Gauge-Invariant Formulation of the Adiabatic Self-Consistent Collective Coordinate Method

Nobuo HINOHARA,[1] Takashi NAKATSUKASA,[2] Masayuki MATSUO[3] and Kenichi MATSUYANAGI[1]

[1] *Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*
[2] *Institute of Physics and Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8571, Japan*
[3] *Department of Physics, Faculty of Science, Niigata University, Niigata 950-2181, Japan*

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The adiabatic self-consistent collective coordinate (ASCC) method is a practical microscopic theory of large-amplitude collective motion in nuclei with superfluidity. We show that its basic equations are invariant under transformations involving the gauge angle in particle-number space. By virtue of this invariance, a clean separation of the large-amplitude collective motion and the pairing rotational motion can be made, and this allows us to restore the particle-number symmetry broken by the Hartree-Fock-Bogoliubov (HFB) approximation. We formulate the ASCC method explicitly in a gauge-invariant form. In solving the ASCC equations, it is necessary to fix the gauge. Applying this new formulation to the multi-$O(4)$ model, we compare different gauge-fixing procedures and demonstrate that calculations using different gauges indeed yield the same results for gauge-invariant quantities, such as the collective path and quantum spectra. We propose a gauge-fixing prescription that seems most convenient in realistic calculations.

§1. Introduction

The construction of a microscopic theory of large-amplitude collective motion is a long-standing and fundamental problem in the study of nuclear many-body systems.[1)–35)] As is well known, pairing correlations play crucial roles in low-lying states of medium and heavy nuclei, and they are taken into account in the Hartree-Fock-Bogoliubov (HFB) mean-field theory by violating the particle number conservation.[36)–38)] The broken particle-number symmetry can be restored, however, by making the self-consistent quasiparticle random-phase approximation (QRPA), on top of the HFB mean field.[36)–38)] It is an advantage of the QRPA that number-conserving collective modes, such as shape-vibrational modes, are exactly decoupled from number-fluctuation modes. The latter modes are associated with the nucleon-number degrees of freedom and are called the 'pairing rotational modes'. It is a unique feature of nuclei as finite quantum systems that such rotational motion in gauge space is actually observed in quantum spectra.[39)] Because the applicability of the QRPA is limited to small-amplitude collective motion, it is highly desirable to extend the QRPA to a general theory which has its decoupling feature. Such a theory should be capable of describing the interplay between large-amplitude collective motion and the pairing rotational modes.

The self-consistent collective coordinate (SCC) method[7)] is a microscopic theory of large-amplitude collective motion based on the time-dependent Hartree-Fock (TDHF) method. This method enables us to extract the collective submanifold in a fully self-consistent manner. The SCC method was originally formulated[7)] for

systems without pairing correlations, and then extended[18] to systems with superfluidity. To extract the collective submanifold embedded in the time-dependent Hartree-Fock-Bogoliubov (TDHFB) phase space, number and angle variables describing the pairing rotational motion are explicitly introduced,[18] in addition to the collective variables describing the large-amplitude collective motion. This extended version of the SCC method has been applied successfully to various kinds of anharmonic vibration and high-spin rotational motion.[40–51] However, obtaining solutions with this method requires use of a technique employing expansion with respect to the collective coordinates and momenta around the HFB states. Thus it is difficult to describe large-amplitude collective motion using this expansion. Recently, the adiabatic SCC (the ASCC) method has been proposed to overcome this difficulty.[52] The ASCC method is an alternative way to solve the SCC basic equations in the case that the large-amplitude collective motion of interest is slow (adiabatic). Under this assumption, the basic equations of the SCC method are expanded up to second order in the collective momentum, but no expansion is carried out with respect to the collective coordinate. This method has been applied[53] to the study of shape-coexistence phenomena[54–56] in which there is large-amplitude collective motion that appears as the transition between the oblate and prolate HFB equilibrium shapes. However, the calculation to determine the collective degrees of freedom often involves a numerical instability, caused by the existence of a redundant degree of freedom in the ASCC equations. This problem has been treated by imposing an additional condition by hand.[57] However we now understand the origin of this redundancy: It is due to the gauge invariance of the ASCC equations.

The main purpose of this paper is to formulate the ASCC method in a manner that makes manifest the invariance under transformations with respect to the angle variable in the gauge space. This invariance is necessary to realize a clean separation of the large-amplitude collective motion and the pairing rotational motion, and to restore the particle-number symmetry broken by the HFB approximation. This new formulation of the ASCC method also provides justification of the prescription adopted in our previous work.[57] In the present work, we apply this method to the multi-$O(4)$ model[57–62] with several choices of the gauge and test the internal consistency of the proposed scheme by carrying out a detailed numerical calculation.

This paper is organized as follows. In §2 the basic equations of the ASCC method are presented. In §3 a gauge-invariant formulation of the ASCC method is given. This formulation is applied to the multi-$O(4)$ model in §4, and the results of numerical calculations testing its validity are reported in §5. Concluding remarks are given in §6.

§2. Basic equations of the ASCC method

2.1. *Basic ideas*

The time evolution of large-amplitude collective motion is described by the time-dependent variational principle expressed as

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

where $|\phi(t)\rangle$ is the time-dependent HFB state vector. Assuming that the time-dependence of the collective motion is governed by the collective coordinate q and

the momentum p, we parameterize the time-dependent HFB state vector as

$$|\phi(t)\rangle = |\phi(q,p,\varphi,n)\rangle\,. \tag{2·2}$$

Here, φ represents the gauge angle conjugate to the particle number $n \equiv N - N_0$. We measure the particle number from a reference value N_0 specified below and assume, for simplicity, that there is one collective coordinate. We define the intrinsic state vector $|\phi(q,p,n)\rangle$ in the particle-number (gauge) space by

$$|\phi(q,p,\varphi,n)\rangle = e^{-i\varphi\tilde{N}}\,|\phi(q,p,n)\rangle\,, \tag{2·3}$$

where $\tilde{N} \equiv \hat{N} - N_0$. Two sets of collective variables, (q,p) and (φ,n), are determined such that the canonical variable conditions

$$\begin{aligned}
\langle\phi(q,p,n)|\, i\frac{\partial}{\partial q}\,|\phi(q,p,n)\rangle &= p + \frac{\partial S}{\partial q}, \quad \langle\phi(q,p,n)|\,\frac{\partial}{i\partial p}\,|\phi(q,p,n)\rangle = -\frac{\partial S}{\partial p},\\
\langle\phi(q,p,n)|\,\tilde{N}\,|\phi(q,p,n)\rangle &= n + \frac{\partial S}{\partial \varphi}, \quad \langle\phi(q,p,n)|\,\frac{\partial}{i\partial n}\,|\phi(q,p,n)\rangle = -\frac{\partial S}{\partial n}
\end{aligned} \tag{2·4}$$

are satisfied. Here, the generating function S is an arbitrary function of q, p, φ, and n. We choose $S = 0$, because it is appropriate for the adiabatic approximation.[15),16),20)] The collective Hamiltonian is defined by

$$\mathcal{H}(q,p,n) = \langle\phi(q,p,\varphi,n)|\,\hat{H}\,|\phi(q,p,\varphi,n)\rangle = \langle\phi(q,p,n)|\,\hat{H}\,|\phi(q,p,n)\rangle\,. \tag{2·5}$$

Note that this collective Hamiltonian is independent of the gauge angle φ, because the original Hamiltonian commutes with the particle number operator $\hat{N}$.

The equation of collective path is obtained by replacing the time derivative term in Eq. (2·1) with derivatives with respect to the four collective variables:

$$\delta\,\langle\phi(q,p,n)|\,\hat{H} - i\left(\frac{\partial\mathcal{H}}{\partial p}\frac{\partial}{\partial q} - \frac{\partial\mathcal{H}}{\partial q}\frac{\partial}{\partial p} + \frac{1}{i}\frac{\partial\mathcal{H}}{\partial n}\tilde{N}\right)|\phi(q,p,n)\rangle = 0. \tag{2·6}$$

Here, the canonical equations of motion for the collective variables (q,p) and (φ,n) are used in order to eliminate the time derivative of the collective variables. Equations (2·4), (2·5) and (2·6) constitute the basic equations of the SCC method.[7),18)]

2.2. *Basic equations of the ASCC method*

Assuming that the large-amplitude collective motion is slow, i.e., that p is small, let us write the TDHFB state vector $|\phi(q,p,n)\rangle$ in the following form:

$$|\phi(q,p,n)\rangle = e^{ip\hat{Q}(q)+in\hat{\Theta}(q)}\,|\phi(q)\rangle\,. \tag{2·7}$$

Here $\hat{Q}(q)$ and $\hat{\Theta}(q)$ are Hermitian one-body operators, which may be written as

$$\hat{Q}(q) = \sum_{\alpha\beta}\left(Q_{\alpha\beta}(q)a^\dagger_\alpha a^\dagger_\beta + Q_{\alpha\beta}(q)^* a_\beta a_\alpha\right), \tag{2·8}$$

$$\hat{\Theta}(q) = i\sum_{\alpha\beta}\left(\Theta_{\alpha\beta}(q)a^\dagger_\alpha a^\dagger_\beta - \Theta_{\alpha\beta}(q)^* a_\beta a_\alpha\right), \tag{2·9}$$

where $a^\dagger_\alpha$ and a_α are the quasiparticle creation and annihilation operators associated with the time-even state vector $|\phi(q)\rangle$, which satisfy $a_\alpha\,|\phi(q)\rangle = 0$, and $n = N - N_0$,

N_0 being the expectation value of the particle number with respect to $|\phi(q)\rangle$. In §3, we show that it is also possible to adopt a slightly different representation for $\hat{Q}(q)$.

Substituting (2·7) into (2·4) and comparing the coefficients of zeroth-order and first-order terms in p and n, we obtain the canonical variable conditions in the adiabatic limit:

$$\langle\phi(q)|\,\hat{P}(q)\,|\phi(q)\rangle = 0, \tag{2·10}$$
$$\langle\phi(q)|\,\hat{Q}(q)\,|\phi(q)\rangle = 0, \tag{2·11}$$
$$\langle\phi(q)|\,\tilde{N}\,|\phi(q)\rangle = 0, \tag{2·12}$$
$$\langle\phi(q)|\,\hat{\Theta}(q)\,|\phi(q)\rangle = 0, \tag{2·13}$$
$$\langle\phi(q)|\,[\hat{\Theta}(q),\tilde{N}]\,|\phi(q)\rangle = i, \tag{2·14}$$
$$\langle\phi(q)|\,[\hat{Q}(q),\hat{\Theta}(q)]\,|\phi(q)\rangle = 0, \tag{2·15}$$
$$\langle\phi(q)|\,\frac{\partial\hat{Q}}{\partial q}\,|\phi(q)\rangle = -1, \tag{2·16}$$

where $\hat{P}(q)$ is the local shift operator defined by

$$\hat{P}(q)\,|\phi(q)\rangle = i\frac{\partial}{\partial q}\,|\phi(q)\rangle\,. \tag{2·17}$$

Differentiating (2·11) and (2·12) with respect to q and using (2·16), we obtain

$$\langle\phi(q)|\,[\hat{Q}(q),\hat{P}(q)]\,|\phi(q)\rangle = i, \tag{2·18}$$
$$\langle\phi(q)|\,[\tilde{N},\hat{P}(q)]\,|\phi(q)\rangle = 0. \tag{2·19}$$

The collective Hamiltonian (2·5) is also expanded up to second order in p and first order in n, and we write

$$\mathcal{H}(q,p,n) = V(q) + \frac{1}{2}B(q)p^2 + \lambda(q)n, \tag{2·20}$$

where the collective potential $V(q)$, the inverse mass parameter $B(q)$, and the chemical potential $\lambda(q)$ are defined by

$$V(q) = \mathcal{H}(q,p,n)\Big|_{p=n=0} = \langle\phi(q)|\,\hat{H}\,|\phi(q)\rangle\,, \tag{2·21}$$
$$B(q) = \frac{1}{2}\frac{\partial^2\mathcal{H}}{\partial p^2}\Big|_{p=n=0} = \langle\phi(q)|\,[[\hat{H},i\hat{Q}(q)],i\hat{Q}(q)]\,|\phi(q)\rangle\,, \tag{2·22}$$
$$\lambda(q) = \frac{\partial\mathcal{H}}{\partial n}\Big|_{p=n=0} = \langle\phi(q)|\,[\hat{H},i\hat{\Theta}(q)]\,|\phi(q)\rangle\,. \tag{2·23}$$

We obtain the ASCC equations by expanding the equation of collective path (2·6) with respect to p and n, and requiring that the variations vanish at each order in p and n. At zeroth order, we obtain the moving-frame HFB equation

$$\delta\,\langle\phi(q)|\,\hat{H}_M(q)\,|\phi(q)\rangle = 0, \tag{2·24}$$

where

$$\hat{H}_M(q) = \hat{H} - \lambda(q)\tilde{N} - \frac{\partial V}{\partial q}\hat{Q}(q) \tag{2·25}$$

is the moving-frame Hamiltonian. At first and second orders, we obtain the moving-frame QRPA equations (also called the local harmonic equations),

$$\delta \langle \phi(q)| [\hat{H}_M(q), i\hat{Q}(q)] - B(q)\hat{P}(q) |\phi(q)\rangle = 0, \tag{2·26}$$

$$\delta \langle \phi(q)| [\hat{H}_M(q), \hat{P}(q)] - iC(q)\hat{Q}(q) - \frac{1}{2B(q)}[[\hat{H}_M(q), \frac{\partial V}{\partial q}\hat{Q}(q)], i\hat{Q}(q)] - i\frac{\partial \lambda}{\partial q}\tilde{N} |\phi(q)\rangle = 0, \tag{2·27}$$

where

$$C(q) = \frac{\partial^2 V}{\partial q^2} + \frac{1}{2B(q)}\frac{\partial B}{\partial q}\frac{\partial V}{\partial q}. \tag{2·28}$$

Note that in Ref. 52) the curvature term $1/2B(q)[[\hat{H}_M(q), \partial V/\partial q\hat{Q}(q)], i\hat{Q}(q)]$ is linearized with respect to $\hat{Q}(q)$ using the relation

$$(\hat{H} - \lambda(q)\hat{N})^A = \frac{\partial V}{\partial q}\hat{Q}(q), \tag{2·29}$$

where the superscript A in Eq. (2·29) denotes the two-quasiparticle creation ($a^\dagger a^\dagger$) and annihilation (aa) part of the operator in the parentheses. Hereafter, we call this part the "A-part" and the $a^\dagger a$ terms the "B-part". The collective variables (q, p) and the collective Hamiltonian $\mathcal{H}(q, p, n)$ are determined by solving the ASCC equations, (2·24), (2·26), and (2·27), under the canonical variable conditions. Note that we can carry out a scale transformation of the collective coordinate q such that $B(q) = 1$. We adopt this choice. Then, $C(q)$ represents the curvature of the collective potential:

$$C(q) = \frac{\partial^2 V(q)}{\partial q^2}. \tag{2·30}$$

§3. Gauge invariance of the ASCC equations with respect to the pairing rotational degree of freedom

3.1. *Gauge invariance at the HFB equilibrium point*

As mentioned in the preceding section, the first step to solve the ASCC equations is to find a solution at one of the HFB equilibrium points, denoted $q = q_0$, which corresponds to the local minimum of the collective potential $V(q)$, satisfying $\partial V/\partial q = 0$. The moving-frame HFB equation reduces to the conventional HFB equation at the equilibrium point:

$$\delta \langle \phi(q_0)| \hat{H} - \lambda(q_0)\tilde{N} |\phi(q_0)\rangle = 0. \tag{3·1}$$

The moving-frame QRPA equations at the equilibrium point are given by

$$\delta \langle \phi(q_0)| [\hat{H} - \lambda(q_0)\tilde{N}, i\hat{Q}(q_0)] - B(q_0)\hat{P}(q_0) |\phi(q_0)\rangle = 0, \tag{3·2}$$

$$\delta \langle \phi(q_0)| [\hat{H} - \lambda(q_0)\tilde{N}, \hat{P}(q_0)] - iC(q_0)\hat{Q}(q_0) - i\frac{\partial \lambda}{\partial q}\tilde{N} |\phi(q_0)\rangle = 0. \tag{3·3}$$

These equations reduce to the QRPA equations if the quantity $\partial\lambda/\partial q$ vanishes. In other words, the QRPA solution corresponds to the special solution of the moving-frame QRPA equations with $\partial\lambda/\partial q = 0$.

Let us consider the following transformations:

$$\hat{Q}(q_0) \to \hat{Q}(q_0) + \alpha \hat{N}^A(q_0), \tag{3·4a}$$

$$\hat{\Theta}(q_0) \to \hat{\Theta}(q_0) + \alpha \hat{P}(q_0), \tag{3·4b}$$

$$\frac{\partial \lambda}{\partial q}(q_0) \to \frac{\partial \lambda}{\partial q}(q_0) - \alpha C(q_0). \tag{3·4c}$$

Here, α is an arbitrary number and $\hat{N}^A$ denotes the A-part of the number operator $\hat{N}$. This is a kind of gauge transformation with respect to the pairing rotational degree of freedom. We can easily confirm that the moving-frame QRPA equations at the HFB equilibrium point, (3·2)–(3·3), and the canonical variable conditions, (2·10)–(2·15) and (2·18)–(2·19), are invariant under this transformation. Due to this invariance, the solution of the moving-frame QRPA equations is not uniquely determined at the HFB equilibrium point. If we choose a value of α such that the relation $\partial\lambda/\partial q = 0$ holds, the moving-frame QRPA equations coincide with the conventional QRPA equations. We can choose other values of α, however, if they are more convenient.

3.2. *Gauge invariance at non-equilibrium points*

At non-equilibrium points, $\partial V/\partial q$ is non-zero, and the moving-frame Hamiltonian (2·25) depends on the collective coordinate operator $\hat{Q}(q)$. However, we can generalize the above considerations applying to the HFB equilibrium point to a general non-equilibrium point q on the collective path. Indeed, it is straightforward to confirm that all the basic equations of the ASCC method [i.e., the collective Hamiltonian $\mathcal{H}(q,p,n)$, (2·20), the inverse mass parameter $B(q)$, (2·22), the moving-frame HFB equation, (2·24), the moving-frame QRPA equations, (2·26)–(2·27), and the canonical variable conditions, (2·10)–(2·15) and (2·18)–(2·19)] are invariant under the transformations with respect to the pairing rotational degree of freedom

$$\hat{Q}(q) \to \hat{Q}(q) + \alpha \tilde{N}, \tag{3·5a}$$

$$\hat{\Theta}(q) \to \hat{\Theta}(q) + \alpha \hat{P}(q), \tag{3·5b}$$

$$\lambda(q) \to \lambda(q) - \alpha \frac{\partial V}{\partial q}(q), \tag{3·5c}$$

$$\frac{\partial \lambda}{\partial q}(q) \to \frac{\partial \lambda}{\partial q}(q) - \alpha C(q) \tag{3·5d}$$

if the collective coordinate operator $\hat{Q}(q)$ is constructed such that it exactly commutes with the number operator $\hat{N}$, i.e.

$$[\hat{Q}(q), \hat{N}] = 0. \tag{3·6}$$

In association with the above transformations of $\hat{Q}(q)$ and $\hat{\Theta}(q)$, the original TDHFB state vector,

$$|\phi(q,p,\varphi,n)\rangle = e^{-i\varphi\tilde{N}} e^{ip\hat{Q}(q)} e^{in\hat{\Theta}(q)} |\phi(q)\rangle\,, \tag{3·7}$$

is transformed as

$$\begin{aligned} |\phi(q,p,\varphi,n)\rangle \to & e^{-i\varphi\tilde{N}} e^{ip(\hat{Q}(q)+\alpha\tilde{N})} e^{in(\hat{\Theta}(q)+\alpha\hat{P}(q))} |\phi(q)\rangle \\ = & e^{-i(\varphi-\alpha p)\tilde{N}} e^{ip\hat{Q}(q)} e^{in\hat{\Theta}(q)} |\phi(q-\alpha n)\rangle\,. \end{aligned} \tag{3·8}$$

Here, the relation

$$|\phi(q+\delta q)\rangle = e^{-i\delta q \hat{P}(q)}\,|\phi(q)\rangle \tag{3·9}$$

is used, and it is assumed that the operators $\hat{\Theta}(q)$ and $\hat{P}(q)$ commute under the adiabatic approximation. We also note that the expression (3·7) is slightly different from (2·7). However, the difference between $e^{ip\hat{Q}(q)+in\hat{\Theta}(q)}$ and $e^{ip\hat{Q}(q)}e^{in\hat{\Theta}(q)}$ gives rise to only higher-order contributions, which are ignored in the adiabatic approximation under consideration. We see that the gauge angle φ changes to $\varphi - \alpha p$ under the transformation (3·5). Thus, hereafter, we refer to the transformations (3·5) as "gauge transformations", the lack of dependence on the choice of α as "gauge invariance", and the choice of the value of α as "gauge fixing."

The commutation relation (3·6) implies that $\hat{Q}(q)$ is a normal one-body operator written in terms of the nucleon creation and annihilation operators $(c^\dagger, c)$ in the following form:

$$\hat{Q}(q) = \sum_{ij} Q_{ij}(q) : c_i^\dagger c_j : \; \equiv \hat{Q}^A(q) + \hat{Q}^B(q). \tag{3·10}$$

Here, the symbol : : denotes the normal product part when $\hat{Q}(q)$ is written in terms of the quasiparticle operators $(a^\dagger, a)$ defined at $|\phi(q)\rangle$, and the coefficients satisfy the relation $Q_{ij}(q) = Q_{ji}(q)^*$, because $\hat{Q}(q)$ is assumed to be Hermitian. Note that this $\hat{Q}(q)$ operator contains the B-part, $\hat{Q}^B(q) = \sum_{kl} Q^B_{kl} a^\dagger_k a_l$, as well as the A-part, $\hat{Q}^A(q) = \sum_{kl} Q^A_{kl} a^\dagger_k a^\dagger_l + \text{h.c.}$ Accordingly, the relation (2·29) does not hold for this $\hat{Q}(q)$ operator.

In this way, we arrive at a new formulation of the ASCC method in which the gauge invariance (3·5) is manifest. The gauge-invariant ASCC method consists of the basic equations, which are the same as those in the original ASCC method,[52] except for the use of Eq. (2·27), and the $\hat{Q}(q)$ operator given in the form of (3·10).

3.3. *Gauge fixing and the numerical algorithm*

The fact that the ASCC equations are invariant under the gauge transformations (3·5) suggests the necessity of choosing a particular gauge for the numerical computation: If the gauge is not fixed, an instability with respect to the gauge degree of freedom might arise during the course of numerical calculation. Let us outline the procedure for the gauge fixing and the numerical algorithm for solving the gauge invariant ASCC equations. We start the calculation by solving the moving-frame QRPA equations at one of the HFB equilibrium points. A solution of the moving-frame QRPA equations at the HFB equilibrium point can be obtained, as discussed in §3.1, by choosing the gauge $\partial\lambda/\partial q = 0$. Hereafter we call this gauge the "QRPA gauge", because under this gauge, the moving-frame QRPA equations at the HFB equilibrium reduce to the conventional QRPA equations. As we see below, numerical calculations using the QRPA gauge encounters a difficulty at inflection points of the collective potential $V(q)$. It is possible, however, to choose another gauge that is free from this difficulty. With the use of the multi-$O(4)$ model, we explicitly show in §5 how this is done.

Since the moving-frame HFB equation at non-equilibrium points contains $\hat{Q}(q)$ that should be determined by the local harmonic equations, we have to resort to an iterative procedure. We proceed in the direction of the lowest energy solution of the moving-frame QRPA equations and successively derive solutions in the following

manner. Suppose that we have already obtained the solution at $q' = q - \delta q$, where δq is the numerical mesh size in the computation. The moving-frame HFB equation at q for the n-th iteration,

$$\delta \left\langle \phi^{(n)}(q) \right| \hat{H}_M^{(n)}(q) \left| \phi^{(n)}(q) \right\rangle = 0, \tag{3·11}$$

$$\hat{H}_M^{(n)}(q) = \hat{H} - \lambda^{(n)}(q)\hat{N} - \frac{\partial V}{\partial q}^{(n)}(q)\hat{Q}^{(n-1)}(q), \tag{3·12}$$

is solved under the constraints

$$\left\langle \phi^{(n)}(q) \right| \hat{N} \left| \phi^{(n)}(q) \right\rangle = N_0, \tag{3·13}$$

$$\left\langle \phi^{(n)}(q) \right| \hat{Q}(q - \delta q) \left| \phi^{(n)}(q) \right\rangle = \delta q, \tag{3·14}$$

which are derived from the canonical variable conditions (2·12) and (2·16), respectively. In starting this iterative procedure at q, the neighboring solution $\hat{Q}(q - \delta q)$ (or a linear combination of the moving-frame QRPA modes at $q - \delta q$) may be used as an initial trial for the operator $\hat{Q}(q)^{(0)}$. The moving-frame QRPA equations for the n-th iteration are written

$$\delta \left\langle \phi^{(n)}(q) \right| [\hat{H}_M^{(n)}(q), i\hat{Q}^{(n)}(q)] - B^{(n)}(q)\hat{P}^{(n)}(q) \left| \phi^{(n)}(q) \right\rangle = 0, \tag{3·15}$$

$$\begin{aligned} \delta \left\langle \phi^{(n)}(q) \right| [\hat{H}_M^{(n)}(q), \hat{P}^{(n)}(q)] - \frac{1}{2B^{(n)}(q)} [[\hat{H}_M^{(n)}(q), \frac{\partial V}{\partial q}\hat{Q}(q)], i\hat{Q}(q)] \\ - iC^{(n)}(q)\hat{Q}^{(n)}(q) - i\frac{\partial \lambda}{\partial q}^{(n)}(q)\hat{N} \left| \phi^{(n)}(q) \right\rangle = 0. \end{aligned} \tag{3·16}$$

As the curvature term is nonlinear with respect to $\hat{Q}(q)$, we replace one of the operators $\hat{Q}(q)$ with that of the previous iteration step, $\hat{Q}^{(n-1)}(q)$. This procedure is discussed in detail for the multi-$O(4)$ model in §4.5. Thus, the moving-frame QRPA equations are linearized with respect to $\hat{Q}^{(n)}(q)$ and $\hat{P}^{(n)}(q)$. Its A-part, $\hat{Q}^{A(n)}(q)$, can be determined in a manner similar to that employed in solving the conventional QRPA equations. After obtaining $\hat{Q}^{A(n)}(q)$, its B-part, $\hat{Q}^{B(n)}(q)$, is determined with the requirement Eq. (3·6). This iterative procedure is repeated until we obtain convergence for $\lambda^{(n)}(q), \hat{Q}^{(n)}(q)$, and $\left|\phi^{(n)}(q)\right\rangle$.

§4. Application of the gauge-invariant ASCC method to the multi-$O(4)$ model

In the following sections, we apply the scheme formulated above to the multi-$O(4)$ model and discuss the gauge-fixing conditions suitable for solving the gauge-invariant ASCC equations. We study excitation spectra and transition strengths in systems with definite particle number $N = N_0$, and for this reason, we set $n = 0$ in the following sections.

4.1. *The multi-$O(4)$ model*

The multi-$O(4)$ model Hamiltonian has been used to test the validity of microscopic theories of nuclear collective motion.[57)–62)] In this work, we employ the model

Hamiltonian used in Ref. 57). The model is constructed in terms of the generators of the $O(4)$ symmetry,

$$\hat{A}_j^\dagger = \sum_{m>0} c_{jm}^\dagger c_{j-m}^\dagger, \qquad \hat{B}_j^\dagger = \sum_{m>0} \sigma_{jm} c_{jm}^\dagger c_{j-m}^\dagger, \tag{4·1}$$

$$\hat{N}_j = \sum_m c_{jm}^\dagger c_{jm}, \qquad \hat{D}_j = \sum_m \sigma_{jm} c_{jm}^\dagger c_{jm}, \tag{4·2}$$

where the nucleon creation and annihilation operators $(c_{jm}^\dagger, c_{jm})$ are used, and the quantity σ_{jm} is given by

$$\sigma_{jm} = \begin{cases} 1 & |m| < \Omega_j/2, \\ -1 & |m| > \Omega_j/2. \end{cases} \tag{4·3}$$

These four operators represent the monopole pair, the (simplified) quadrupole pair, the particle number, and the (simplified) quadrupole operators for each j-shell, respectively. The model Hamiltonian is written in the form

$$\hat{H} = \hat{h}_0 - \frac{1}{2} G_0 (\hat{A}^\dagger \hat{A} + \hat{A}\hat{A}^\dagger) - \frac{1}{2} G_2 (\hat{B}^\dagger \hat{B} + \hat{B}\hat{B}^\dagger) - \frac{1}{2}\chi \hat{D}^2, \tag{4·4}$$

$$\hat{h}_0 = \sum_j e_j^0 \hat{N}_j,$$

where

$$\hat{A}^\dagger = \sum_j \hat{A}_j^\dagger, \quad \hat{B}^\dagger = \sum_j d_j \hat{B}_j^\dagger, \quad \hat{N} = \sum_j \hat{N}_j, \quad \hat{D} = \sum_j d_j \hat{D}_j, \tag{4·5}$$

and d_j represents the quadrupole matrix element. The first term on the right-hand side of Eq. (4·4) is the single-particle Hamiltonian, giving a spherical single-particle energy e_j^0 for each j-shell, which possesses $(2\Omega_j)$-fold degeneracy ($2\Omega_j = 2j+1$). The other terms represent the residual two-body interactions: the monopole-pairing interaction, the quadrupole-type pairing interaction, and the quadrupole-type particle-hole interaction. Their interaction strengths are denoted G_0, G_2, and χ, respectively. Here, the operators $\hat{A}$ and $\hat{N}$ are the monopole-pair and the number operators, while $\hat{B}$ and $\hat{D}$ represent the simplified quadrupole-pair and quadrupole particle-hole operators, respectively.

The residual interactions of this model are separable, and we can always write such a separable Hamiltonian in the form

$$\hat{H} = \hat{h}_0 - \frac{1}{2}\sum_s \kappa_s \hat{F}_s^{(+)} \hat{F}_s^{(+)} + \frac{1}{2}\sum_s \kappa_s \hat{F}_s^{(-)} \hat{F}_s^{(-)}, \tag{4·6}$$

where

$$\hat{F}_s^{(\pm)} \equiv (\hat{F}_s \pm \hat{F}_s^\dagger)/2 = \pm \hat{F}_s^{(\pm)\dagger}. \tag{4·7}$$

Here, the superscript $(+)$ indicates that the bilinear operator $\hat{F}$ is Hermitian and $(-)$ indicates that it is anti-Hermitian. The multi-$O(4)$ model Hamiltonian under consideration contains three kinds of residual interactions. The subscripts s =1, 2, and 3 on the operators $\hat{F}$ and the interaction strengths κ_s indicate the monopole-pairing, the quadrupole-pairing and the quadrupole particle-hole interactions, respectively: $\hat{F}_{s=1} = A, \hat{F}_{s=2} = B$, $\hat{F}_{s=3} = \hat{D}$, $\kappa_1 = 2G_0, \kappa_2 = 2G_2$ and $\kappa_3 = \chi$.

4.2. *Quasiparticle representation*

To solve the ASCC equations, it is convenient to use the quasiparticle basis defined locally with respect to the state $|\phi(q)\rangle$ on the collective path. For the multi-$O(4)$ model, the Bogoliubov transformation to the quasiparticle creation and annihilation operators, $a_i^\dagger(q)$ and $a_i(q)$, satisfying the vacuum condition $a_i(q)\,|\phi(q)\rangle = 0$ is written

$$\begin{pmatrix} a_i^\dagger(q) \\ a_{-i}(q) \end{pmatrix} \equiv \begin{pmatrix} u_i(q) & -v_i(q) \\ v_i(q) & u_i(q) \end{pmatrix} \begin{pmatrix} c_i^\dagger \\ c_{-i} \end{pmatrix}. \tag{4·8}$$

Here, the indices $\pm i$ represent the set of angular momentum quantum numbers $(j, \pm m)$. The Bogoliubov transformation is locally determined on the collective path by the moving-frame HFB equation for a given collective coordinate operator $\hat{Q}(q)$.

Using the quasiparticle bilinear operators

$$\boldsymbol{A}_i^\dagger(q) = a_i^\dagger(q) a_{-i}^\dagger(q), \tag{4·9}$$

$$\boldsymbol{N}_i(q) = a_i^\dagger(q) a_i(q) + a_{-i}^\dagger(q) a_{-i}(q), \tag{4·10}$$

the nucleon bilinear operators $\hat{A}_i^\dagger$ and $\hat{N}_i$ can be rewritten as

$$\hat{A}_i^\dagger = u_i(q)v_i(q) + u_i^2(q)\boldsymbol{A}_i^\dagger(q) - v_i^2(q)\boldsymbol{A}_i(q) - u_i(q)v_i(q)\boldsymbol{N}_i(q), \tag{4·11}$$

$$\hat{N}_i = 2v_i^2(q) + 2u_i(q)v_i(q)(\boldsymbol{A}_i^\dagger(q) + \boldsymbol{A}_i(q)) + (u_i^2(q) - v_i^2(q))\boldsymbol{N}_i(q). \tag{4·12}$$

The quasiparticle bilinear operators $\boldsymbol{A}_i^\dagger(q), \boldsymbol{A}_i(q)$, and $\boldsymbol{N}_i(q)$ satisfy the following commutation relations:

$$\left[\boldsymbol{A}_i(q), \boldsymbol{A}_{i'}^\dagger(q)\right] = \delta_{ii'}(1 - \boldsymbol{N}_i(q)), \tag{4·13}$$

$$\left[\boldsymbol{N}_i(q), \boldsymbol{A}_{i'}^\dagger(q)\right] = 2\delta_{ii'}\boldsymbol{A}_{i'}^\dagger(q). \tag{4·14}$$

The particle number N_0, the quadrupole deformation $D(q)$, the monopole-pairing gap $\Delta_0(q)$, and the quadrupole-pairing gap $\Delta_2(q)$ are given by the expectation values of the corresponding operators with respect to the mean-field state vector $|\phi(q)\rangle$:

$$N_0 = \langle\phi(q)|\,\hat{N}\,|\phi(q)\rangle = 2\sum_{i>0} v_i^2(q), \tag{4·15}$$

$$D(q) = \langle\phi(q)|\,\hat{D}\,|\phi(q)\rangle = 2\sum_{i>0} d_i\sigma_i v_i^2(q), \tag{4·16}$$

$$\Delta_0(q) = G_0\,\langle\phi(q)|\,\hat{A}^\dagger\,|\phi(q)\rangle = G_0\sum_{i>0} u_i(q)v_i(q), \tag{4·17}$$

$$\Delta_2(q) = G_2\,\langle\phi(q)|\,\hat{B}^\dagger\,|\phi(q)\rangle = G_2\sum_{i>0} d_i\sigma_i u_i(q)v_i(q). \tag{4·18}$$

Below, we often omit q as the argument of such functions, for example, writing $\boldsymbol{A}_i(q)$ as $\boldsymbol{A}_i$. It should be kept in mind, however, that these quantities are locally defined with respect to the quasiparticle vacuum $|\phi(q)\rangle$ and depend on q.

4.3. *The ASCC equations for separable interactions*

The ASCC equations for the separable Hamiltonian are given by

$$\delta\,\langle\phi(q)|\,\hat{h}_M(q)\,|\phi(q)\rangle = 0, \tag{4·19}$$

$$\delta \langle\phi(q)| [\hat{h}_M(q), \hat{Q}(q)] - \sum_s f^{(-)}_{Q,s} \hat{F}^{(-)}_s - \frac{1}{i} B(q) \hat{P}(q) |\phi(q)\rangle = 0, \tag{4·20}$$

$$\begin{aligned}\delta \langle\phi(q)| \left[\hat{h}_M(q), \frac{1}{i} B(q) \hat{P}(q)\right] - \sum_s f^{(+)}_{P,s}(q) \hat{F}^{(+)}_s - B(q)C(q)\hat{Q}(q) - \sum_s f^{(+)}_{R,s}(q) \hat{F}^{(+)}_s \\ - \frac{1}{2}[[\hat{h}_M(q), \frac{\partial V}{\partial q}\hat{Q}(q)], \hat{Q}(q)] \\ + \sum_s \left[\hat{F}^{(-)}_s, \frac{\partial V}{\partial q}\hat{Q}(q)\right] f^{(-)}_{Q,s} - f_N(q)\tilde{N} |\phi(q)\rangle = 0,\end{aligned} \tag{4·21}$$

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

$$\hat{h}_M(q) = \hat{h}(q) - \lambda(q)\tilde{N} - \frac{\partial V}{\partial q}\hat{Q}(q), \tag{4·22}$$

with

$$\hat{h}(q) = \hat{h}_0 - \sum_s \kappa_s \hat{F}^{(+)}_s \langle\phi(q)| \hat{F}^{(+)}_s |\phi(q)\rangle . \tag{4·23}$$

We also define the following quantities:

$$f^{(-)}_{Q,s}(q) = -\kappa_s \langle\phi(q)| [\hat{F}^{(-)}_s, \hat{Q}(q)] |\phi(q)\rangle , \tag{4·24}$$

$$f^{(+)}_{P,s}(q) = \kappa_s \langle\phi(q)| [\hat{F}^{(+)}_s, \frac{1}{i} B(q) \hat{P}(q)] |\phi(q)\rangle , \tag{4·25}$$

$$f^{(+)}_{R,s}(q) = -\frac{1}{2}\kappa_s \langle\phi(q)| \left[\left[\hat{F}^{(+)}_s, \frac{\partial V}{\partial q}\hat{Q}(q)\right], \hat{Q}(q)\right] |\phi(q)\rangle , \tag{4·26}$$

$$f_N(q) = B(q)\frac{\partial \lambda}{\partial q}. \tag{4·27}$$

Note that all matrix elements are real, and then $\langle\phi(q)| \hat{F}^{(-)}_s |\phi(q)\rangle = 0$. The fifth term in Eq.(4·21) appears only in the gauge-invariant formulation of the ASCC equations, because there is a contribution from this term only if $\hat{Q}(q)$ contains the B-part.

4.4. *The moving-frame HFB equation*

The moving-frame HFB equation (4·19) at a given q determines the time-even TDHB state vector $|\phi(q)\rangle$. The variation of Eq. (4·19) is taken with respect to two arbitrary quasiparticle states:

$$\delta |\phi(q)\rangle = a^\dagger_i(q) a^\dagger_j(q) |\phi(q)\rangle . \tag{4·28}$$

If we know the operator $\hat{Q}(q)$, we can solve this equation using the gradient method so as to eliminate the two-quasiparticle terms proportional to $\boldsymbol{A}^\dagger_i$ and $\boldsymbol{A}_i$. The quantities $\lambda(q)$ and $\partial V/\partial q$ can be regarded as Lagrange multipliers, which are determined by the following two constraints. The first is the particle number constraint given by (4·15). This constraint specifies the location in particle-number space. The second constraint is written as (3·14). For the $\hat{Q}$ operator defined by (3·10), this equation yields

$$\langle\phi(q)| \hat{Q}(q - \delta q) |\phi(q)\rangle = 2\sum_{i>0} Q_i(q - \delta q)(v_i(q)^2 - v_i(q - \delta q)^2) = \delta q. \tag{4·29}$$

4.5. *The moving-frame QRPA equations*

We solve the moving-frame QRPA equations to obtain the operators $\hat{Q}(q)$ and $\hat{P}(q)$. The collective coordinate operator $\hat{Q}(q)$ is written

$$\hat{Q}(q) = \sum_i Q_i(q) : \hat{N}_i := \sum_{i>0} \left\{ Q_i^A(q)(\boldsymbol{A}_i^\dagger + \boldsymbol{A}_i) + Q_i^B(q)\boldsymbol{N}_i \right\}, \tag{4·30}$$

while the collective momentum operator $\hat{P}(q)$ is expressed as

$$\hat{P}(q) = i \sum_{i>0} P_i(q)(\boldsymbol{A}_i^\dagger - \boldsymbol{A}_i). \tag{4·31}$$

As mentioned in the preceding section, the B-part of the operator $\hat{P}(q)$ is unnecessary in second order with respect to the collective momentum p.

We solve the moving-frame QRPA equations in the following way. First, we assume that the solution $\hat{Q}^{(n-1)}(q)$ (obtained in the previous iteration step) of the moving-frame QRPA equations and the solutions, such as $|\phi(q)\rangle$ and $V(q)$, of the moving-frame HFB equation are known. [The superscript n is omitted, except on $\hat{Q}(q)$.] In solving the moving-frame QRPA equations, we note that the moving-frame Hamiltonian $\hat{h}_M(q)$ and the operators $\hat{F}_s^{(\pm)}$ can be expressed in terms of the quasiparticle bilinear operators $\boldsymbol{A}_i^\dagger$, $\boldsymbol{A}_i$, and $\boldsymbol{N}_i$ as

$$\hat{h}_M(q) = V(q) + \sum_{i>0} E_i(q)\boldsymbol{N}_i, \tag{4·32}$$

$$\begin{aligned}\hat{F}_s^{(+)} &= \langle\phi(q)|\, \hat{F}_s^{(+)}\, |\phi(q)\rangle + \hat{F}_{A,s}^{(+)} + \hat{F}_{B,s}^{(+)} \\ &= \langle\phi(q)|\, \hat{F}_s^{(+)}\, |\phi(q)\rangle + \sum_{i>0} F_{A,s}^{(+)}(i)(\boldsymbol{A}_i^\dagger + \boldsymbol{A}_i) + \sum_{i>0} F_{B,s}^{(+)}(i)\boldsymbol{N}_i,\end{aligned} \tag{4·33}$$

$$\hat{F}_s^{(-)} = \sum_{i>0} F_{A,s}^{(-)}(i)(\boldsymbol{A}_i^\dagger - \boldsymbol{A}_i). \tag{4·34}$$

Here, we have

$$F_{A,1}^{(+)}(i) = \frac{1}{2}(u_i^2 - v_i^2), \quad F_{A,2}^{(+)}(i) = \frac{1}{2} d_i\sigma_i(u_i^2 - v_i^2), \quad F_{A,3}^{(+)}(i) = 2d_i\sigma_i u_i v_i, \tag{4·35}$$

$$F_{A,1}^{(-)}(i) = -\frac{1}{2}, \quad F_{A,2}^{(-)}(i) = -\frac{1}{2} d_i\sigma_i, \quad F_{A,3}^{(-)}(i) = 0, \tag{4·36}$$

$$F_{B,1}^{(+)}(i) = -u_i v_i, \quad F_{B,2}^{(+)}(i) = -d_i\sigma_i u_i v_i, \quad F_{B,3}^{(+)}(i) = d_i\sigma_i(u_i^2 - v_i^2), \tag{4·37}$$

$$\begin{aligned}E_i(q) = (u_i^2 - v_i^2)\left(e_i - \chi d_i\sigma_i D(q) - \lambda(q) - \frac{\partial V}{\partial q} Q_i^{(n-1)}(q) \right) \\ - 2(\Delta_0(q) + d_i\sigma_i\Delta_2(q))u_i v_i.\end{aligned} \tag{4·38}$$

These quantities are determined by solving the moving-frame HFB equation (4·19). For later convenience, we define the following quasiparticle bilinear operators:

$$\hat{R}_s^{(\pm)} \equiv \left[\hat{F}_s^{(\pm)}, \frac{\partial V}{\partial q}\hat{Q}^{(n-1)}(q) \right] = 2\sum_{i>0} R_{A,s}^{(\pm)}(i)(\boldsymbol{A}_i^\dagger \mp \boldsymbol{A}_i), \tag{4·39}$$

with

$$R^{(+)}_{A,s}(i) = \frac{\partial V}{\partial q}\left(F^{(+)}_{B,s}(i)Q^{A(n-1)}_i(q) - F^{(+)}_{A,s}(i)Q^{B(n-1)}_i(q)\right), \tag{4·40}$$

$$R^{(-)}_{A,s}(i) = -\frac{\partial V}{\partial q}F^{(-)}_{A,s}(i)Q^{B(n-1)}_i(q). \tag{4·41}$$

We can express the matrix elements $Q^{A(n)}_i$ and P_i in terms of $f^{(-)}_{Q,s}$, $f^{(+)}_{P,s}$, $f^{(+)}_{R,s}$ and f_N by substituting Eqs. (4·30) and (4·31) into Eqs. (4·20) and (4·21). This yields

$$\begin{aligned} Q^{A(n)}_i =& \frac{1}{(2E_i)^2 - \omega^2 + 2\frac{\partial V}{\partial q}E_iQ^{B(n-1)}_i} \\ & \left\{2E_i\sum_s F^{(-)}_{A,s}(i)f^{(-)}_{Q,s} + \sum_s\left(F^{(+)}_{A,s}(i)f^{(+)}_{PR,s} - 2R^{(-)}_{A,s}(i)f^{(-)}_{Q,s}\right) + N_if_N\right\}, \end{aligned} \tag{4·42}$$

$$\begin{aligned} P_i =& \frac{2E_i}{(2E_i)^2 - \omega^2 + 2\frac{\partial V}{\partial q}E_iQ^{B(n-1)}_i}\left\{\sum_s\left(F^{(+)}_{A,s}(i)f^{(+)}_{PR,s} - 2R^{(-)}_{A,s}(i)f^{(-)}_{Q,s}\right) + N_if_N\right\} \\ & + \frac{\omega^2 - 2\frac{\partial V}{\partial q}E_iQ^{B(n-1)}_i}{(2E_i)^2 - \omega^2 + 2\frac{\partial V}{\partial q}E_iQ^{B(n-1)}_i}\sum_s F^{(-)}_{A,s}(i)f^{(-)}_{Q,s}, \end{aligned} \tag{4·43}$$

where

$$N_i = 2u_i(q)v_i(q), \tag{4·44}$$

$$f^{(+)}_{PR,s} = f^{(+)}_{P,s}(q) + f^{(+)}_{R,s}(q), \tag{4·45}$$

$$\omega = \sqrt{B(q)C(q)}. \tag{4·46}$$

Substituting Eqs. (4·30), (4·31) and (4·39) into Eqs. (4·24), (4·25) and (4·26), we obtain

$$f^{(-)}_{Q,s} = 2\kappa_s\sum_{i>0}F^{(-)}_{A,s}(i)Q^{A(n)}_i, \tag{4·47}$$

$$f^{(+)}_{PR,s} = 2\kappa_s\sum_{i>0}\left\{F^{(+)}_{A,s}(i)P_i + R^{(+)}_{A,s}(i)Q^{A(n)}_i\right\}. \tag{4·48}$$

Note that $f^{(-)}_{Q,3} = 0$. From the canonical variable condition, the orthogonality of the collective and number fluctuation modes is required, i.e.

$$\langle\phi(q)|[\tilde{N}, \hat{P}(q)]|\phi(q)\rangle = 2i\sum_{i>0}N_iP_i = 0. \tag{4·49}$$

Eliminating $Q^{A(n)}_i$ and P_i from Eqs. (4·47), (4·48), and (4·49) with use of Eqs. (4·42) and (4·43), we finally obtain the dispersion equation

$$\boldsymbol{S}(\omega^2)\cdot\boldsymbol{f} = 0, \tag{4·50}$$

for the quantity $\boldsymbol{f} = \boldsymbol{f}(q) = \{f^{(-)}_{Q,1},\, f^{(-)}_{Q,2},\, f^{(+)}_{PR,1},\, f^{(+)}_{PR,2},\, f^{(+)}_{PR,3},\, f_N\}$. Here $\boldsymbol{S} = \{S_{ij}\}$ is a 6×6 matrix whose elements are given by

$$S_{11} = 2\kappa_1 \left\{ S^{(1)}(F^{(-)}_{A,1}, F^{(-)}_{A,1}) - 2S^{(2)}(F^{(-)}_{A,1}, R^{(-)}_{A,1}) \right\} - 1, \tag{4·51a}$$

$$S_{12} = 2\kappa_1 \left\{ S^{(1)}(F^{(-)}_{A,1}, F^{(-)}_{A,2}) - 2S^{(2)}(F^{(-)}_{A,1}, R^{(-)}_{A,2}) \right\}, \tag{4·51b}$$

$$S_{13} = 2\kappa_1 S^{(2)}(F^{(-)}_{A,1}, F^{(+)}_{A,1}), \tag{4·51c}$$

$$S_{14} = 2\kappa_1 S^{(2)}(F^{(-)}_{A,1}, F^{(+)}_{A,2}), \tag{4·51d}$$

$$S_{15} = 2\kappa_1 S^{(2)}(F^{(-)}_{A,1}, F^{(+)}_{A,3}), \tag{4·51e}$$

$$S_{16} = 2\kappa_1 S^{(2)}(F^{(-)}_{A,1}, N), \tag{4·51f}$$

$$S_{21} = 2\kappa_2 \left\{ S^{(1)}(F^{(-)}_{A,2}, F^{(-)}_{A,1}) - 2S^{(2)}(F^{(-)}_{A,2}, R^{(-)}_{A,1}) \right\}, \tag{4·52a}$$

$$S_{22} = 2\kappa_2 \left\{ S^{(1)}(F^{(-)}_{A,2}, F^{(-)}_{A,2}) - 2S^{(2)}(F^{(-)}_{A,2}, R^{(-)}_{A,2}) \right\} - 1, \tag{4·52b}$$

$$S_{23} = 2\kappa_2 S^{(2)}(F^{(-)}_{A,2}, F^{(+)}_{A,1}), \tag{4·52c}$$

$$S_{24} = 2\kappa_2 S^{(2)}(F^{(-)}_{A,2}, F^{(+)}_{A,2}), \tag{4·52d}$$

$$S_{25} = 2\kappa_2 S^{(2)}(F^{(-)}_{A,2}, F^{(+)}_{A,3}), \tag{4·52e}$$

$$S_{26} = 2\kappa_2 S^{(2)}(F^{(-)}_{A,2}, N), \tag{4·52f}$$

$$\begin{aligned} S_{31} = 2\kappa_1 \Big\{ & \omega^2 S^{(2)}(F^{(+)}_{A,1}, F^{(-)}_{A,1}) - S^{(1)}(F^{(+)}_{A,1}, R^{(-)}_{A,1}) \\ & + S^{(1)}(R^{(+)}_{A,1}, F^{(-)}_{A,1}) - 2S^{(2)}(R^{(+)}_{A,1}, R^{(-)}_{A,1}) \Big\}, \end{aligned} \tag{4·53a}$$

$$\begin{aligned} S_{32} = 2\kappa_1 \Big\{ & \omega^2 S^{(2)}(F^{(+)}_{A,1}, F^{(-)}_{A,2}) - S^{(1)}(F^{(+)}_{A,1}, R^{(-)}_{A,2}) \\ & + S^{(1)}(R^{(+)}_{A,1}, F^{(-)}_{A,2}) - 2S^{(2)}(R^{(+)}_{A,1}, R^{(-)}_{A,2}) \Big\}, \end{aligned} \tag{4·53b}$$

$$S_{33} = 2\kappa_1 \left\{ S^{(1)}(F^{(+)}_{A,1}, F^{(+)}_{A,1}) + S^{(2)}(R^{(+)}_{A,1}, F^{(+)}_{A,1}) \right\} - 1, \tag{4·53c}$$

$$S_{34} = 2\kappa_1 \left\{ S^{(1)}(F^{(+)}_{A,1}, F^{(+)}_{A,2}) + S^{(2)}(R^{(+)}_{A,1}, F^{(+)}_{A,2}) \right\}, \tag{4·53d}$$

$$S_{35} = 2\kappa_1 \left\{ S^{(1)}(F^{(+)}_{A,1}, F^{(+)}_{A,3}) + S^{(2)}(R^{(+)}_{A,1}, F^{(+)}_{A,3}) \right\}, \tag{4·53e}$$

$$S_{36} = 2\kappa_1 \left\{ S^{(1)}(F^{(+)}_{A,1}, N) + S^{(2)}(R^{(+)}_{A,1}, N) \right\}, \tag{4·53f}$$

$$\begin{aligned} S_{41} = 2\kappa_2 \Big\{ & \omega^2 S^{(2)}(F^{(+)}_{A,2}, F^{(-)}_{A,1}) - S^{(1)}(F^{(+)}_{A,2}, R^{(-)}_{A,1}) \\ & + S^{(1)}(R^{(+)}_{A,2}, F^{(-)}_{A,1}) - 2S^{(2)}(R^{(+)}_{A,2}, R^{(-)}_{A,1}) \Big\}, \end{aligned} \tag{4·54a}$$

$$\begin{aligned} S_{42} = 2\kappa_2 \Big\{ & \omega^2 S^{(2)}(F^{(+)}_{A,2}, F^{(-)}_{A,2}) - S^{(1)}(F^{(+)}_{A,2}, R^{(-)}_{A,2}) \\ & + S^{(1)}(R^{(+)}_{A,2}, F^{(-)}_{A,2}) - 2S^{(2)}(R^{(+)}_{A,2}, R^{(-)}_{A,2}) \Big\}, \end{aligned} \tag{4·54b}$$

$$S_{43} = 2\kappa_2 \left\{ S^{(1)}(F^{(+)}_{A,2}, F^{(+)}_{A,1}) + S^{(2)}(R^{(+)}_{A,2}, F^{(+)}_{A,1}) \right\}, \tag{4·54c}$$

$$S_{44} = 2\kappa_2 \left\{ S^{(1)}(F^{(+)}_{A,2}, F^{(+)}_{A,2}) + S^{(2)}(R^{(+)}_{A,2}, F^{(+)}_{A,2}) \right\} - 1, \tag{4·54d}$$

$$S_{45} = 2\kappa_2 \left\{ S^{(1)}(F^{(+)}_{A,2}, F^{(+)}_{A,3}) + S^{(2)}(R^{(+)}_{A,2}, F^{(+)}_{A,3}) \right\}, \tag{4·54e}$$

$$S_{46} = 2\kappa_2 \left\{ S^{(1)}(F^{(+)}_{A,2}, N) + S^{(2)}(R^{(+)}_{A,2}, N) \right\}, \tag{4·54f}$$

$$S_{51} = 2\kappa_3 \Big\{ \omega^2 S^{(2)}(F^{(+)}_{A,3}, F^{(-)}_{A,1}) - S^{(1)}(F^{(+)}_{A,3}, R^{(-)}_{A,1}) + S^{(1)}(R^{(+)}_{A,3}, F^{(-)}_{A,1}) - 2S^{(2)}(R^{(+)}_{A,3}, R^{(-)}_{A,1}) \Big\}, \tag{4·55a}$$

$$S_{52} = 2\kappa_3 \Big\{ \omega^2 S^{(2)}(F^{(+)}_{A,3}, F^{(-)}_{A,2}) - S^{(1)}(F^{(+)}_{A,3}, R^{(-)}_{A,2}) + S^{(1)}(R^{(+)}_{A,3}, F^{(-)}_{A,2}) - 2S^{(2)}(R^{(+)}_{A,3}, R^{(-)}_{A,2}) \Big\}, \tag{4·55b}$$

$$S_{53} = 2\kappa_3 \left\{ S^{(1)}(F^{(+)}_{A,3}, F^{(+)}_{A,1}) + S^{(2)}(R^{(+)}_{A,3}, F^{(+)}_{A,1}) \right\}, \tag{4·55c}$$

$$S_{54} = 2\kappa_3 \left\{ S^{(1)}(F^{(+)}_{A,3}, F^{(+)}_{A,2}) + S^{(2)}(R^{(+)}_{A,3}, F^{(+)}_{A,2}) \right\}, \tag{4·55d}$$

$$S_{55} = 2\kappa_3 \left\{ S^{(1)}(F^{(+)}_{A,3}, F^{(+)}_{A,3}) + S^{(2)}(R^{(+)}_{A,3}, F^{(+)}_{A,3}) \right\} - 1, \tag{4·55e}$$

$$S_{56} = 2\kappa_3 \left\{ S^{(1)}(F^{(+)}_{A,3}, N) + S^{(2)}(R^{(+)}_{A,3}, N) \right\}, \tag{4·55f}$$

$$S_{61} = \omega^2 S^{(2)}(N, F^{(-)}_{A,1}) - S^{(1)}(N, R^{(-)}_{A,1}), \qquad S_{62} = \omega^2 S^{(2)}(N, F^{(-)}_{A,2}) - S^{(1)}(N, R^{(-)}_{A,2}), \tag{4·56a}$$

$$S_{63} = S^{(1)}(N, F^{(+)}_{A,1}), \qquad S_{64} = S^{(1)}(N, F^{(+)}_{A,2}), \tag{4·56b}$$

$$S_{65} = S^{(1)}(N, F^{(+)}_{A,3}), \qquad S_{66} = S^{(1)}(N, N). \tag{4·56c}$$

Here, the quantities $S^{(1)}$ and $S^{(2)}$ are defined by

$$S^{(1)}(X, Y) = \sum_{i>0} \frac{2E_i(q)}{(2E_i(q))^2 - \omega^2(q) + 2\frac{\partial V}{\partial q} E_i Q_i^{(B(n-1))}} X_i Y_i, \tag{4·57}$$

$$S^{(2)}(X, Y) = \sum_{i>0} \frac{1}{(2E_i(q))^2 - \omega^2(q) + 2\frac{\partial V}{\partial q} E_i Q_i^{(B(n-1))}} X_i Y_i. \tag{4·58}$$

The unknown quantities in the dispersion equation (4·50) are $\boldsymbol{f}(q)$ and $\omega^2(q)$. The squared frequency $\omega^2(q)$ can be determined by the condition that the matrix $\boldsymbol{S}(\omega^2(q))$ has no inverse:

$$\det \boldsymbol{S}(\omega^2(q)) = 0. \tag{4·59}$$

In the case that there are many solutions $\omega^2(q)$ satisfying this equation, we choose the smallest of these (including negative values) as the collective mode. Once the value of $\omega^2(q)$ and, consequently, the matrix $\boldsymbol{S}(q)$ is specified, the direction of the

vector $\boldsymbol{f}(q)$ is known. Then, its absolute value is fixed by the normalization condition for the collective mode,

$$\langle\phi(q)|\left[\hat{Q}^{(n)}(q),\hat{P}(q)\right]|\phi(q)\rangle = 2i\sum_{i>0} Q_i^{A(n)}(q)P_i(q) = i. \tag{4·60}$$

The choice of the signs of $\hat{Q}^{(n)}(q)$ and $\hat{P}(q)$ are still arbitrary. This choice specifies the "rear" and "front" of the one-dimensional collective path.

The B-part of $\hat{Q}(q)$ is automatically determined in terms of its A-part according to its definition (4·30):

$$Q_i^{B(n)}(q) = \frac{u_i^2 - v_i^2}{2u_iv_i} Q_i^{A(n)}(q). \tag{4·61}$$

4.6. *Gauge fixing*

Under the gauge transformation (3·5), the quantities, $f_{Q,1}^{(-)}(q)$, $f_{Q,2}^{(-)}(q)$, and $f_N(q)$ appearing in the dispersion equation (4·50) transform as

$$f_{Q,1}^{(-)}(q) \to f_{Q,1}^{(-)}(q) - 4\alpha\Delta_0(q), \tag{4·62}$$

$$f_{Q,2}^{(-)}(q) \to f_{Q,2}^{(-)}(q) - 4\alpha\Delta_2(q), \tag{4·63}$$

$$f_N(q) \to f_N(q) - \alpha\omega^2(q). \tag{4·64}$$

These properties clearly indicate that one of the above three quantities can be eliminated: By choosing an appropriate value for α (gauge fixing), we can reduce the dispersion equation (4·50) to a 5×5 matrix equation. In other words, Eq. (4·50) is redundant, and the gauge fixing is equivalent to the reduction of its dimension. The QRPA gauge corresponds to setting $f_N(q) = 0$. In Ref. 57), we set $f_{Q,1}^{(-)}(q) = 0$, which corresponds to another gauge. Because the quantity $f_{Q,1}^{(-)}(q)$ represents the contribution from the time-odd component of the monopole-pairing interaction, let us call this gauge the "ETOP (eliminating time-odd pairing) gauge"

4.7. *Requantization*

The solution of the ASCC equations yields the classical collective Hamiltonian:

$$\mathcal{H}(q,p) = \frac{1}{2}p^2 + V(q). \tag{4·65}$$

We can thus obtain the quantum collective Hamiltonian by carrying out the canonical quantization $\mathcal{H}(q,p) \to \mathcal{H}\left(q, \frac{1}{i}\frac{\partial}{\partial q}\right)$. Note that, in this quantization step, there is no ambiguity associated with the ordering of q and p, because the coordinate scale is chosen such that the inverse mass function is unity, i.e., $B(q) = 1$.

§5. Numerical test of the internal consistency of the proposed scheme

5.1. *Details of numerical calculation*

We numerically solved the gauge-invariant ASCC equations for the multi-$O(4)$ model with the same parameters as in Refs. 57) and 62). The system consists of 28 particles (one kind of fermion). The model space consists of three j-shells, labeled j_1, j_2 and j_3, with the pair degeneracies $\Omega_{j_i} = 14, \Omega_{j_2} = 10$ and $\Omega_{j_3} = 4$, single-particle energies $e_{j_1} = 0, e_{j_2} = 1.0$ and $e_{j_3} = 3.5$, and the single-particle quadrupole

moments $d_{j_1} = 2$ and $d_{j_2} = d_{j_3} = 1$. Within this model space, the deformation $D = \langle\phi(q)|\,\hat{D}\,|\phi(q)\rangle$ ranges from $D_{\min} = -42$ to $D_{\max} = 42$. The calculation was done with the quadrupole-interaction strength $\chi = 0.04$ and the monopole-pairing-interaction strengths $G_0 = 0.14, 0.16$ and 0.20. The nature of the system changes from a double-well ($G_0 = 0.14$) to a spherical vibrator ($G_0 = 0.20$) as the value of G_0 is changed. The effect of the quadrupole pairing is studied by comparing the results for $G_2 = 0.00, 0.02$ and 0.04. As pointed out in Ref. 57), the quadrupole pairing has a strong effect on the collective mass. However, it need not be considered for investigation of the gauge-fixing condition. Therefore, we present the results for $G_2 = 0$ in the next subsection and show its effect in the final subsection only. The calculation starts from one of the HFB equilibrium states, labeled by $q = 0$ (see Fig. 2). For the deformed cases ($G_0 = 0.14$ and 0.16), the HFB equilibrium state with positive (prolate) deformation is chosen as the starting point.

5.2. *Comparison of the two gauge fixing conditions*

Let us examine whether or not we can find a gauge independent solution of the ASCC equations. The existence of the collective path that simultaneously satisfies all equations of the ASCC method is not self-evident. The aim of the numerical calculation here is to check the internal consistency of the equations presented in the preceding section. We solve the gauge-invariant ASCC equations with two different gauge fixing conditions: the QRPA gauge [$f_N(q) = 0$] and the ETOP gauge [$f^{(-)}_{Q,1}(q) = 0$]. In the QRPA gauge, the chemical potential $\lambda(q)$ along the collective path is set to a constant, while in the ETOP gauge, the time-odd contribution of the monopole pairing interaction is fully eliminated from the ASCC equations.

Figure 1 displays the collective potential $V(q)$ and the monopole pairing gap $\Delta_0(q)$ as functions of the quadrupole deformation $D(q)$. Figure 2 displays the relation between the collective variables q and the quadrupole deformation D, as well as the squared frequency $\omega^2(q)$ obtained by solving the local-harmonic equations. The collective mass $M(D(q)) = (dq/dD)^2$, which is derived by transforming the collective kinetic energy as a function of the velocity $\dot{D}$ under the condition $B(q) = 1$,[57] is plotted as a function of D in Fig. 3. We find that the calculation using the ETOP gauge encounters no difficulties, and the collective path connecting the two local (oblate and prolate) minima with different signs of the deformation are successfully obtained. By contrast, the calculation using the QRPA gauge encounters a point beyond which we cannot proceed. In the region where the solutions have been found for both gauges, they are consistent. This should be the case, because these are gauge invariant quantities. The cause of the difficulty encountered in the QRPA gauge can be understood as follows.

Figures 4 and 5 display the chemical potential $\lambda(q)$ and the quantities $f^{(-)}_{Q,1}(q)$ and $f_N(q)$, respectively. Their values depend on the gauge adopted. If the QRPA gauge is used, $\lambda(q)$ should be constant along the path, because of the condition $f_N(q) = B(q)\partial\lambda/\partial q = 0$. We find, however, that $\lambda(q)$ diverges near the inflection point of the collective potential, where $\omega(q)^2 = \partial^2 V/\partial q^2 = 0$. This divergence occurs because the inflection point is a singularity for the gauge transformation (4·64), where an arbitrary α gives the same $f_N(q)$. Thus, the calculation using the QRPA gauge stops at the inflection point. Contrastingly, we can go over the inflection point using the ETOP gauge, because the gauge transformation for $f^{(-)}_{Q,1}(q)$, (4·62), involves only the monopole pairing gap $\Delta_0(q)$, which always takes finite values along

the collective path (except at the limit of the model space). In these figures, we also present the results that obtained with the following procedure. After determining the collective paths employing the ETOP gauge, we calculate the gauge-dependent quantities $\lambda(q), f^{(-)}_{Q,1}(q)$ and $f_N(q)$ by switching to the QRPA gauge using the relations

$$f^{(-)}_{Q,1(\mathrm{QRPA})} = -\frac{4f_N(q)_{(\mathrm{ETOP})}\Delta_0(q)}{\omega^2(q)}, \tag{5·1a}$$

$$\lambda(q)_{(\mathrm{QRPA})} = \lambda(q)_{(\mathrm{ETOP})} - \frac{4f_N(q)_{(\mathrm{ETOP})}}{\omega^2(q)}\frac{\partial V}{\partial q}. \tag{5·1b}$$

We see in Figs. 4 and 5 that the results obtained by this procedure are consistent with those calculated using the QRPA gauge [$f_N(q) = 0$] from the beginning [in the region of deformation $D(q)$, where the collective path can be obtained using the QRPA gauge]. This agreement demonstrates that the collective paths determined by using different gauge fixing conditions are the same, as should be the case. Nevertheless, there is a particularly suitable gauge fixing condition for finding solutions of the ASCC equations and constructing the collective path. For the multi-$O(4)$ model with superfluidity, we find that the ETOP gauge is more useful than the QRPA gauge, because the gauge transformation (4·62) is well-defined as long as the pairing gap $\Delta_0(q)$ is non-zero.

5.3. *Comparison with the previous calculation*

In a previous paper,[57] we employed the ETOP gauge condition [$f^{(-)}_{Q,1}(q) = 0$], but the B-part of $\hat{Q}(q)$ was ignored. Let us evaluate the error caused by this approximation. The results of these calculations are also presented in Figs. 1-4 and compared with those of the full calculations. We see that they differ little, which indicates that the approximation made by ignoring the B-part is rather good.

In Fig. 5, we present the quantity

$$f^{(-)}_{Q,1}(q) = -\kappa_1 \langle\phi(q)|\,[\hat{F}^{(-)}_1, \hat{Q}(q)]\,|\phi(q)\rangle = -\kappa_1 \sum_{i>0} Q^A_i(q), \tag{5·2}$$

evaluated using the $\hat{Q}(q)$ operator that is obtained by ignoring the B-part in the process of solving the ASCC equations. This quantity should be zero if the $\hat{Q}(q)$ operator determined by the gauge-invariant ASCC equations is used. We see that the deviation from zero is negligible (except near the limit of the model space), again indicating that the approximation is good.

The quantum spectra and transition strengths are displayed in Fig. 6. These were obtained by solving the Schrödinger equation for the quantized collective Hamiltonian. In this figure, the effects of the quadrupole pairing interaction are also shown. We see that the results of the previous calculation [in which the B-part of $\hat{Q}(q)$ is ignored] are quite similar to those of the full calculation (including the B-part), and both results accurately reproduce the trend of the excitation spectra obtained through the exact diagonalization of the microscopic Hamiltonian (Fig. 7). The numerical calculation discussed above thus suggests that the approximation of ignoring the B-part of $\hat{Q}(q)$, adopted in Ref. 57), is valid, and it may serve as an economical way of determining the collective path.

§6. Concluding remarks

We have shown that the basic equations of the ASCC method are invariant under transformations involving the angle in the gauge space conjugate to the particle number. By virtue of this invariance, a clean separation of the large-amplitude collective motion and the pairing rotational motion can be realized. This allows us to restore the particle-number symmetry broken by the HFB approximation. We have formulated the ASCC method explicitly in a gauge-invariant form. Then, we applied it to the multi-$O(4)$ model using different gauge-fixing procedures. The calculations using different gauges indeed yield the same results for gauge-invariant quantities, such as the collective path, the collective mass parameter, and the spectra obtained by requantizing the collective Hamiltonian. We suggested a gauge-fixing prescription that can be used in realistic calculations.

The explicit gauge invariance requires the B-part ($a^\dagger a$ part) of the collective coordinate operator $\hat{Q}(q)$. Actually, it is stated in Ref. 27) that the separation of the Nambu-Goldstone modes in the local harmonic formulation requires higher-order terms in the collective coordinate. This is consistent with the present conclusion in the gauge-invariant formalism. We have also demonstrated that the approximation made by ignoring the B-part leads to results almost identical to those obtained in the full calculation, at least for the multi-$O(4)$ model.

We are presently investigating oblate-prolate shape coexistence phenomena[54)–56)] in nuclei around ^{68}Se with the pairing-plus-quadrupole interactions[63)–65)] using a prescription based on the new formulation of the ASCC method proposed in this paper. The result will be reported in the near future.

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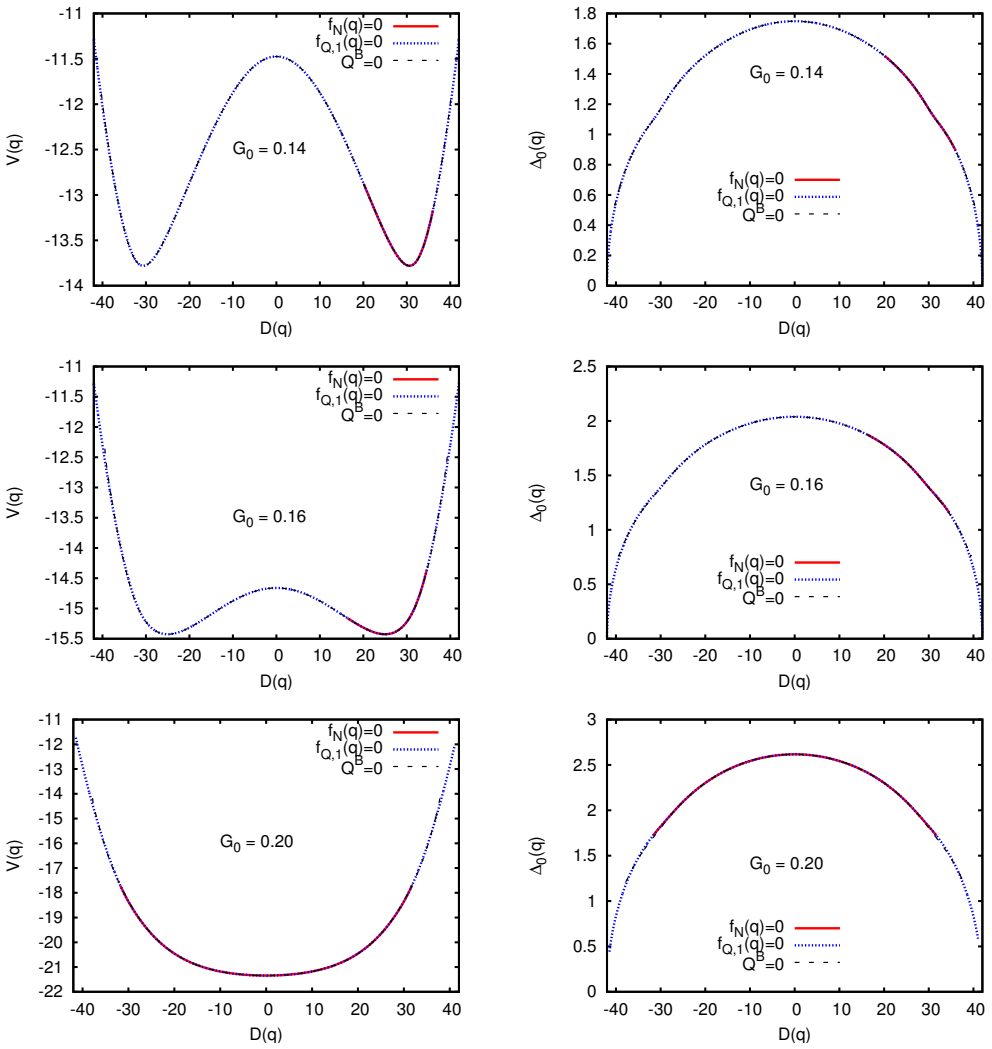

Fig. 1. Collective potentials $V(q)$ and monopole pairing gaps $\Delta_0(q)$ plotted as functions of the quadrupole deformation D. The upper, middle and lower panels display the results for $G_0 = 0.14, 0.16$ and 0.20, respectively. In each graph, results obtained from different calculations are compared. Those obtained using the QRPA gauge [$f_N(q) = 0$] and the ETOP gauge [$f^{(-)}_{Q,1}(q) = 0$] are plotted by solid (red) and dotted (blue) curves, respectively, while those obtained ignoring the B-part of $\hat{Q}(q)$ [i.e., setting $Q^B_i(q) = 0$] are plotted by the dashed curves.

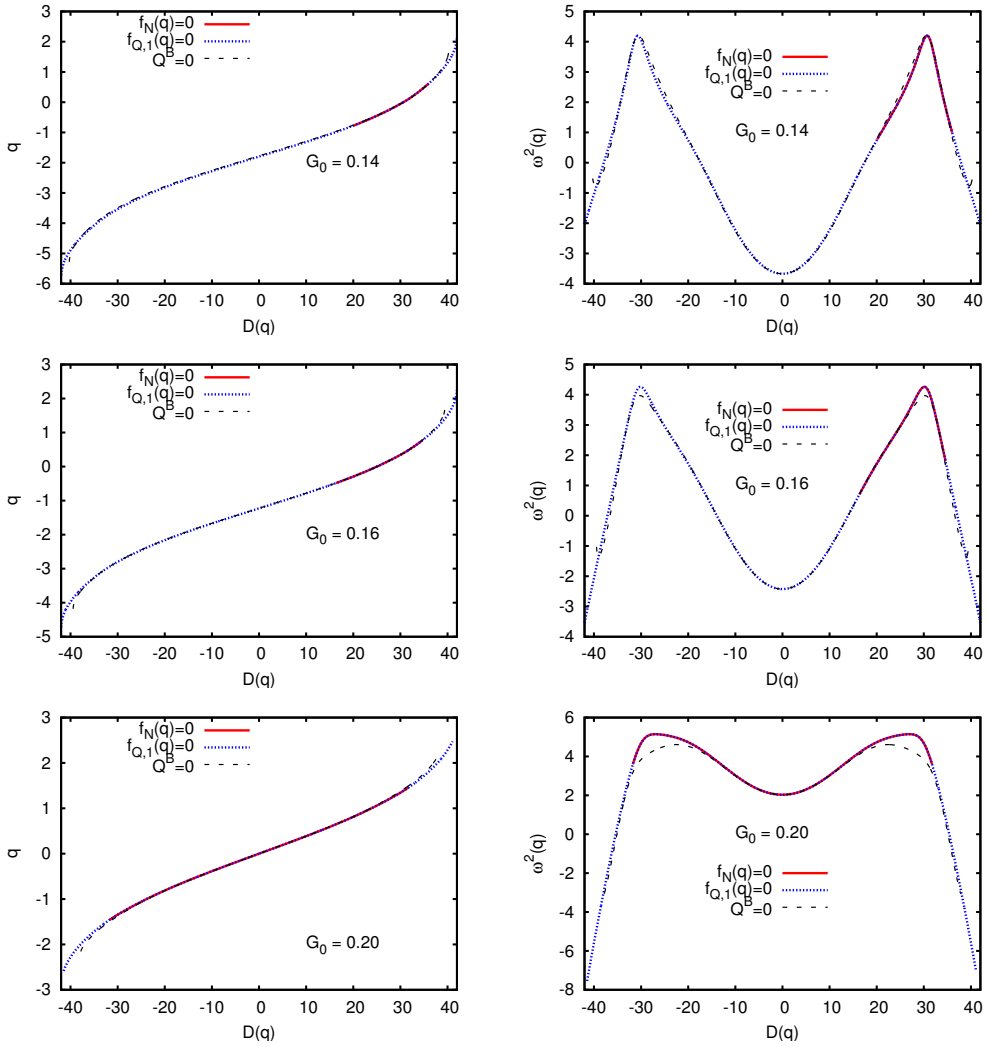

Fig. 2. *Left column*: Relation between the collective coordinate q and the quadrupole deformation $D(q) = \langle\phi(q)|\,\hat{D}\,|\phi(q)\rangle$. The point $q = 0$ corresponds to the HFB equilibrium, which is the starting point of the numerical calculation. *Right column*: Squared frequencies $\omega^2(q)$ of the moving-frame QRPA equations, plotted as functions of D. Note that they are negative; i.e., $\omega(q)$ is purely imaginary in the region where the curvature of the collective potential is negative. The upper, middle and lower rows display the results for $G_0 = 0.14, 0.16$ and 0.20, respectively. (See the caption of Fig. 1.)

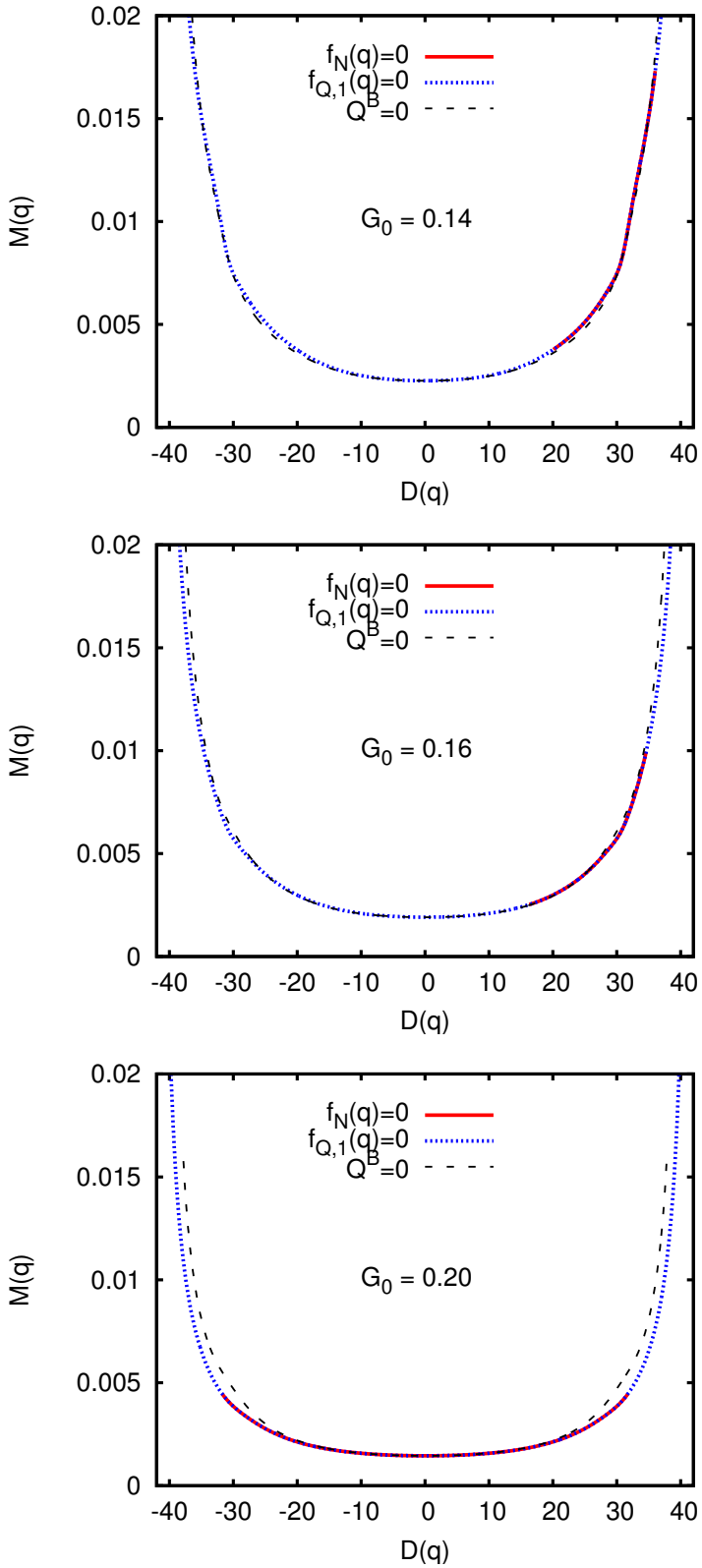

Fig. 3. The ASCC collective mass $M(q(D))$ as functions of the deformation D. The upper, middle and lower rows display the results for $G_0 = 0.14$, 0.16 and 0.20, respectively. (See the caption of Fig. 1.)

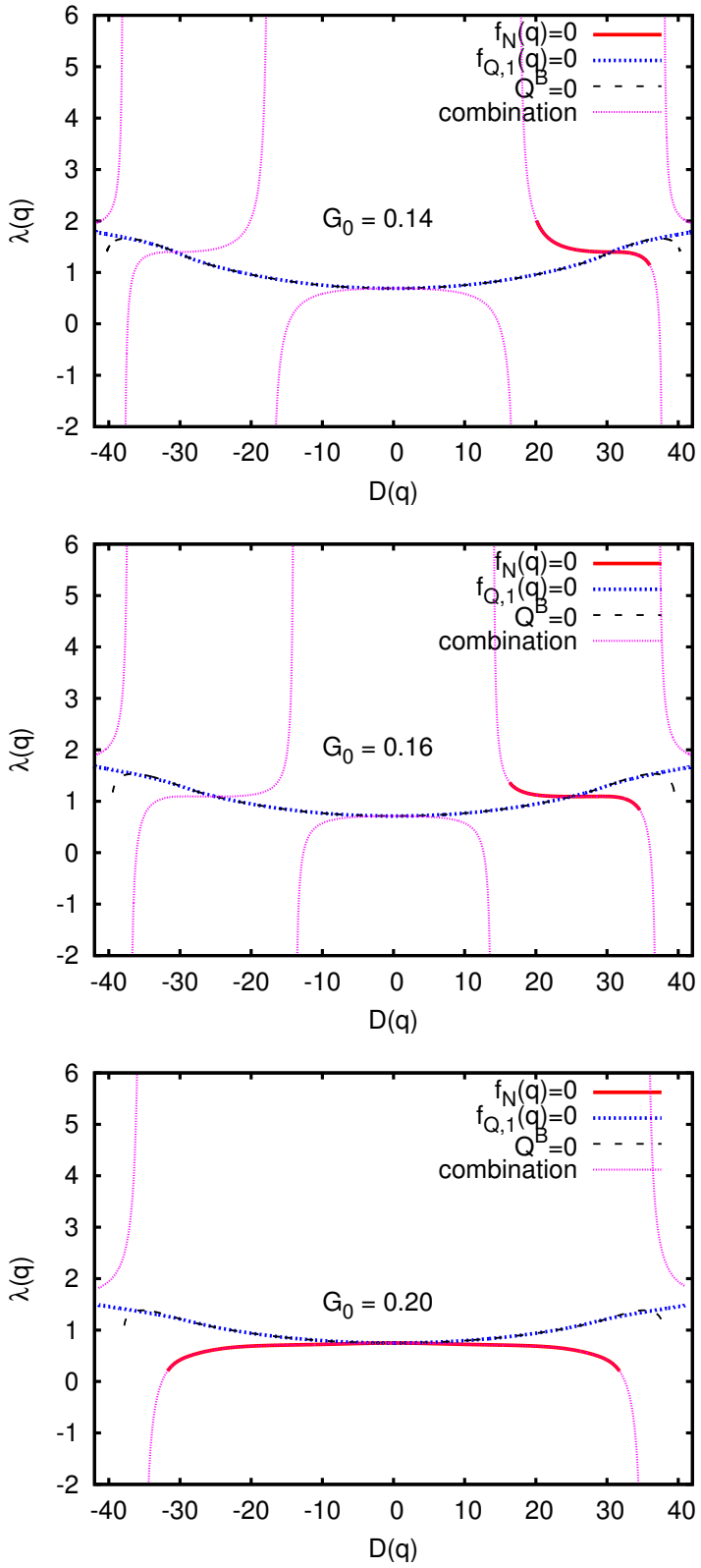

Fig. 4. The chemical potentials $\lambda(q)$ as functions of the deformation D. The upper, middle and lower rows display the results for $G_0 = 0.14$, 0.16 and 0.20, respectively. In each graph, the results obtained from different calculations are compared. The solid (red) and dotted (blue) curves represent the results obtained using the QRPA gauge [$f_N(q) = 0$] and the ETOP gauge [$f^{(-)}_{Q,1}(q) = 0$], respectively, while the dashed curves represent those obtained using the ETOP gauge but ignoring the B-part of $\hat{Q}(q)$ [i.e., setting $Q^B_i(q) = 0$]. The dotted (purple) curves labeled "combination" represent the results calculated by switching to the QRPA gauge after the collective path is determined using the ETOP gauge.

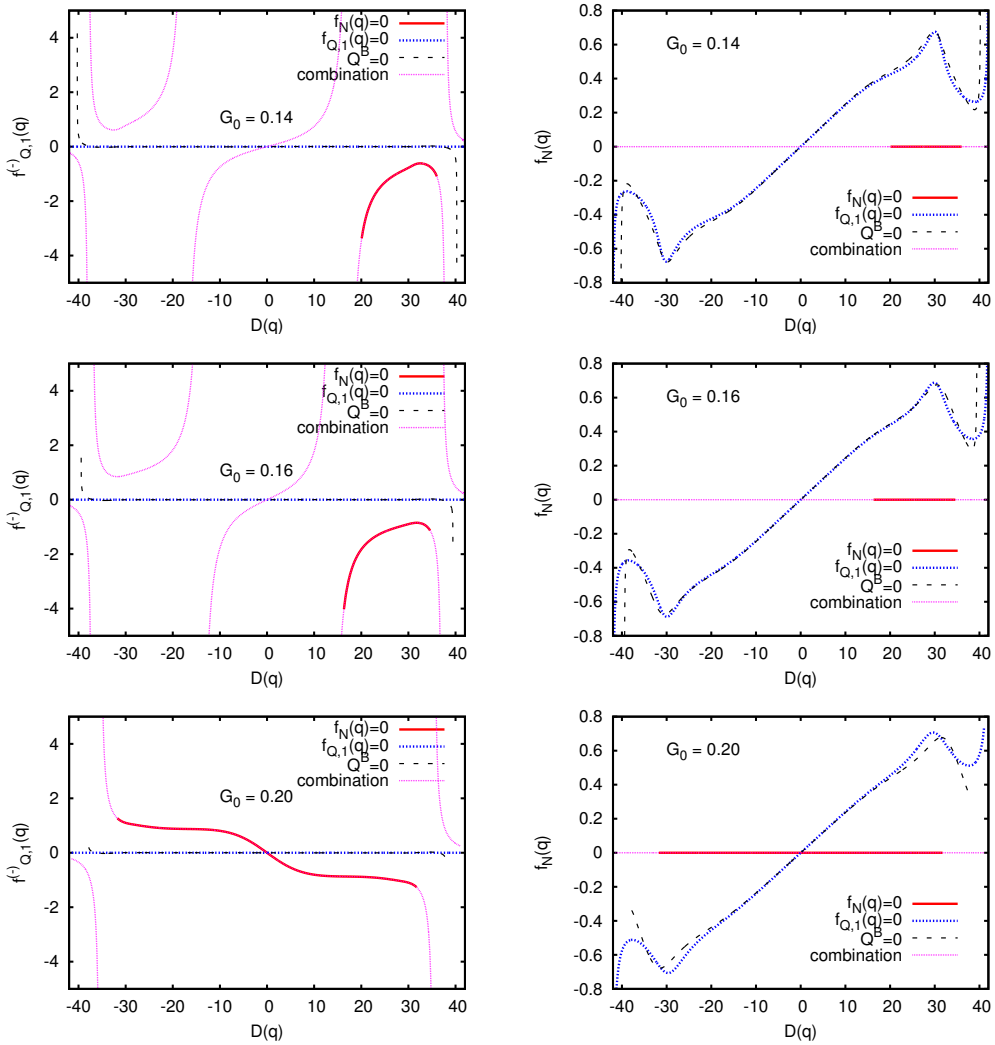

Fig. 5. The gauge dependent quantities $f^{(-)}_{Q,1}(q)$ (*left column*) and $f_N(q)$ (*right column*) plotted as functions of the deformation D. The upper, middle and lower rows display the results for $G_0 = 0.14, 0.16$ and 0.20, respectively. (See the caption of Fig. 4.)

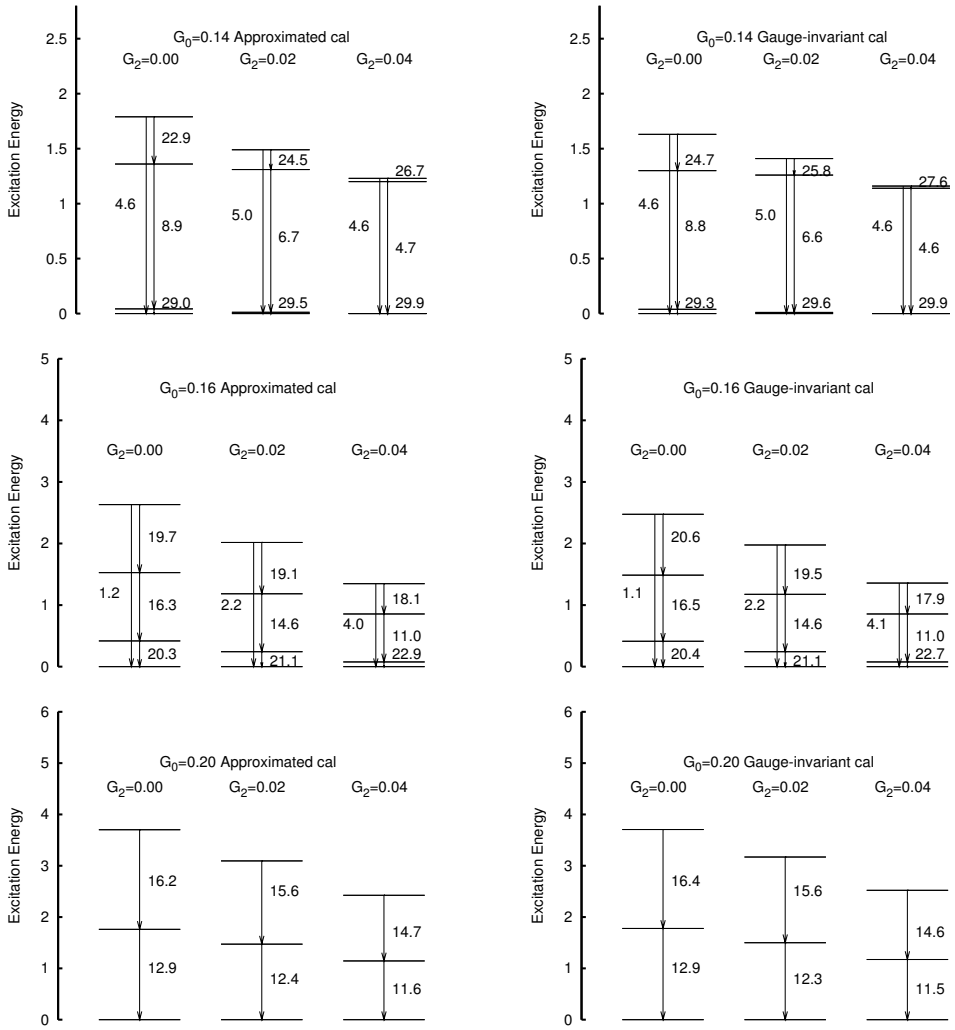

Fig. 6. Excitation spectra and quadrupole transition matrix elements. *Left column*: The result obtained using the ETOP gauge [$f^{(-)}_{Q,1}(q) = 0$] but ignoring the B-part of the collective coordinate operator $\hat{Q}(q)$. This is the same as that presented in Ref. 57). *Right column*: The result obtained by solving the gauge-invariant ASCC equations using the ETOP gauge. The upper, middle and lower rows display the results for $G_0 = 0.14$, 0.16 and 0.20, respectively. In each row, the results for $G_2 = 0.00, 0.02$ and 0.04 are compared. The numbers adjacent to the vertical lines are the absolute values of the transition matrix elements. The matrix elements between the doublets are indicated beside them.

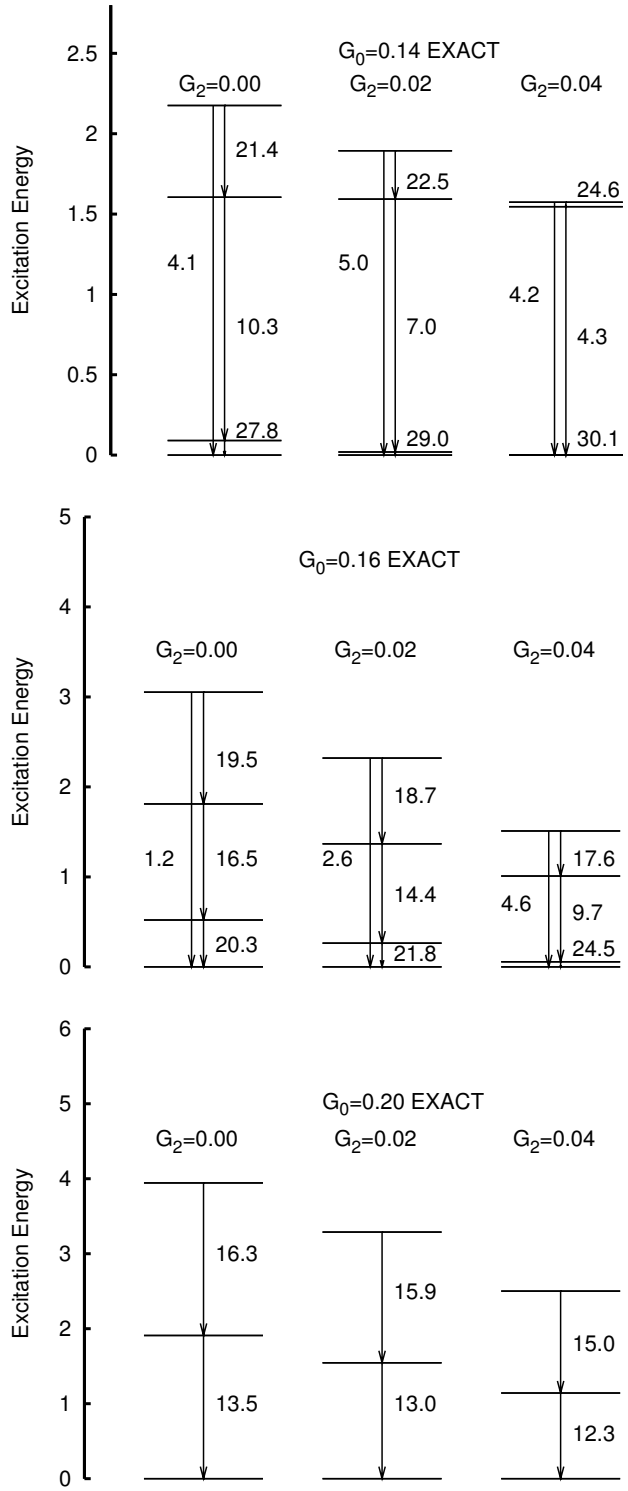

Fig. 7. Excitation spectra calculated with the exact diagonalization of the multi-$O(4)$ model Hamiltonian. The upper, middle and lower rows display the results for $G_0 = 0.14$, 0.16, and 0.20, respectively. In each row, the results for $G_2 = 0.00, 0.02, 0.04$ are compared. The numbers adjacent to vertical lines indicate the transition matrix elements. The matrix elements between the doublets are indicated beside them.