal{H}(q, p, \varphi, N)$ . As discussed above, the variable  $\varphi$  is introduced to represent the gauge angle. This requirement is easily satisfied<sup>15)</sup> if one uses the parameterization

$$|\phi(q, p, \varphi, N)\rangle = e^{-i\varphi\hat{N}} |\phi(q, p, N)\rangle, \quad (2.2)$$

where  $\hat{N}$  is the number operator of particles. Here  $|\phi(q, p, N)\rangle$  represents an intrinsic state that rotates in the gauge space.

The basic equations of the SCCM consist of a canonical variable condition and an invariance principle of the time-dependent Schrödinger equation (TDHFB equation in our case). The canonical variable condition is, in general, given by

$$\langle\phi(q, p, \varphi, N)| i \frac{\partial}{\partial q} |\phi(q, p, \varphi, N)\rangle = p + \frac{\partial S}{\partial q}, \quad (2.3a)$$

$$\langle\phi(q, p, \varphi, N)| \frac{\partial}{i\partial p} |\phi(q, p, \varphi, N)\rangle = -\frac{\partial S}{\partial p}, \quad (2.3b)$$

$$\langle\phi(q, p, \varphi, N)| i \frac{\partial}{\partial \varphi} |\phi(q, p, \varphi, N)\rangle = N + \frac{\partial S}{\partial \varphi}, \quad (2.3c)$$

$$\langle\phi(q, p, \varphi, N)| \frac{\partial}{i\partial N} |\phi(q, p, \varphi, N)\rangle = -\frac{\partial S}{\partial N}, \quad (2.3d)$$

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\*) For simplicity, here we assume a single kind of particles. Extension to systems with many kinds (e.g., protons and neutrons in nuclei) is straightforward.

for the collective subspace parameterized by two sets of coordinates  $(q, \varphi)$  and momenta  $(p, N)$ . Although  $S$  is an arbitrary function of  $\{q, p, \varphi, N\}$ , we choose  $S = 0$ , which is appropriate for the adiabatic approximation.<sup>6)</sup> Then the canonical variable condition can be rewritten as equations for the state  $|\phi(q, p, N)\rangle$ :

$$\langle \phi(q, p, N) | i \frac{\partial}{\partial q} | \phi(q, p, N) \rangle = p, \quad (2.4a)$$

$$\langle \phi(q, p, N) | \frac{\partial}{i \partial p} | \phi(q, p, N) \rangle = 0, \quad (2.4b)$$

$$\langle \phi(q, p, N) | \hat{N} | \phi(q, p, N) \rangle = N, \quad (2.4c)$$

$$\langle \phi(q, p, N) | \frac{\partial}{i \partial N} | \phi(q, p, N) \rangle = 0. \quad (2.4d)$$

The third equation requires that the collective variable  $N$  be identical to the expectation value of the number operator. In other words, the particle number expectation value does not depend on the collective variables  $(q, p)$  for the LACM under consideration. This is nothing but the condition of particle number conservation.

The collective Hamiltonian is defined as the value of the total energy in the collective subspace, given by

$$\mathcal{H} = \langle \phi(q, p, \varphi, N) | \hat{H} | \phi(q, p, \varphi, N) \rangle \quad (2.5a)$$

$$= \langle \phi(q, p, N) | \hat{H} | \phi(q, p, N) \rangle. \quad (2.5b)$$

Since the Hamiltonian  $\hat{H}$  commutes with the number operator  $\hat{N}$ , the collective Hamiltonian does not depend on the gauge angle  $\varphi$ . Therefore,  $\varphi$  becomes cyclic, as we expect.

The invariance principle of the TDHFB equation plays a central role in determining the collective subspace, which requires that the TDHFB state vector  $|\phi(q(t), p(t), \varphi(t), N(t))\rangle$  evolving in time within the collective subspace obey the full TDHFB equation, Eq. (2.1). This is equivalent to the condition that the collective subspace is an invariant subspace of the TDHFB equations of motion. Inserting Eq. (2.2) into the time-dependent variational principle, Eq. (2.1), we obtain

$$\delta \langle \phi(q, p, N) | \hat{H} - \frac{dq}{dt} \overset{\circ}{P} + \frac{dp}{dt} \overset{\circ}{Q} + \frac{dN}{dt} \overset{\circ}{\Theta} - \frac{d\varphi}{dt} \hat{N} | \phi(q, p, N) \rangle = 0, \quad (2.6)$$

where the infinitesimal generators defined by

$$\overset{\circ}{P} | \phi(q, p, N) \rangle = i \frac{\partial}{\partial q} | \phi(q, p, N) \rangle, \quad (2.7a)$$

$$\overset{\circ}{Q} | \phi(q, p, N) \rangle = \frac{1}{i} \frac{\partial}{\partial p} | \phi(q, p, N) \rangle, \quad (2.7b)$$

$$\overset{\circ}{\Theta} | \phi(q, p, N) \rangle = \frac{1}{i} \frac{\partial}{\partial N} | \phi(q, p, N) \rangle \quad (2.7c)$$

have been used. These operators are one-body operators which can be written as linear combinations of bilinear products  $\{a_{\alpha}^{\dagger} a_{\beta}^{\dagger}, a_{\beta} a_{\alpha}, a_{\alpha}^{\dagger} a_{\beta}\}$  of the quasiparticle op-

erators defined with respect to  $|\phi(q, p, N)\rangle$ . Because of the canonical variable conditions, these infinitesimal generators satisfy the commutation relations

$$\langle\phi(q, p, N)|[\hat{Q}, \hat{P}]|\phi(q, p, N)\rangle = i, \quad (2.8a)$$

$$\langle\phi(q, p, N)|[\hat{\Theta}, \hat{N}]|\phi(q, p, N)\rangle = i, \quad (2.8b)$$

and commutators of other combinations of  $\hat{Q}, \hat{P}, \hat{\Theta}$  and  $\hat{N}$  give zero expectation value. By taking the variation as  $\delta|\phi(q, p, N)\rangle = \{\hat{P}, \hat{Q}, \hat{\Theta}, \hat{N}\}|\phi(q, p, N)\rangle$ , Eq. (2.6) produces the canonical equations of motion for the collective variables:

$$\frac{dq}{dt} = \frac{\partial\mathcal{H}}{\partial p} = i\langle\phi(q, p, N)|[\hat{H}, \hat{Q}]|\phi(q, p, N)\rangle, \quad (2.9a)$$

$$\frac{dp}{dt} = -\frac{\partial\mathcal{H}}{\partial q} = i\langle\phi(q, p, N)|[\hat{H}, \hat{P}]|\phi(q, p, N)\rangle, \quad (2.9b)$$

$$\frac{d\varphi}{dt} = \frac{\partial\mathcal{H}}{\partial N} = i\langle\phi(q, p, N)|[\hat{H}, \hat{\Theta}]|\phi(q, p, N)\rangle, \quad (2.9c)$$

$$\frac{dN}{dt} = -\frac{\partial\mathcal{H}}{\partial\varphi} = 0. \quad (2.9d)$$

Using Eq. (2.9), Eq. (2.6) reduces to an *equation of collective subspace*:

$$\delta\langle\phi(q, p, N)|\hat{H} - \frac{\partial\mathcal{H}}{\partial p}\hat{P} - \frac{\partial\mathcal{H}}{\partial q}\hat{Q} - \frac{\partial\mathcal{H}}{\partial N}\hat{N}|\phi(q, p, N)\rangle = 0. \quad (2.10)$$

If we take a variation  $\delta_{\perp}$  that is orthogonal to the infinitesimal generators  $\{\hat{P}, \hat{Q}, \hat{\Theta}, \hat{N}\}$ , we can immediately show  $\delta_{\perp}\langle\phi(q, p, N)|\hat{H}|\phi(q, p, N)\rangle = 0$ , which implies that the energy expectation value is stationary in the collective subspace with respect to all the variations, except for those along directions tangent to the collective subspace. In other words, the collective mode is decoupled from the other modes of excitation.

We remark here that the above basic equations of the SCCM are invariant under point transformations of the collective coordinate

$$q \rightarrow q' = q'(q), \quad (2.11a)$$

$$p \rightarrow p' = p \times (dq'/dq)^{-1}. \quad (2.11b)$$

The basic principles, i.e. the canonical variable condition, Eq. (2.3), and the invariance principle of the TDHFB equation, Eq. (2.6), are not affected by the general canonical transformations of collective variables  $\{q, p, \varphi, N\} \rightarrow \{q', p', \varphi', N'\}$ . By taking the parameterization, Eq. (2.2), and the specific choice of  $S = 0$  in Eq. (2.3), the allowed canonical transformations are restricted to the point transformations.<sup>6)</sup>

## 2.2. Adiabatic approximation

Assuming that the LACM described by the collective variables  $\{q, p\}$  is slow motion, we here introduce the adiabatic approximation to the SCCM. Namely, we expand the basic equations with respect to the collective momentum  $p$ , which is

appropriate for small values of momentum. Since the particle number variable  $N$  is a momentum variable in the present formulation, we also expand the basic equations with respect to  $n = N - N_0$  when we consider a system with particle number  $N_0$ .

Let us first consider the expansion of the TDHFB state vector  $|\phi(q, p, N)\rangle$  in the collective subspace. The origin of the expansion is the state  $|\phi(q)\rangle \equiv |\phi(q, p, N)\rangle|_{p=0, N=N_0}$ . We can assume that this is a time-even state, i.e.,  $\mathcal{T}|\phi(q)\rangle = |\phi(q)\rangle$  under the time-reversal operation  $\mathcal{T}$ . (Here we consider system of an even number of particles.) Thanks to the generalized Thouless theorem, the state vector  $|\phi(q, p, N)\rangle$  can be expressed as

$$|\phi(q, p, N)\rangle = e^{i\hat{G}(q,p,n)} |\phi(q)\rangle \tag{2.12}$$

by using the unitary transformation  $e^{i\hat{G}(q,p,n)}$ . Here the Hermitian operator  $\hat{G}$  is given by

$$\hat{G}(q, p, n) = \sum_{\alpha>\beta} \left( G_{\alpha\beta}(q, p, n) a_\alpha^\dagger a_\beta^\dagger + G_{\alpha\beta}^*(q, p, n) a_\beta a_\alpha \right) = \hat{G}(q, p, n)^\dagger. \tag{2.13}$$

Here and hereafter, the quasiparticle operators  $\{a_\alpha^\dagger, a_\alpha\}$  are always defined locally at each value of  $q$  and satisfy the condition  $a_\alpha |\phi(q)\rangle = 0$ . We now expand the operator  $\hat{G}(q, p, n)$  in powers of  $p$  and  $n$  and keep only the lowest order term. We have

$$\hat{G}(q, p, n) = p\hat{Q}(q) + n\hat{\Theta}(q), \tag{2.14a}$$

$$\hat{Q}(q) = \sum_{\alpha>\beta} \left( Q_{\alpha\beta}(q) a_\alpha^\dagger a_\beta^\dagger + Q_{\alpha\beta}^*(q) a_\beta a_\alpha \right) = \hat{Q}(q)^\dagger, \tag{2.14b}$$

$$\hat{\Theta}(q) = \sum_{\alpha>\beta} \left( \Theta_{\alpha\beta}(q) a_\alpha^\dagger a_\beta^\dagger + \Theta_{\alpha\beta}^*(q) a_\beta a_\alpha \right) = \hat{\Theta}(q)^\dagger. \tag{2.14c}$$

If we require that time-reversal of  $|\phi(q, p, N)\rangle$  causes sign inversion of the collective momentum  $p$ , i.e.  $\mathcal{T}|\phi(q, p, N)\rangle = |\phi(q, -p, N)\rangle$ , the operators  $\hat{Q}(q)$  and  $\hat{\Theta}(q)$  must be time-even ( $\mathcal{T}\hat{Q}(q)\mathcal{T}^{-1} = \hat{Q}(q)$ ) and time-odd ( $\mathcal{T}\hat{\Theta}(q)\mathcal{T}^{-1} = -\hat{\Theta}(q)$ ), respectively. If we set  $n = 0$  (i.e.  $N = N_0$ ), the parameterization Eq. (2.12) together with Eq. (2.14) reduces to  $|\phi(q, p)\rangle = e^{ip\hat{Q}(q)} |\phi(q)\rangle$ , which has the same form as that introduced by Villars and is often used in the ATDHF theories.<sup>1), 3), 7)</sup>

The collective Hamiltonian is expanded as

$$\mathcal{H}(q, p, N) = V(q) + \frac{1}{2}B(q)p^2 + \lambda(q)n, \tag{2.15a}$$

$$V(q) = \mathcal{H}(q, p, N)|_{p=0, N=N_0} = \langle \phi(q) | \hat{H} | \phi(q) \rangle, \tag{2.15b}$$

$$\begin{aligned} B(q) &= \frac{1}{2} \frac{\partial^2 \mathcal{H}(q, p, N)}{\partial p^2} \Big|_{p=0, N=N_0} \\ &= - \langle \phi(q) | [[\hat{H}, \hat{Q}(q)], \hat{Q}(q)] | \phi(q) \rangle, \end{aligned} \tag{2.15c}$$

$$\lambda(q) = \frac{\partial \mathcal{H}(q, p, N)}{\partial N} \Big|_{p=0, N=N_0} = \langle \phi(q) | [\hat{H}, i\hat{\Theta}(q)] | \phi(q) \rangle, \tag{2.15d}$$

where we have kept terms up to second order in the collective momentum  $p$ , and up to the first order in  $n$ . The collective Hamiltonian for the system with  $N = N_0$  particles ( $n = 0$ ) is given by

$$\mathcal{H}(q, p, N_0) = V(q) + \frac{1}{2}B(q)p^2 \tag{2.16}$$

as the sum of the collective potential  $V(q)$  and the collective kinetic energy (the second term).

We next expand the infinitesimal generators. It is convenient for this purpose to define the unitary transformations  $\hat{P}' = e^{-i\hat{G}}\hat{P}e^{i\hat{G}}$ ,  $\hat{Q}' = e^{-i\hat{G}}\hat{Q}e^{i\hat{G}}$  and  $\hat{\Theta}' = e^{-i\hat{G}}\hat{\Theta}e^{i\hat{G}}$  of the infinitesimal generators  $\hat{P}$ ,  $\hat{Q}$  and  $\hat{\Theta}$ . They are expanded as

$$\hat{P}' = \hat{P}(q) + e^{-i\hat{G}}i\frac{\partial}{\partial q}e^{i\hat{G}} = \hat{P}(q) - p\frac{\partial\hat{Q}}{\partial q} - n\frac{\partial\hat{\Theta}}{\partial q} + \dots, \tag{2.17}$$

$$\hat{Q}' = e^{-i\hat{G}}\frac{\partial}{i\partial p}e^{i\hat{G}} = \hat{Q}(q) + \frac{i}{2}[\hat{Q}, p\hat{Q} + n\hat{\Theta}] + \dots, \tag{2.18}$$

$$\hat{\Theta}' = e^{-i\hat{G}}\frac{\partial}{i\partial N}e^{i\hat{G}} = \hat{\Theta}(q) + \frac{i}{2}[\hat{\Theta}, p\hat{Q} + n\hat{\Theta}] + \dots, \tag{2.19}$$

with use of the general expansion formula

$$e^{-i\hat{G}}\partial e^{i\hat{G}} = i\partial\hat{G} + \frac{1}{2!}[i\partial\hat{G}, i\hat{G}] + \frac{1}{3!}[[i\partial\hat{G}, i\hat{G}], i\hat{G}] + \dots \tag{2.20}$$

The operator  $\hat{P}(q)$  is the infinitesimal generator with respect to  $|\phi(q)\rangle$  defined by

$$\hat{P}(q)|\phi(q)\rangle = i\frac{\partial}{\partial q}|\phi(q)\rangle. \tag{2.21}$$

Similarly, we introduce the unitary transformation of the number operator and expand it as

$$\hat{N}' \equiv e^{-i\hat{G}}\hat{N}e^{i\hat{G}} = \hat{N} + i[\hat{N}, p\hat{Q} + n\hat{\Theta}] + \dots \tag{2.22}$$

Substituting these operators into the canonical variable condition, Eq. (2.4), we have

$$\langle\phi(q)|\hat{P}'(q, p, N)|\phi(q)\rangle = p, \tag{2.23a}$$

$$\langle\phi(q)|\hat{Q}'(q, p, N)|\phi(q)\rangle = 0, \tag{2.23b}$$

$$\langle\phi(q)|\hat{\Theta}'(q, p, N)|\phi(q)\rangle = 0, \tag{2.23c}$$

$$\langle\phi(q)|\hat{N}'(q, p, N)|\phi(q)\rangle = N. \tag{2.23d}$$

Now we expand these equations with respect to the momenta  $p$  and  $n$ , and obtain the following equations.

The zeroth order canonical variable conditions:

$$\langle\phi(q)|\hat{P}(q)|\phi(q)\rangle = \langle\phi(q)|i\frac{\partial}{\partial q}|\phi(q)\rangle = 0, \tag{2.24}$$

$$\langle\phi(q)|\hat{Q}(q)|\phi(q)\rangle = 0, \tag{2.25}$$

$$\langle\phi(q)|\hat{\Theta}(q)|\phi(q)\rangle = 0, \tag{2.26}$$

$$\langle\phi(q)|\hat{N}|\phi(q)\rangle = N_0. \tag{2.27}$$

Equations (2.25) and (2.26) are automatically fulfilled by the definition Eq. (2.14) of the operators  $\hat{Q}(q)$  and  $\hat{\Theta}(q)$ . Equation (2.24) can be satisfied if the  $q$ -dependent phase of  $|\phi(q)\rangle$  is properly chosen. Equation (2.27) is the constraint on  $|\phi(q)\rangle$  for the conservation of the average particle number.

The first order canonical variable conditions:

$$\langle\phi(q)|\frac{\partial\hat{Q}(q)}{\partial q}|\phi(q)\rangle = -1, \tag{2.28}$$

$$\langle\phi(q)|[\hat{Q}(q),\hat{\Theta}(q)]|\phi(q)\rangle = 0, \tag{2.29}$$

$$\langle\phi(q)|[\hat{Q}(q),\hat{N}]|\phi(q)\rangle = 0. \tag{2.30}$$

One finds

$$\langle\phi(q)|[\hat{Q}(q),\hat{P}(q)]|\phi(q)\rangle = i, \tag{2.31}$$

which can be derived by differentiating Eq. (2.25) with respect to  $q$  and using Eq. (2.28). One can also derive from Eq. (2.27)

$$\langle\phi(q)|[\hat{P}(q),\hat{N}]|\phi(q)\rangle = 0. \tag{2.32}$$

These equations give constraints on the infinitesimal generators  $\hat{Q}(q)$  and  $\hat{P}(q)$  concerning the normalization, Eq. (2.31), and the orthogonality to the particle number operator, Eq. (2.32).

Next we expand the equation of collective subspace, Eq. (2.10), to obtain a complete set of the basic equations for the adiabatic approximation. After rewriting Eq. (2.10) as

$$\delta\langle\phi(q)|e^{-i\hat{G}}\hat{H}e^{i\hat{G}} - \frac{\partial\mathcal{H}}{\partial p}\hat{P}' - \frac{\partial\mathcal{H}}{\partial q}\hat{Q}' - \frac{\partial\mathcal{H}}{\partial N}\hat{N}'|\phi(q)\rangle = 0, \tag{2.33}$$

we can expand each term with respect to  $p$  and  $n$  with use of the equations listed above.

The zeroth order equation of collective subspace:

$$\delta\langle\phi(q)|\hat{H} - \lambda(q)\hat{N} - \frac{\partial V}{\partial q}\hat{Q}(q)|\phi(q)\rangle = 0. \tag{2.34}$$

The first order equation of collective subspace:

$$\delta\langle\phi(q)|[\hat{H} - \lambda(q)\hat{N},\hat{Q}(q)] - \frac{1}{i}B(q)\hat{P}(q)|\phi(q)\rangle = 0. \tag{2.35}$$

These equations are similar to the equations of path in Villars' ATDHF theory,<sup>1)</sup> except that the present paper deals with the superconducting Hartree-Fock-Bogoliubov (HFB) state and that the Hamiltonian accompanies the  $q$ -dependent chemical potential term  $-\lambda(q)\hat{N}$ . As mentioned in §1, the ATDHF theory has the problem that the solution satisfying these two equations is not uniquely determined.<sup>4),5)</sup> Although an additional validity condition was introduced to further constrain the solutions,<sup>3),4)</sup> the procedure of Ref. 3) does not fully solve the problem since the method does not work around the HF minima.

The non-uniqueness problem has been investigated in recent studies of the adiabatic theories, and in our opinion they can be classified into two different approaches. The first one represented by Ref. 6) asserts that the solution is uniquely determined if an RPA boundary condition is specified at the HF minimum and if the analyticity of the collective path as a function of  $q$  is imposed together with the canonical variable condition. The solution, however, needs to be constructed in an analytic way or by means of a Taylor expansion method with respect to the collective coordinate  $q$ . We do not adopt this approach since we wish to construct a method applicable to systems exhibiting large excursions from the HFB minimum. We rather follow the other approach, represented by Refs. 7)–9). These theories require the additional condition that the equation of collective subspace (corresponding to the decoupling condition in Ref. 8)) should be satisfied up to the next order of the adiabatic expansion. In the present formulation, this second order condition is expressed as follows.

The second order equation of collective subspace:

$$\delta \langle \phi(q) | \frac{1}{2} [[\hat{H} - \lambda(q)\hat{N}, \hat{Q}(q)], \hat{Q}(q)] - B(q)\Delta\hat{Q}(q) | \phi(q) \rangle = 0, \quad (2\cdot36)$$

where

$$\Delta\hat{Q}(q) = \frac{\partial\hat{Q}}{\partial q} + \Gamma(q)\hat{Q}(q), \quad (2\cdot37)$$

$$\Gamma(q) = -\frac{1}{2B(q)} \frac{\partial B}{\partial q}. \quad (2\cdot38)$$

This equation is equivalent in its mathematical form to the one given in Ref. 7) if the chemical potential term  $-\lambda(q)\hat{N}$  is neglected. The last term  $-B(q)\Delta\hat{Q}(q)$ , often called a curvature term, was simply neglected in the original version of the local harmonic approximation.<sup>12),13)</sup> In the next subsection, instead of neglecting this curvature term, we rewrite  $\Delta\hat{Q}(q)$  and change Eq. (2·36) into a workable form.

It is worth noting here the invariance of the adiabatic equations with respect to the coordinate transformation. The collective momentum  $p$  undergoes a linear homogeneous transformation under the point transformation, Eq. (2·11). Therefore, different orders of the expansion with respect to the power of  $p$  are not mixed under the point transformation. The invariance property of the basic equations of SCCM is thus inherited by each equation of the adiabatic approximation listed above. One can also confirm this property by seeing that the quantities appearing in the equations transform as

$$\hat{Q}(q) \rightarrow \hat{Q}'(q') = \hat{Q}(q(q')) \left( \frac{dq'}{dq} \right), \quad (2\cdot39a)$$

$$\hat{P}(q) \rightarrow \hat{P}'(q') = \hat{P}(q(q')) \left( \frac{dq'}{dq} \right)^{-1}, \quad (2\cdot39b)$$

$$\frac{\partial V}{\partial q} \rightarrow \frac{\partial V'}{\partial q'} = \frac{\partial V}{\partial q} \left( \frac{dq'}{dq} \right)^{-1}, \quad (2\cdot39c)$$

$$B \rightarrow B'(q') = B(q(q')) \left( \frac{dq'}{dq} \right)^2, \quad (2.39d)$$

$$\Delta\hat{Q}(q) \rightarrow \Delta\hat{Q}'(q') = \Delta\hat{Q}(q). \quad (2.39e)$$

### §3. Local harmonic approximation to collective subspace

#### 3.1. Local harmonic equations

In this section we present a concrete procedure to construct an approximate solution of the adiabatic SCC method. To this end, we first derive, from the adiabatic equations, another set of equations of collective subspace which can be solved in a manner similar to that for the RPA equation.

We first take the derivative of the zeroth order equation, Eq. (2.34), with respect to  $q$ . This leads to

$$\delta \langle \phi(q) | \left[ \hat{H} - \lambda(q)\hat{N}, \frac{1}{i}\hat{P}(q) \right] - C(q)\hat{Q}(q) - \frac{\partial V}{\partial q} \Delta\hat{Q}(q) - \frac{\partial \lambda}{\partial q} \hat{N} | \phi(q) \rangle = 0, \quad (3.1)$$

$$C(q) = \frac{\partial^2 V}{\partial q^2} - \Gamma(q) \frac{\partial V}{\partial q}, \quad (3.2)$$

where  $\Delta\hat{Q}(q)$  and  $\Gamma(q)$  are given by Eqs. (2.37) and (2.38), respectively. Using Eq. (2.36), we eliminate  $\Delta\hat{Q}(q)$  and rewrite Eq. (3.1) as

$$\delta \langle \phi(q) | \left[ \hat{H} - \lambda(q)\hat{N}, \frac{1}{i}\hat{P}(q) \right] - C(q)\hat{Q}(q) - \frac{1}{2B(q)} \left[ \left[ \hat{H} - \lambda(q)\hat{N}, \frac{\partial V}{\partial q} \hat{Q}(q) \right], \hat{Q}(q) \right] - \frac{\partial \lambda}{\partial q} \hat{N} | \phi(q) \rangle = 0. \quad (3.3)$$

Furthermore, due to Eq. (2.34), we find

$$\frac{\partial V}{\partial q} \hat{Q} = (\hat{H} - \lambda\hat{N})_A, \quad (3.4)$$

where  $(\hat{H} - \lambda\hat{N})_A$  represents the  $a^\dagger a^\dagger$  and  $aa$  part of the operator  $\hat{H} - \lambda\hat{N}$  containing two-quasiparticle creation and annihilation in the normal-ordered expression.

We thus replace Eqs. (2.34)–(2.36) by the equivalent set

$$\delta \langle \phi(q) | \hat{H}_M(q) | \phi(q) \rangle = 0, \quad (3.5)$$

$$\delta \langle \phi(q) | [\hat{H}_M(q), \hat{Q}(q)] - \frac{1}{i}B(q)\hat{P}(q) | \phi(q) \rangle = 0, \quad (3.6)$$

$$\delta \langle \phi(q) | \left[ \hat{H}_M(q), \frac{1}{i}\hat{P}(q) \right] - C(q)\hat{Q}(q) - \frac{1}{2B(q)} [[\hat{H}_M(q), (\hat{H} - \lambda(q)\hat{N})_A], \hat{Q}(q)] - \frac{\partial \lambda}{\partial q} \hat{N} | \phi(q) \rangle = 0. \quad (3.7)$$

In Eqs. (3·6) and (3·7),  $\hat{H} - \lambda\hat{N}$  has been replaced by

$$\hat{H}_M(q) = \hat{H} - \lambda(q)\hat{N} - \frac{\partial V}{\partial q}\hat{Q}(q), \quad (3\cdot8)$$

since the last term has no influence. The operator  $\hat{H}_M(q)$  may be regarded as the Hamiltonian in the moving frame. The second and third terms can be identified with generalized cranking terms associated with the pairing rotation and the LACM, respectively.

Equations (3·6) and (3·7) are linear equations with respect to the one-body operators  $\hat{Q}(q)$  and  $\hat{P}(q)$ . They have essentially the same structure as the standard RPA equations, except for the last two terms in Eq. (3·7). The quantity  $C(q)$  is the local stiffness parameter defined as the second (covariant) derivative of the collective potential  $V(q)$ . The infinitesimal generators  $\hat{Q}(q)$  and  $\hat{P}(q)$  are thus closely related to the harmonic normal modes locally defined for  $|\phi(q)\rangle$  and the moving frame Hamiltonian  $\hat{H}_M(q)$ . These equations may be called *local harmonic equations*.

It was shown in Ref. 7) that the zeroth, first and second order equations of AT-DHF give a valley line of a potential energy surface in a multi-dimensional configuration space associated with the TDHF states. Similarly, the local harmonic equations we have obtained, Eqs. (3·5)–(3·7), define the valley of the multi-dimensional potential energy surface. The solution of these equations will be uniquely determined if a suitable boundary condition is specified. These features are similar to the formulation of Ref. 8) where the valley equation of the potential energy surface is derived from the decoupling condition.

We remark again that the local harmonic equations in the present paper differ from those of Rowe-Bassermann<sup>12)</sup> and Marumori<sup>13)</sup> with respect to the third and fourth terms of Eq. (3·7), which arise from the curvature term (derivative of the generator) and the particle number constraint, respectively. It is important to keep the curvature term in order to maintain the relation between the collective subspace and the valley of the potential surface. We also note that the present formalism is invariant with respect to the point transformation of the collective coordinate, as is the formulation of Ref. 8).

### 3.2. Matrix formulation of local harmonic equations

Let us now give a procedure to find the operators  $\hat{Q}(q)$  and  $\hat{P}(q)$  that satisfy the local harmonic equations, (3·6) and (3·7), for a given state  $|\phi(q)\rangle$ . Since these are linear equations with respect to these operators, this can be done in a manner analogous to that for the standard RPA. To show this, we first express the operator  $\hat{P}(q)$  and  $\hat{N}$  in terms of the quasiparticle operators:

$$\hat{P}(q) = i \sum_{\alpha>\beta} \left( P_{\alpha\beta}(q) a_{\alpha}^{\dagger} a_{\beta}^{\dagger} - P_{\alpha\beta}^{*}(q) a_{\beta} a_{\alpha} \right) = \hat{P}(q)^{\dagger}, \quad (3\cdot9)$$

$$\hat{N} = \sum_{\alpha>\beta} \left( N_{\alpha\beta}(q) a_{\alpha}^{\dagger} a_{\beta}^{\dagger} + N_{\alpha\beta}^{*}(q) a_{\beta} a_{\alpha} \right). \quad (3\cdot10)$$

Note that the  $a^{\dagger}a$  and  $c$ -number parts are neglected here since they do not change the state vector  $|\phi(q)\rangle$ , except for the phase. The Hamiltonian  $\hat{H}$  can also be expressed

in terms of the same quasiparticle operators. Assuming that the matrix elements  $Q_{\alpha\beta}$  and  $P_{\alpha\beta}$  are real, the local harmonic equations can be written as the following matrix equations:

$$(\mathbf{A} - \mathbf{B})\mathbf{Q} - B(q)\mathbf{P} = 0, \quad (3.11a)$$

$$(\mathbf{A} + \mathbf{B})\mathbf{P} - C(q)\mathbf{Q} - \frac{1}{B(q)}\mathbf{D}\mathbf{Q} - \lambda'\mathbf{N} = 0, \quad (3.11b)$$

$$\mathbf{P}^T\mathbf{N} = 0, \quad (3.11c)$$

$$2\mathbf{Q}^T\mathbf{P} = 1, \quad (3.11d)$$

$$\lambda' = \frac{\partial\lambda}{\partial q}. \quad (3.11e)$$

Here all quantities are functions of  $q$  while  $\mathbf{Q} = (\dots, Q_{\alpha\beta}, \dots)^T$ ,  $\mathbf{P} = (\dots, P_{\alpha\beta}, \dots)^T$  and  $\mathbf{N} = (\dots, N_{\alpha\beta}, \dots)^T$  form the vector representation of the matrix elements with  $\alpha > \beta$ .  $\mathbf{A}$  and  $\mathbf{B}$  are the matrices whose elements are given by

$$(\mathbf{A})_{\alpha\beta,\gamma\delta} = \delta_{\alpha\gamma}\delta_{\beta\delta}(e_\alpha + e_\beta) + v_{\alpha\beta,\gamma\delta}^{22}, \quad (3.12a)$$

$$(\mathbf{B})_{\alpha\beta,\gamma\delta} = v_{\alpha\beta\gamma\delta}^{40}, \quad (3.12b)$$

in terms of the matrix elements of the moving frame Hamiltonian,

$$\hat{H}_M(q) = \sum_{\alpha} e_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \quad (3.13a)$$

$$+ \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta}^{22} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (3.13b)$$

$$+ \frac{1}{4!} \sum_{\alpha\beta\gamma\delta} \left( v_{\alpha\beta\gamma\delta}^{40} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma}^{\dagger} a_{\delta}^{\dagger} + v_{\alpha\beta\gamma\delta}^{04} a_{\delta} a_{\gamma} a_{\beta} a_{\alpha} \right) \quad (3.13c)$$

$$+ \frac{1}{3!} \sum_{\alpha\beta\gamma\delta} \left( v_{\alpha\beta\gamma,\delta}^{31} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma}^{\dagger} a_{\delta} + v_{\delta,\alpha\beta\gamma}^{13} a_{\delta}^{\dagger} a_{\gamma} a_{\beta} a_{\alpha} \right). \quad (3.13d)$$

Here, due to Eq. (2.34), the  $a^{\dagger}a^{\dagger}$  and  $aa$  parts of  $\hat{H}_M(q)$  vanish, and the  $a^{\dagger}a$  part of  $\hat{H}_M(q)$  is diagonalized. The matrix elements of the residual interactions in Eqs. (3.13b)–(3.13d) are antisymmetrized with respect to the quasiparticle indices. The matrices  $\mathbf{A}$  and  $\mathbf{B}$  have the same structures as those defined in the quasiparticle RPA formalism.<sup>17)</sup> The matrix  $\mathbf{D}$  is defined by

$$(\mathbf{D})_{\alpha\beta,\gamma\delta} = \frac{1}{2} \langle \phi(q) | [ [\hat{H}_M(q), (\hat{H} - \lambda(q)\hat{N})_A], a_{\alpha}^{\dagger} a_{\beta}^{\dagger} + a_{\beta} a_{\alpha}], a_{\gamma} a_{\delta} ] | \phi(q) \rangle. \quad (3.14)$$

These matrix elements can be expressed also in terms of the Hamiltonian matrix elements as

$$(\mathbf{D})_{\alpha\beta,\gamma\delta} = (d_{\alpha\beta,\gamma\delta}^{22} - d_{\alpha\beta\gamma\delta}^{40} + d_{\alpha\gamma}^{11}\delta_{\beta\delta} - d_{\beta\gamma}^{11}\delta_{\alpha\delta} - d_{\alpha\delta}^{11}\delta_{\beta\gamma} + d_{\beta\delta}^{11}\delta_{\alpha\gamma})/2, \quad (3.15a)$$

$$d_{\alpha\beta,\gamma\delta}^{22} = \sum_{\epsilon} (v_{\alpha\beta\epsilon,\gamma}^{31} h_{\delta\epsilon} - v_{\alpha\beta\epsilon,\delta}^{31} h_{\gamma\epsilon} - v_{\alpha,\epsilon\gamma\delta}^{13} h_{\beta\epsilon} + v_{\beta,\epsilon\gamma\delta}^{13} h_{\alpha\epsilon}), \quad (3.15b)$$

$$d_{\alpha\beta\gamma\delta}^{40} = \sum_{\epsilon} (v_{\alpha\beta\gamma,\epsilon}^{31} h_{\epsilon\delta} - v_{\beta\gamma\delta,\epsilon}^{31} h_{\epsilon\alpha} + v_{\gamma\delta\alpha,\epsilon}^{31} h_{\epsilon\beta} - v_{\delta\alpha\beta,\epsilon}^{31} h_{\epsilon\gamma}), \quad (3.15c)$$

$$d_{\alpha\beta}^{11} = \sum_{\gamma>\delta} (v_{\alpha,\beta\gamma\delta}^{13} h_{\gamma\delta} - v_{\gamma\delta\alpha,\beta}^{31} h_{\gamma\delta}), \quad (3.15d)$$

where  $h_{\alpha\beta}$  represents the matrix elements of  $(\hat{H} - \lambda\hat{N})_A$  defined by

$$(\hat{H} - \lambda\hat{N})_A = \sum_{\alpha>\beta} h_{\alpha\beta} (a_{\alpha}^{\dagger} a_{\beta}^{\dagger} + a_{\beta} a_{\alpha}). \quad (3.16)$$

Note that  $\mathbf{D}$  contains the matrix elements of the types  $v^{13}$  and  $v^{31}$ . These terms of the Hamiltonian do not contribute to the standard RPA equations.

The solution of the matrix equations is obtained as follows. From Eq. (3.11), we obtain

$$\mathbf{Q} = \lambda' B(q) ((\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) - \mathbf{D} - \Omega)^{-1} \mathbf{N}, \quad (3.17a)$$

$$\mathbf{P} = \lambda' (\mathbf{A} - \mathbf{B}) ((\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) - \mathbf{D} - \Omega)^{-1} \mathbf{N}, \quad (3.17b)$$

with

$$\Omega = B(q)C(q). \quad (3.18)$$

The condition that the collective mode is orthogonal to the number operator, Eq. (3.11c), gives the following equation:

$$S(\Omega) \equiv \mathbf{N}^T (\mathbf{A} - \mathbf{B}) ((\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) - \mathbf{D} - \Omega)^{-1} \mathbf{N} = 0. \quad (3.19)$$

The quantity  $\Omega = B(q)C(q)$  represents the square of the frequency  $\omega = \sqrt{BC}$  of the local harmonic mode, which is not necessarily positive. This equation can be regarded as a dispersion equation to determine  $\Omega = \omega^2$  as a zero point of  $S(\Omega)$ . The normalization condition, Eq. (3.11d), then gives a constraint on the value of  $\lambda'^2 B(q)$ . The value of the mass parameter  $B(q)$  is arbitrary, being related to the invariance under the point transformation Eq. (2.11). The choice of the coordinate  $q$  specifies the value of the mass parameter,  $B(q)$ . In practice, the coordinate is often scaled so as to make the mass parameter unity.

When the residual interactions are separable forces, such as the monopole pairing and the quadruple-quadrupole forces, the local harmonic equations reduce to a simpler form. The dispersion equation for the separable interaction does not require a matrix inversion as in Eq. (3.19). The details of these points are discussed in the Appendix.

Reference 10) discusses a problem of spurious (Nambu-Goldstone) modes for local harmonic approaches, and it is stated there that the RPA equation at non-equilibrium points must be extended in order to guarantee separation of the spurious modes. However, no practical way of solving the equation was given because the equation has parameters for which we do not have a method to calculate. In our present formulation, the RPA equation is indeed extended to assure the number conservation.

### 3.3. Construction of collective subspace

Let us finally give algorithms to construct the collective subspace  $|\phi(q)\rangle$  as a function of the collective coordinate  $q$ . Note that the local harmonic equations, Eqs. (3.5)–(3.7), are regarded as local equations in the sense that the equations can be solved independently for different values of  $q$ . At the HFB ground state,  $|\phi_0\rangle$ , defined by the HFB equation

$$\delta \langle \phi_0 | \hat{H} - \lambda_0 \hat{N} | \phi_0 \rangle = 0, \quad (3.20)$$

we find  $\partial V / \partial q = 0$ . Therefore,  $|\phi_0\rangle$  is always a state in the collective subspace because Eq. (3.5) is automatically satisfied. Equations (3.6) and (3.7) reduce to the standard RPA equations at  $|\phi_0\rangle$  since the last two terms in Eq. (3.7) vanish. The operators  $\hat{Q}$  and  $\hat{P}$  are then determined as one of the normal modes of the RPA equation.

For non-equilibrium states, in general, Eq. (3.5) and the other two equations, (3.6) and (3.7), are coupled. We may solve the coupled equations in an iterative way. As discussed in §3.2, we can find the operators  $\hat{Q}(q)^{(n)}$  and  $\hat{P}(q)^{(n)}$  by solving Eqs. (3.6) and (3.7) for a given trial state  $|\phi(q)\rangle^{(n)}$  ( $n$  denoting the iteration step). This defines the moving frame Hamiltonian  $\hat{H}_M(q)^{(n+1)} = \hat{H} - \lambda(q)^{(n+1)} \hat{N} - \left(\frac{\partial V}{\partial q}\right)^{(n)} \hat{Q}(q)^{(n)}$ , which can be used to construct a trial state  $|\phi(q)\rangle^{(n+1)}$  for the next iteration. If the iteration converges, we obtain a state  $|\phi(q)\rangle$  for which Eqs. (3.5)–(3.7) are simultaneously satisfied. Repeating the same procedure for different values of  $q$ , one finally obtains the collective subspace  $|\phi(q)\rangle$  and the collective Hamiltonian as a function of  $q$ .

We remark here that the operator  $\hat{P}(q)$  thus determined does not guarantee Eq. (2.21), although the other equations are satisfied. In this sense, the local harmonic solution is an approximate solution. The exact solution satisfying all the basic equations in §2.2 may not exist in realistic situations. Only when the system is “exactly decoupled”<sup>8)</sup> does the above procedure give the exact solution.

It is possible to choose another algorithm which satisfies Eq. (2.21), at the expense of introducing errors into Eq. (3.5). Let  $|\phi(q_0)\rangle$  be a solution that satisfies the basic equations at  $q = q_0$ . The infinitesimal generators  $\hat{Q}(q_0)$  and  $\hat{P}(q_0)$  are determined by solving Eqs. (3.6) and (3.7). Then we can generate the state  $|\phi(q_0 + \delta q)\rangle$  for an infinitesimal shift of the collective coordinate as

$$|\phi(q_0 + \delta q)\rangle = e^{-i\delta q \hat{P}(q_0)} |\phi(q_0)\rangle. \quad (3.21)$$

Repeating this procedure, we can construct a collective subspace. This solution should coincide with that solved by the previous method if the system is exactly decoupled.

The two methods described above give different solutions in situations where the exact decoupling is not satisfied. In such cases, one can evaluate the quality of decoupling for the collective subspace or the validity of the local harmonic approximation by comparing the two solutions. We note also that the second method can be used to provide an initial guess,  $|\phi(q)\rangle^{(0)}$ , for the iteration of the first method.

#### §4. Extension to multi-dimensional collective subspace

In this section we extend the adiabatic SCC method to the case of a multi-dimensional collective subspace described by  $D$  collective coordinates and conjugate momenta,  $\{q^i, p_i; i = 1, \dots, D\}$ .

One can easily derive the basic equations of the adiabatic SCC method in parallel to the derivation given in §2 by noting first that Eqs. (2·12) and (2·14) are now extended to

$$|\phi(q, p, N)\rangle = e^{i\hat{G}(q,p,n)} |\phi(q)\rangle, \quad (4.1)$$

$$\hat{G} = p_i \hat{Q}^i(q) + n \hat{\Theta}(q), \quad (4.2)$$

where the operator  $\hat{Q}^i(q)$  now has  $D$  components with the coordinate label  $i$ . It is implied here and hereafter that any coordinate index ( $i$  in the above expression) appearing both as the superscript and subscript is summed over. The infinitesimal generator  $\hat{P}_i(q)$  also has  $D$  components, each of which is related to the derivative  $i \frac{\partial}{\partial q^i} |\phi(q)\rangle$ . In the following, the coordinate dependence is often omitted. For instance,  $B^{ij}(q)$  and  $\hat{Q}^i(q)$  will be simply denoted by  $B^{ij}$  and  $\hat{Q}^i$ .

The adiabatic collective Hamiltonian is expressed as

$$\mathcal{H}(q, p, N) = V(q) + \frac{1}{2} B^{ij}(q) p_i p_j + \lambda(q) n. \quad (4.3)$$

The zeroth and the first order equations of the collective subspace are derived as

$$\delta \langle \phi(q) | \hat{H} - \lambda(q) \hat{N} - \frac{\partial V}{\partial q^i} \hat{Q}^i | \phi(q) \rangle = 0, \quad (4.4)$$

$$\delta \langle \phi(q) | [\hat{H} - \lambda(q) \hat{N}, \hat{Q}^i] - \frac{1}{i} B^{ij} \hat{P}_j | \phi(q) \rangle = 0, \quad (4.5)$$

while the second order equation becomes

$$\begin{aligned} \delta \langle \phi(q) | \frac{1}{2} [\hat{H} - \lambda(q) \hat{N}, \hat{Q}^i, \hat{Q}^j] + \frac{1}{6} \left[ \frac{\partial V}{\partial q^k} \hat{Q}^k, \hat{Q}^i, \hat{Q}^j \right] \\ - \frac{1}{2} (B^{ik} \hat{Q}_{;k}^j + B^{jk} \hat{Q}_{;k}^i) | \phi(q) \rangle = 0 \end{aligned} \quad (4.6)$$

with

$$\hat{Q}_{;j}^i = \frac{\partial \hat{Q}^i}{\partial q^j} + \Gamma_{kj}^i \hat{Q}^k, \quad (4.7)$$

$$\Gamma_{kj}^i = \frac{1}{2} B^{il} \left( \frac{\partial B_{lk}}{\partial q^j} + \frac{\partial B_{lj}}{\partial q^k} - \frac{\partial B_{kj}}{\partial q^l} \right), \quad (4.8)$$

where  $B_{ij}$  is the inverse matrix of  $B^{ij}$ , and the bracket including the three operators is defined by

$$[A, B, C] = \frac{1}{2} ([ [A, B], C ] + [ [A, C], B ]). \quad (4.9)$$

Expanding the canonical variable condition with respect to  $p_i$  and  $n$ , the following equations are derived:

$$\langle \phi(q) | \hat{P}_i | \phi(q) \rangle = 0, \tag{4.10}$$

$$\langle \phi(q) | \hat{N} | \phi(q) \rangle = N_0, \tag{4.11}$$

and

$$\langle \phi(q) | [\hat{Q}^i, \hat{P}_j] | \phi(q) \rangle = i\delta_{ij}, \tag{4.12}$$

$$\langle \phi(q) | [\hat{Q}^i, \hat{N}] | \phi(q) \rangle = 0, \tag{4.13}$$

$$\langle \phi(q) | [\hat{P}_i, \hat{N}] | \phi(q) \rangle = 0. \tag{4.14}$$

These basic equations are invariant under the point transformation of the collective variables:

$$q^i \rightarrow q'^i = q'^i(q), \tag{4.15a}$$

$$p_i \rightarrow p'_i = p_j \times \left( \partial q^j / \partial q'^i \right). \tag{4.15b}$$

We have adopted the vector-tensor notation<sup>20)</sup> to make clear the transformation properties under the point transformation. Quantities with a coordinate index as the subscript (superscript) have the transformation properties of the *covariant* (*contravariant*) vectors. For example,

$$\hat{Q}^i \rightarrow \hat{Q}'^i = \hat{Q}^j \times \left( \partial q'^i / \partial q^j \right), \tag{4.16}$$

$$\hat{P}_i \rightarrow \hat{P}'_i = \hat{P}_j \times \left( \partial q^j / \partial q'^i \right). \tag{4.17}$$

The mass tensor  $B^{ij}$  is the contravariant tensor of second rank. The operator  $\hat{Q}^i_{;j}$  defined by Eq. (4.7) is the covariant derivative of  $\hat{Q}^i$ , and  $\Gamma^i_{kj}$  is the Christoffel symbol, where the mass tensor  $B_{ij}$  plays the role of metric tensor.

Let us now derive local harmonic equations of the collective subspace. Taking the  $q$ -derivative, the zeroth order equation (4.4) leads to

$$\delta \langle \phi(q) | \left[ \hat{H} - \lambda(q)\hat{N}, \frac{1}{i}\hat{P}_i \right] - C_{ij}(q)\hat{Q}^j - \frac{\partial V}{\partial q^j}\hat{Q}^j_{;i} - \frac{\partial \lambda}{\partial q^i}\hat{N} | \phi(q) \rangle = 0, \tag{4.18}$$

$$C_{ij}(q) = \frac{\partial^2 V}{\partial q^i \partial q^j} - \Gamma^k_{ij} \frac{\partial V}{\partial q^k}. \tag{4.19}$$

As we have done for the  $D = 1$  case, we would like to eliminate the covariant derivative  $\hat{Q}^j_{;i}$  in Eq. (4.18) in order to give a feasible form of the local harmonic equation. This was done for the  $D = 1$  case with the help of the second order equation of the collective subspace. The corresponding equations (4.6) give  $D(D + 1)/2$  constraints, while the number of unknown parameters,  $\hat{Q}^j_{;i}$ , is  $D^2$ . In fact, Eq. (4.6) is equivalent to

$$\delta \langle \phi(q) | \frac{1}{2} [[\hat{H} - \lambda(q)\hat{N}, \hat{Q}^j], \hat{Q}^i] + \frac{1}{6} \left[ \left[ \frac{\partial V}{\partial q^k} \hat{Q}^k, \hat{Q}^j \right], \hat{Q}^i \right] - (B^{ik}\hat{Q}^j_{;k} + \hat{R}^{ij}) | \phi(q) \rangle = 0, \tag{4.20}$$

where  $\hat{R}^{ij}$  are arbitrary one-body operators which are antisymmetric with respect to exchange of indices  $i$  and  $j$ . If we choose  $\hat{R}^{ij} = 0$ , we can eliminate the derivative term  $\frac{\partial V}{\partial q^i} \hat{Q}_i^j$ . Then, Eq. (4.18) leads to

$$\delta \langle \phi(q) | \left[ \hat{H} - \lambda(q) \hat{N}, \frac{1}{i} \hat{P}_i \right] - C_{ij} \hat{Q}^j - \frac{1}{2} [[\hat{H} - \lambda(q) \hat{N}, (\hat{H} - \lambda(q) \hat{N})_A], B_{ij} \hat{Q}^j] - \frac{\partial \lambda}{\partial q^i} \hat{N} | \phi(q) \rangle = 0. \quad (4.21)$$

This equation is an analog of Eq. (3.7) and is linear in the infinitesimal generators  $\hat{Q}^i$  and  $\hat{P}_i$ . We can numerically solve Eqs. (4.4), (4.5) and (4.21) in the same manner as discussed in §§3.2 and 3.3.

It should be remarked that the local harmonic equation Eq. (4.21) for  $D > 1$  is derived from Eqs. (4.4) and (4.6), but with the additional condition  $\hat{R}^{ij} = 0$  in Eq. (4.20). This condition is introduced to obtain the local harmonic equations parallel to the one-dimensional case.

## §5. Conclusions

We have formulated the adiabatic approximation of the general framework of the selfconsistent collective coordinate method in order to describe large amplitude collective motion in superconducting nuclei. The formalism, based on the TDHFB equations of motion, guarantees the conservation of particle number in a transparent way. We have shown that the equations of collective subspace are reduced to local linear equations for the infinitesimal generators, which can be solved with use of the quasiparticle representation of the Hamiltonian matrix elements. This provides a concrete procedure to determine the states  $e^{ip\hat{Q}(q)} |\phi(q)\rangle$  in the collective subspace and the collective Hamiltonian  $\mathcal{H}(q, p) = V(q) + \frac{1}{2} B(q) p^2$  as functions of the collective coordinate  $q$  and momentum  $p$ . A possible extension to the case of multi-dimensional collective coordinates was also discussed.

We emphasize that the equations given in this paper are solvable by means of the matrix method similar to the standard RPA. We hope that the present adiabatic theory is useful to solve a number of open questions in realistic studies of large amplitude collective motion in nuclear systems.

## Appendix A

### — Solution for the Separable Interactions —

In this appendix, we give solutions of the local harmonic equations of collective subspace for the case in which the two-body interaction is given by separable forces. We assume that the Hamiltonian is given by

$$\hat{H} = \hat{h}_0 - \frac{\kappa}{2} \hat{F}^\dagger \hat{F}, \quad (A.1)$$

where  $\hat{h}_0(= \hat{h}_0^\dagger)$  and  $\hat{F}$  are one-body operators. Equivalently, one may write

$$\hat{H} = \hat{h}_0 - \frac{\kappa}{2} \hat{F}^{(+)} \hat{F}^{(+)} + \frac{\kappa}{2} \hat{F}^{(-)} \hat{F}^{(-)}, \quad (\text{A}\cdot 2)$$

$$\hat{F}^{(\pm)} \equiv (\hat{F} \pm \hat{F}^\dagger)/2 = \pm \hat{F}^{(\pm)\dagger}. \quad (\text{A}\cdot 3)$$

For separable forces, it is customary to neglect the Fock term of the forces. This approximation is easily and consistently implemented in the SCCM by assuming that the equation of motion for the time-dependent mean-field state  $|\phi(t)\rangle$  is now given by the time-dependent Hartree-Bogoliubov equation without the Fock terms,

$$\delta \langle \phi(t) | i \frac{\partial}{\partial t} - \hat{h}(t) | \phi(t) \rangle = 0, \quad (\text{A}\cdot 4)$$

$$\hat{h}(t) = \hat{h}_0 - \kappa \hat{F}^{(+)} \langle \phi(t) | \hat{F}^{(+)} | \phi(t) \rangle + \kappa \hat{F}^{(-)} \langle \phi(t) | \hat{F}^{(-)} | \phi(t) \rangle. \quad (\text{A}\cdot 5)$$

The local harmonic equations (3·5)–(3·7) then become

$$\delta \langle \phi(q) | \hat{h}_M(q) | \phi(q) \rangle = 0, \quad (\text{A}\cdot 6)$$

$$\delta \langle \phi(q) | [\hat{h}_M(q), \hat{Q}(q)] - f_Q^{(-)} \hat{F}^{(-)} - \frac{1}{i} B(q) \hat{P}(q) | \phi(q) \rangle = 0, \quad (\text{A}\cdot 7)$$

$$\begin{aligned} \delta \langle \phi(q) | \left[ \hat{h}_M(q), \frac{1}{i} B(q) \hat{P}(q) \right] - f_P^{(+)} \hat{F}^{(+)} - B(q) C(q) \hat{Q}(q) - f_R^{(+)} \hat{F}^{(+)} \\ - f_Q^{(-)} [\hat{F}^{(-)}, (\hat{h}(q) - \lambda(q) \hat{N})_A] - f_N \hat{N} | \phi(q) \rangle = 0, \end{aligned} \quad (\text{A}\cdot 8)$$

where  $\hat{h}_M(q)$  is the mean-field Hamiltonian in the moving frame defined by

$$\hat{h}_M(q) = \hat{h}(q) - \frac{\partial V}{\partial q} \hat{Q}(q) - \lambda(q) \hat{N}, \quad (\text{A}\cdot 9)$$

$$\hat{h}(q) = \hat{h}_0 - \kappa \hat{F}^{(+)} \langle \phi(q) | \hat{F}^{(+)} | \phi(q) \rangle, \quad (\text{A}\cdot 10)$$

and the definitions of the other symbols are

$$f_Q^{(-)} = -\kappa \langle \phi(q) | [\hat{F}^{(-)}, \hat{Q}(q)] | \phi(q) \rangle, \quad (\text{A}\cdot 11\text{a})$$

$$f_P^{(+)} = \kappa \langle \phi(q) | \left[ \hat{F}^{(+)}, \frac{1}{i} B(q) \hat{P}(q) \right] | \phi(q) \rangle, \quad (\text{A}\cdot 11\text{b})$$

$$f_R^{(+)} = -\kappa \langle \phi(q) | [[\hat{F}^{(+)}, (\hat{h}(q) - \lambda(q) \hat{N})_A], \hat{Q}(q)] | \phi(q) \rangle / 2, \quad (\text{A}\cdot 11\text{c})$$

$$f_N = B(q) \frac{\partial \lambda}{\partial q}. \quad (\text{A}\cdot 11\text{d})$$

We express all operators in the above equations in terms of the quasiparticle operators  $\{a_\alpha^\dagger, a_\alpha\}$  defined for  $\hat{h}_M(q)$  and  $|\phi(q)\rangle$ . For example, we have

$$\hat{h}_M(q) = \sum_\alpha e_\alpha a_\alpha^\dagger a_\alpha, \quad (\text{A}\cdot 12)$$

$$\hat{F}^{(+)} = \sum_{\alpha>\beta} F_{\alpha\beta}^{(+)} (a_\alpha^\dagger a_\beta^\dagger + a_\beta a_\alpha) + \sum_{\alpha\beta} F_{B,\alpha\beta}^{(+)} a_\alpha^\dagger a_\beta, \quad (\text{A}\cdot 13)$$

$$\hat{F}^{(-)} = \sum_{\alpha>\beta} F_{\alpha\beta}^{(-)} (a_\alpha^\dagger a_\beta^\dagger - a_\beta a_\alpha) + \sum_{\alpha\beta} F_{B,\alpha\beta}^{(-)} a_\alpha^\dagger a_\beta. \quad (\text{A}\cdot 14)$$

We have assumed here that all matrix elements are real. Equations (A·7) and (A·8) can then be reduced to linear equations for the matrix elements  $Q_{\alpha\beta}$  and  $P_{\alpha\beta}$  of the infinitesimal generators  $\hat{Q}(q)$  and  $\hat{P}(q)$ . They are easily solved to give the expression

$$Q_{\alpha\beta} = \frac{e_\alpha + e_\beta}{(e_\alpha + e_\beta)^2 - \Omega} F_{\alpha\beta}^{(-)} f_Q^{(-)} + \frac{1}{(e_\alpha + e_\beta)^2 - \Omega} \left( F_{\alpha\beta}^{(+)} f_{PR}^{(+)} + R_{\alpha\beta}^{(-)} f_Q^{(-)} + N_{\alpha\beta} f_N \right), \quad (\text{A}\cdot 15)$$

$$BP_{\alpha\beta} = \frac{e_\alpha + e_\beta}{(e_\alpha + e_\beta)^2 - \Omega} \left( F_{\alpha\beta}^{(+)} f_{PR}^{(+)} + R_{\alpha\beta}^{(-)} f_Q^{(-)} + N_{\alpha\beta} f_N \right) + \frac{\Omega}{(e_\alpha + e_\beta)^2 - \Omega} F_{\alpha\beta}^{(-)} f_Q^{(-)}, \quad (\text{A}\cdot 16)$$

$$f_{PR}^{(+)} = f_P^{(+)} + f_R^{(+)}, \quad (\text{A}\cdot 17)$$

where we have introduced the one-body operator

$$\hat{R}(q)^{(\pm)} \equiv [\hat{F}_B^{(\pm)}(q), (\hat{h}(q) - \lambda(q)\hat{N})_A] = \sum_{\alpha>\beta} R_{\alpha\beta}^{(\pm)} (a_\alpha^\dagger a_\beta^\dagger \mp a_\beta a_\alpha), \quad (\text{A}\cdot 18)$$

with  $\hat{F}_B^{(\pm)}(q)$  being the last terms of  $\hat{F}^{(\pm)}$  in Eqs. (A·13) and (A·14).

Inserting this expression for the definition of  $f_{PR}^{(+)}$  and  $f_Q^{(-)}$ , we obtain equations for the unknown quantities  $f_{PR}^{(+)}$ ,  $f_Q^{(-)}$  and  $f_N$ . Similarly, the condition of orthogonality to the number operator Eq. (3·11c) gives another equation for  $f_{PR}^{(+)}$ ,  $f_Q^{(-)}$  and  $f_N$ . These equations can be written in a  $3 \times 3$  matrix form:

$$\begin{pmatrix} S_{xx'}(\Omega) \end{pmatrix} \begin{pmatrix} f_{PR}^{(+)} \\ f_Q^{(-)} \\ f_N \end{pmatrix} = 0, \quad (\text{A}\cdot 19)$$

where

$$S_{11} = 2S_{F^{(+)}F^{(+)}}^{(1)} + S_{R^{(+)}F^{(+)}}^{(2)} - \frac{1}{\kappa}, \quad (\text{A}\cdot 20\text{a})$$

$$S_{12} = 2\Omega S_{F^{(+)}F^{(-)}}^{(2)} + 2S_{F^{(+)}R^{(-)}}^{(1)} + S_{R^{(+)}F^{(-)}}^{(1)} + S_{R^{(+)}R^{(-)}}^{(2)}, \quad (\text{A}\cdot 20\text{b})$$

$$S_{13} = 2S_{F^{(+)}N}^{(1)} + S_{R^{(+)}N}^{(2)}, \quad (\text{A}\cdot 20\text{c})$$

$$S_{21} = 2S_{F^{(-)}F^{(+)}}^{(2)}, \quad (\text{A}\cdot 20\text{d})$$

$$S_{22} = 2S_{F^{(-)}F^{(-)}}^{(1)} + 2S_{F^{(-)}R^{(-)}}^{(2)} - \frac{1}{\kappa}, \quad (\text{A}\cdot 20\text{e})$$

$$S_{23} = 2S_{F^{(-)}N}^{(2)}, \quad (\text{A}\cdot 20\text{f})$$

$$S_{31} = S_{NF^{(+)}}^{(1)}, \quad (\text{A}\cdot 20\text{g})$$

$$S_{32} = \Omega S_{NF^{(-)}}^{(2)} + S_{NR^{(-)}}^{(1)}, \quad (\text{A}\cdot 20\text{h})$$

$$S_{33} = S_{NN}^{(1)}. \quad (\text{A}\cdot 20\text{i})$$

The functions  $S_{XY}^{(1)}$  with the symbols  $X$  and  $Y$  denoting  $(X, Y) = (F^{(+)}, F^{(+)})$ ,  $(F^{(+)}, R^{(-)})$ ,  $(F^{(+)}, N)$ ,  $(R^{(+)}, F^{(-)})$ ,  $(F^{(-)}, F^{(-)})$ ,  $(N, N)$ ,  $(N, F^{(+)})$ ,  $(N, R^{(-)})$  are given by

$$S_{XY}^{(1)} = \sum_{\alpha > \beta} \frac{e_{\alpha} + e_{\beta}}{(e_{\alpha} + e_{\beta})^2 - \Omega} X_{\alpha\beta} Y_{\alpha\beta}, \quad (\text{A}\cdot\text{21})$$

while the functions  $S_{XY}^{(2)}$  with  $(X, Y) = (F^{(+)}, F^{(-)})$ ,  $(R^{(+)}, F^{(+)})$ ,  $(R^{(+)}, R^{(-)})$ ,  $(R^{(+)}, N)$ ,  $(F^{(-)}, F^{(+)})$ ,  $(F^{(-)}, R^{(-)})$ ,  $(F^{(-)}, N)$ ,  $(N, F^{(-)})$  are given by

$$S_{XY}^{(2)} = \sum_{\alpha > \beta} \frac{1}{(e_{\alpha} + e_{\beta})^2 - \Omega} X_{\alpha\beta} Y_{\alpha\beta}. \quad (\text{A}\cdot\text{22})$$

The value of  $\Omega$  is determined by finding the zero point of the dispersion equation

$$\det\{S_{xx'}(\Omega)\} = 0. \quad (\text{A}\cdot\text{23})$$

Normalizations of  $f_{PR}^{(+)}$ ,  $f_Q^{(-)}$  and  $f_N$  are fixed by the condition Eq. (3-11d). It is straightforward to extend the above procedure to the case in which the two-body interaction is given by a sum of the separable forces.

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