Relation of $a^\dagger a$ terms to higher-order terms in the adiabatic expansion for large-amplitude collective motion

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We investigate the relation of $a^\dagger a$ terms in the collective operator to the higher-order terms in the adiabatic self-consistent collective coordinate (ASCC) method. In the ASCC method, a state vector is written as $e^{i\hat{G}(q,p,n)}|\phi(q)\rangle$ with $\hat{G}(q,p,n)$ which is a function of collective coordinate $q$, its conjugate momentum $p$ and the particle number $n$. According to the generalized Thouless theorem, $\hat{G}$ can be written as a linear combination of two-quasiparticle creation and annihilation operators $a^\dagger_\mu a^\dagger_\nu$ and $a_\nu a_\mu$. We show that, if $a^\dagger a$ terms are included in $\hat{G}(q,p,n)$, it corresponds to the higher-order terms in the adiabatic expansion of $\hat{G}$. This relation serves as a prescription to determine the higher-order collective operators from the $a^\dagger a$ part of the collective operator, once it is given without solving the higher-order equations of motion.

1. Introduction

According to the generalized Thouless theorem (Refs. [1–5]), a Hartree–Fock–Bogoliubov-type state vector (a generalized Slater determinant) can be written in a unitary form as

$$|\psi\rangle = e^{i\hat{G}}|\phi\rangle, \quad \hat{G} = \sum_{\mu\nu} \left( Z_{\mu\nu} a^\dagger_\mu a^\dagger_\nu + Z^*_{\mu\nu} a_\nu a_\mu \right), \quad (1.1)$$

where $|\phi\rangle$ is the vacuum with respect to quasiparticle operator $a_\mu$ ($a_\mu|\phi\rangle = 0$). The purpose of this paper is to investigate the role of $a^\dagger a$ terms, if included in $\hat{G}$, in the context of adiabatic approximation to time-dependent Hartree–Fock–Bogoliubov (TDHFB) theory. In a recent paper (Ref. [6]), we analyzed the higher-order collective coordinate operators and their roles in the gauge invariance of the adiabatic self-consistent collective coordinate (ASCC) method (Ref. [7]), which can be regarded as an advanced version of the adiabatic TDHFB (ATDHFB) theory.

In this paper, we investigate the relation between the $a^\dagger a$ terms and the higher-order collective coordinate operators in the adiabatic expansion. We shall call $a^\dagger a^\dagger$ and $aa$ terms A-terms and $a^\dagger a$ and $aa^\dagger$ (or equivalently $a^\dagger a$ and constant terms) B-terms, respectively. With this terminology, the generalized Thouless theorem states that $\hat{G}$ is uniquely given by a linear combination of A-terms. The (generalized) Thouless theorem is useful to express the Hartree–Fock–Bogoliubov-type state vectors and plays an important role in the time-dependent mean-field theory (Ref. [8]).
In contrast with the theorem, in the ASCC method, B-terms were introduced in $\hat{G}$ (Refs. [9–11]), and it is closely related to the gauge invariance of the theory as we shall explain below. In Ref. [6], we analyzed the gauge symmetry and its breaking in the ASCC method, and showed that the gauge invariance is (partially) broken by the adiabatic approximation and that one needs the higher-order collective operators to retain the gauge invariance. In this paper, we show that the introduction of B-terms in $\hat{G}$ is equivalent to that of a certain kind of higher-order operators, which are written in terms of the B-terms.

The ASCC method (Ref. [7]) is a practical method for describing the large-amplitude collective motion of atomic nuclei with superfluidity. It is an adiabatic approximation to the self-consistent collective coordinate (SCC) method, which was originally formulated by Marumori et al (Ref. [2]), and can be regarded as an advanced version of the ATDHF theory. The ASCC method overcomes the difficulties, which several versions of the ATDHF(B) theory encountered [see Refs. [12–14] for a review], and enables one to describe the large-amplitude collective dynamics which cannot be treated by the $(\eta, \eta^*)$ expansion of the SCC method.

The ASCC method was first pointed out by Hinohara et al (Ref. [9]). They encountered numerical instability in the calculation of the one-dimensional ASCC method. (We mean by the $D$-dimensional ASCC method that the dimension of the collective coordinate $q$ is $D$.) They found that the instability was caused by the symmetry associated with some continuous transformation under which the basic equations of the theory are invariant. As the transformation changes the phase of the state vector, they called this symmetry the "gauge" symmetry and proposed a prescription for the numerical stability ("gauge fixing"), which led them to successful calculation. After the successful application of the one-dimensional ASCC method by Hinohara et al., an approximate version of the two-dimensional ASCC method, which is called the constrained Hartree–Fock–Bogoliubov (HFB) plus local quasiparticle random phase approximation (QRPA) method, was developed and applied to a variety of quadrupole shape dynamics (Refs. [16–22]). However, little progress had been made in the understanding of the gauge symmetry. Recently, we analyzed the gauge symmetry in the ASCC method on the basis of the Dirac–Bergmann theory of the constrained systems (Refs. [23–25]), which shed a new light (Refs. [6, 26]). It is worth mentioning that the one-dimensional ASCC method without pairing correlation was also successfully applied to the nuclear reaction studies (Ref. [27]).

In the ASCC method, a state vector is written in the form of

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

(1.2)

Here, $(q,p)$ are the collective coordinate and conjugate collective momentum. $n$ is the particle number measured by the mean value $N_0$ ($n = N - N_0$), and $\varphi$ is the gauge angle conjugate to $n$. Hinohara et al (Refs. [9–11]) employed $\hat{G}$ expanded up to the first order of $(p,n)$: $\hat{G} = p\hat{Q}(q) + n\hat{\Theta}(q)$. As mentioned above, they encountered the numerical instability, and their prescription for the numerical stability is as follows. They require the commutativity of the collective-coordinate and the particle-number operators $[\hat{Q}, \hat{N}] = 0$ for the gauge symmetry of moving-frame HFB & QRPA equations, which are the equations of motion in the ASCC method, and then fix the gauge. However, the requirement of $[\hat{Q}, \hat{N}] = 0$ implies that they needed to include B-terms in $\hat{Q}(q)$, in contrast with the original formulation of the ASCC method in Ref. [7], which respects the generalized Thouless theorem.
In Ref. [6], we showed that the gauge symmetry in the ASCC method is broken by two sources: the decomposition of the equation of collective submanifold depending on the order of $p$ and the truncation of the adiabatic expansion of $\hat{G}$ to a certain order of $(p, n)$. We showed that the gauge symmetry broken by the truncation is retained by including the higher-order operators as in Eq. (2.2). In this approach with the higher-order operators, the condition $[\hat{Q}, \hat{N}] = 0$ is not necessary for the gauge symmetry, and one does not need B-terms in the collective operators.

Thus, there are two approaches to conserve the gauge symmetry. One is the approach with higher-order operators consisting of only A-terms, and the other with only the first-order operator containing B-terms as well as the A-terms, requiring $[\hat{Q}, \hat{N}] = 0$. Let us call the former Approach A and the latter Approach B. Note that, as shown in Ref. [6], the gauge symmetry in the canonical-variable conditions, which are conditions for the collective variables to be canonical, is broken in Approach B, while it is not in Approach A. It is noteworthy that, in Approach A, the collective operators consists of A-terms but that the gauge transformation mixes A-terms and B-terms.

When the ASCC method is applied to the translational motion, the collective coordinate and momentum operators $\hat{Q}$ and $\hat{P}$ correspond to the center-of-mass position and momentum, respectively, and their exact operator forms are known. Whereas the state vector can be written without the B-terms according to the generalized Thouless theorem, $\hat{Q}$ for the translational motion contains B-terms in the quasiparticle representation. With the B-terms included, $\hat{G}$ expanded up to the first order would give the exact solution for the translational motion. Although the state vector could be written without B-terms, if the B-terms are neglected, one might need to take into account the higher-order operators at the level of the equations of motion after the adiabatic expansion. Thus, it is no trivial whether or not one should include B-terms and/or higher-order terms in $\hat{G}$. To address this point, one must investigate the relation between the two approaches.

Concerning the higher-order terms and B-terms in the adiabatic expansion for large-amplitude collective motion, the following two things are worthy of note. First, in his paper on the ATDHF in 1977 (Ref. [28]), Villars mentioned the extension of his ATDHF theory including the higher-order operator (more strictly, the extension with the first- and third-order operators and no second-order operator) and preannounced a publication on it: "Ref. 17) A. Toukan and F. Villars, to be published" in Ref. [28]. However, as far as the author knows, it was not published after all. Second, in the ATDHF theory by Baranger and Vénéroni (Ref. [29]), they proposed the density matrix in the form of $\rho(t) = e^{i\chi(t)}\rho_0(t)e^{-\chi(t)}$ with Hermitian and time-even $\rho_0(t)$ and $\chi(t)$. They emphasized that $\chi(t)$ can be written in terms of A-terms only, but included B-terms as well as A-terms in the treatment of the translational motion. In this paper, we attempt to clarify the relation between the higher-order terms and B-terms.

The paper is organized as follows. In Sect. 2, after giving a brief explanation of the formulation of the ASCC method, we compare the moving-frame HFB & QRPA equations between the two approaches. We shall find some correspondence between the higher-order operators and the (multiple) commutators of the A-part and B-part of the first-order operators. This comparison is useful for understanding the contribution of the B-part of the collective coordinate operator $\hat{Q}(q)$ to the equations of motion. In Sect. 3, we illustrates how to obtain
the correspondence between the higher-order operators and the multiple commutators of the first-order operators in general. By comparing the state vectors in the two approaches directly, we show that the inclusion of B-terms is equivalent to that of a certain kind of the higher-order operators and give the explicit expression of the corresponding higher-order operators. This correspondence gives a prescription to determine the higher-order collective operators from the B-part of the first-order collective coordinate operator \( \hat{Q}_B(q) \). In Sect. 4, we compare the inertial masses and confirm that, if we determine the higher-order operators with the above-mentioned prescription, the two approaches give the same results. Concluding remarks are given in Sect. 5. In Appendix, some formulae of commutators of fermion operators are given, which helps understand the derivation in the text.

2. Comparison of the equations of motion

In this section, we give a minimal explanation of the formulation of the ASCC method which is necessary for the purpose of this paper. (For details, see Refs. [6, 7].) Then we shall compare the moving-frame HFB & QRPA equations in the two approaches. Although we compare the state vectors in the two approaches directly in the next section, the comparison of the moving-frame equations in this section is useful to understand how the B-part of \( \hat{G} \) contribute to the equations of motion.

The state vector in the ASCC method is written as

\[
|\phi(q,p,\varphi,n)\rangle = e^{-i\varphi \hat{N}} e^{i\hat{G}(q,p,n)} |\phi(q)\rangle. \tag{2.1}
\]

We assume the \( \varphi \)-dependence of the state vector as above, which guarantees the conservation of the expectation value of the particle number \( \hat{N} \). Although there are two components, neutrons and protons, in atomic nuclei, we consider the ASCC method with a single component for simplicity. We show below \( \hat{G} \) expanded up to the third order in Approach A,

\[
\hat{G}(q,p,n) = p\hat{Q}^{(1)}(q) + n\hat{\Theta}^{(1)}(q) + \frac{1}{2} p^2 \hat{Q}^{(2)}(q) + \frac{1}{2} n^2 \hat{\Theta}^{(2)}(q) + pm\hat{X}
\]

\[
+ \frac{1}{3!} p^3 \hat{Q}^{(3)}(q) + \frac{1}{3!} n^3 \hat{\Theta}^{(3)}(q) + \frac{1}{2} p^2 n\hat{O}^{(2,1)}(q) + \frac{1}{2} pn^2 \hat{O}^{(1,2)}(q). \tag{2.2}
\]

All the operators in Eq. (2.2) consist of A-terms only. For example, \( \hat{Q}^{(i)}(q) \) is defined by

\[
\hat{Q}^{(i)}(q) = \sum_{\alpha\beta} Q^{(i)}_{\alpha\beta}(q) a^\dagger_\alpha a_\beta + Q^{(i)*}_{\alpha\beta}(q) a_\beta a_\alpha \quad (i = 1, 2, 3). \tag{2.3}
\]

The other operators are defined similarly.

In Approach B, \( \hat{G} \) is expanded up to the first order as

\[
\hat{G}(q,p,n) = p\hat{Q}(q) + n\hat{\Theta}(q). \tag{2.4}
\]

We omit the superscripts indicating the order of expansion in Approach B. In Approach B, while \( \hat{\Theta}(q) \) consists of only A-terms as in Approach A, \( \hat{Q} \) contains B-terms.

\[
\hat{Q}(q) = \hat{Q}_A(q) + \hat{Q}_B(q), \tag{2.5}
\]

\[
\hat{Q}_A(q) = \sum_{\alpha\beta} Q_{A\alpha\beta}(q) a^\dagger_\alpha a_\beta + Q^{*}_{A\alpha\beta}(q) a_\beta a_\alpha, \tag{2.6}
\]

\[
\hat{Q}_B(q) = \sum_{\alpha\beta} Q_{B\alpha\beta}(q) a^\dagger_\alpha a_\beta. \tag{2.7}
\]
where $Q_B$ is a Hermitian matrix. [We denote the $A(B)$-part of an operator $\hat{O}$ by $\hat{O}_{A(B)}$ hereinafter.] One might wonder if $\hat{Q}_B$ could be written in a more general form

$$\hat{Q}_B = \sum_{\mu \nu} Q_{B}^{\mu \nu} a_\mu^\dagger a_\nu + \sum_{\mu} \tilde{Q}_{B}^{\mu} a_\mu^\dagger a_\nu, \tag{2.8}$$

with Hermitian matrices $Q_B$ and $\tilde{Q}_B$, and it can be rewritten as

$$\hat{Q}_B = \sum_{\mu \nu} (Q_{B}^{\mu \nu} - \tilde{Q}_{B}^{\mu}) a_\mu^\dagger a_\nu + \sum_{\mu} \tilde{Q}_{B}^{\mu}. \tag{2.9}$$

$(Q_B - \tilde{Q}_B^T)$ is also Hermitian, and it implies that the right-hand side of Eq. (2.7) could have a constant term. However, the collective coordinate operator $\hat{Q}$ should satisfy the canonical-variable conditions (Ref. [7]), and the zeroth-order canonical-variable condition is given by

$$\langle \phi(2)|\hat{Q}(2)|\phi(2)\rangle = \langle \phi(2)|\hat{Q}_B(2)|\phi(2)\rangle = 0, \tag{2.10}$$

which implies that there is no constant term in Eq. (2.7).

The equations of motion in the ASCC method is derived from the invariance principle of time-dependent Schrödinger equation

$$\delta \langle \phi(q,p,\varphi,n)|i\partial_t - \hat{H}|\phi(q,p,\varphi,n)\rangle = 0, \tag{2.11}$$

which is rewritten as the equation of collective submanifold,

$$\delta \langle \phi(q,p,\varphi,n)|\hat{H} - i \frac{\partial \mathcal{H}}{\partial p} \partial_q - \frac{1}{i} \frac{\partial \mathcal{H}}{\partial q} \partial_p - \frac{1}{i} \frac{\partial \mathcal{H}}{\partial \varphi} \partial_n - \frac{\partial \mathcal{H}}{\partial n} \hat{N}|\phi(q,p,\varphi,n)\rangle = 0, \tag{2.12}$$

with the collective Hamiltonian $\mathcal{H} = \langle \phi(q,p,\varphi,n)|\hat{H}|\phi(q,p,\varphi,n)\rangle$. We substitute the state vector (2.1), expand in powers of $(p,n)$ (adiabatic expansion), and decompose the above equation (2.12) depending on the order of $p$. From the equations of $O(1)$, $O(p)$ and $O(p^2)$, the moving-frame HFB & QRPA equations are derived, which are the equation of motion in the ASCC method. When $\hat{G}$ is expanded up to $O(p^3)$ in Approach A, the moving-frame HFB & QRPA equations are given by

Moving-frame HFB equation

$$\delta \langle \phi(q)|\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}^{(1)}|\phi(q)\rangle = 0, \tag{2.13}$$

Moving-frame QRPA equations

$$\delta \langle \phi(q)||\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}^{(1)}, \hat{Q}^{(1)}| - \frac{1}{i} B(q) \hat{P} - \frac{1}{i} \partial_q V \hat{Q}^{(2)}|\phi(q)\rangle = 0, \tag{2.14}$$

$$\delta \langle \phi(q)||\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}^{(1)}|\hat{P} - C(q) \hat{Q}^{(1)} - \partial_q \lambda \hat{N}$$

$$- \frac{1}{2B} \partial_q V \left\{ [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}^{(1)}, \hat{Q}^{(1)}], \hat{Q}^{(1)} \right\} - i [\hat{H} - \lambda \hat{N}, \hat{Q}^{(2)}]$$

$$+ \partial_q V \left[ \hat{Q}^{(3)} - \frac{i}{2} [\hat{Q}^{(1)}, \hat{Q}^{(2)}] \right] \right\} |\phi(q)\rangle = 0. \tag{2.15}$$

Note that the moving-frame QRPA equation of $O(p)$ (2.14) contains the second-order operator $\hat{Q}^{(2)}(q)$, and the moving-frame QRPA equation of $O(p^2)$ (2.15) does the third-order
operator \( \hat{Q}^{(3)}(q) \) as well as \( \hat{Q}^{(2)}(q) \). Here \( \hat{Q}^{(i)}(i = 1, 2, 3) \) and \( \hat{P} \) contain only A-terms. Eqs. (2.13) and (2.14) are derived from the \( O(1) \) and \( O(p) \) terms of Eq. (2.11), respectively. Eq. (2.15) are derived using the \( O(1) \) and \( O(p^2) \) terms.

In Approach B, the moving-frame HFB & QRPA equations are given by

Moving-frame HFB equation

\[
\delta \langle \phi(q) | \hat{H} - \lambda \hat{N} - \partial_q V \hat{Q} | \phi(q) \rangle = 0,
\]

(2.16)

Moving-frame QRPA equations

\[
\delta \langle \phi(q) | [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}, \frac{1}{i} \hat{P}] - C(q) \hat{\mathcal{Q}} - \partial_q \lambda \hat{N} \\
- \frac{1}{2B} \partial_q V \{ [[\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}, \hat{\mathcal{Q}}], \hat{\mathcal{Q}}] \} | \phi(q) \rangle = 0.
\]

(2.17)

Note that \( \hat{Q} \) is the first-order operator.

As shown in Ref. [6], Eqs. (2.13)–(2.15) are invariant under the following transformation:

\[
\hat{Q}^{(1)} \rightarrow \hat{Q}^{(1)} + \alpha \hat{N},
\]

(2.19)

\[
\hat{Q}^{(2)} \rightarrow \hat{Q}^{(2)} + i\alpha [\hat{N}, \hat{Q}^{(1)}],
\]

(2.20)

\[
\hat{Q}^{(3)} \rightarrow \hat{Q}^{(3)} + \frac{3}{2} \alpha i [\hat{N}, \hat{Q}^{(2)}] - \frac{1}{2} \alpha [\hat{Q}^{(1)}, [\hat{Q}^{(1)}, \hat{N}]],
\]

(2.21)

\[
\lambda \rightarrow \lambda - \alpha \partial_q V,
\]

(2.22)

\[
\partial_q \lambda \rightarrow \partial_q \lambda - \alpha C.
\]

(2.23)

On the other hand, if \( [\hat{Q}, \hat{N}] = 0 \), Eqs. (2.16)–(2.18) are invariant under the transformation

\[
\hat{Q} \rightarrow \hat{Q} + \alpha \hat{N},
\]

(2.24)

\[
\lambda \rightarrow \lambda - \alpha \partial_q V,
\]

(2.25)

\[
\partial_q \lambda \rightarrow \partial_q \lambda - \alpha C.
\]

(2.26)

[Here, we have not shown the transformations of the operators which are not involved in the moving-frame HFB & QRPA equations (2.13)–(2.18) above. However, to consider the gauge symmetry in the canonical-variable conditions, the transformations of the operators not shown here are needed. See Ref. [6] for the complete list of the transformations.]

Before comparing the moving-frame equations between the two approaches, we shall give some remarks. In the ASCC method, we take only the variation in the form of \( \delta | \phi \rangle = a^\dagger \mu a_\nu | \phi \rangle \).

Therefore, the A-terms can directly contribute to the moving-frame HFB & QRPA equation, but the variation of B-terms automatically vanishes.

\[
\delta \langle \phi(q) | (B\text{-terms}) | \phi(q) \rangle = 0.
\]

(2.27)

The B-terms contribute only through commutators, e.g., [A-terms, B-terms]. Concerning the commutators, the following rules are readily understood from Eqs. (A1)–(A4) and are useful
for the investigation below.

\[
[A\text{-terms, A\text{-terms}}] = B\text{-terms,} \tag{2.28}
\]

\[
[A\text{-terms, B\text{-terms}}] = A\text{-terms,} \tag{2.29}
\]

\[
[B\text{-terms, B\text{-terms}}] = B\text{-terms.} \tag{2.30}
\]

One can also see that the variation of the normally ordered fourth-order operators \((a^{\dagger}a^{\dagger}a^{\dagger}a^{\dagger},a^{\dagger}a^{\dagger}a,\ldots)\) vanishes.

\[
\delta \langle \phi(q) | (\text{normally ordered fourth-order terms}) | \phi(q) \rangle = 0. \tag{2.31}
\]

Let us substitute \(\hat{Q} = \hat{Q}_A + \hat{Q}_B\) into the moving-frame HFB & QRPA equations in Approach B and compare them with those in Approach A. First, one can see that \(\hat{Q}_B\) does not contribute to the moving-frame HFB equation (2.16).

\[
\delta \langle \phi(q) | \hat{H} - \lambda \hat{N} - \partial_q V \hat{Q} | \phi(q) \rangle = 0,
\]

\[
\Leftrightarrow \delta \langle \phi(q) | \hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A | \phi(q) \rangle = 0. \tag{2.32}
\]

As a matter of course, \(\hat{Q}_A\) corresponds to \(\hat{Q}^{(1)}\):

\[
\hat{Q}^{(1)} \Leftrightarrow \hat{Q}_A. \tag{2.33}
\]

Next, the moving-frame QRPA equation of \(O(p)\) (2.17) reads

\[
\delta \langle \phi(q) | [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A - \partial_q V \hat{Q}_B, \hat{Q}_A + \hat{Q}_B] - \frac{1}{i} B(q) \hat{P} | \phi(q) \rangle = 0,
\]

\[
\Leftrightarrow \delta \langle \phi(q) | [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A, \hat{Q}_A] - \frac{1}{i} B(q) \hat{P} - \partial_q V [\hat{Q}_B, \hat{Q}_A] | \phi(q) \rangle = 0. \tag{2.34}
\]

Here, we have used that \(\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A\) does not contain A-terms, which follows from the moving-frame HFB equation (2.16), and that the commutator of the normally ordered fourth-order terms of \((a^{\dagger},a)\) (from the residual interaction part of \(\hat{H}\)) with the B-term does not contribute, i.e.,

\[
\delta \langle \phi(q) | [\text{normally ordered forth-order terms, B\text{-terms}}] | \phi(q) \rangle = 0. \tag{2.35}
\]

This can easily seen with Eqs. (A5)–(A7), their Hermitian conjugates, and Eq. (2.31).

By comparing Eq. (2.34) with Eq. (2.14), one finds the correspondence as follows.

\[
\hat{Q}^{(2)} \Leftrightarrow i[\hat{Q}_B, \hat{Q}_A]. \tag{2.36}
\]

Then, we consider the moving-frame QRPA equation of \(O(p^2)\) (2.18). From Eq. (2.17), we have

\[
\frac{1}{i} \hat{P} = \frac{1}{B} [\hat{H}_M, \hat{Q}^A] = \frac{1}{B} [\hat{H}_M, \hat{Q}_A], \tag{2.37}
\]

with

\[
\hat{H}_M := \hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}. \tag{2.38}
\]

In the second equality in Eq. (2.37), we have used Eqs. (2.30) and (A5)–(A7).
Thus the moving-frame QRPA equation (2.18) is rewritten as

\[
\delta\langle q \rangle [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A, \frac{1}{i} \hat{P}] - \partial_q V [\hat{Q}_B, \frac{1}{i} \hat{P}] - C(q) \hat{Q}_A - \partial_q \lambda \hat{N}
\]

\[
- \frac{1}{2B} \partial_q V \left\{ [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}], \hat{Q} \right\} |\phi(q)\rangle = 0,
\]

\[
\leftrightarrow \delta\langle q \rangle [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A, \frac{1}{i} \hat{P}] - C(q) \hat{Q}_A - \partial_q \lambda \hat{N}
\]

\[
- \frac{1}{B} \partial_q V [\hat{Q}_B, [\hat{H}_M, \hat{Q}_A]] - \frac{1}{2B} \partial_q V [\hat{H}_M, \hat{Q}], \hat{Q} |\phi(q)\rangle = 0. \quad (2.39)
\]

The fourth term is rewritten as

\[
\delta\langle q \rangle \frac{1}{B} \partial_q V [\hat{H}_M, \hat{Q}_A, \hat{Q}_B] |\phi(q)\rangle = \delta\langle q \rangle \frac{1}{B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_B] |\phi(q)\rangle,
\]

\[
= \delta\langle q \rangle \frac{1}{B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_B] |\phi(q)\rangle, \quad (2.40)
\]

where we have used that $[\hat{H}_M, \hat{Q}_A]$ contains B-terms and normally ordered fourth-order terms but that they do not contribute because of Eqs. (2.27) (2.30) and (2.35). Similarly, one can easily see that

\[
\delta\langle q \rangle [\hat{H}_M, \hat{Q}_B] |\phi(q)\rangle = 0. \quad (2.41)
\]

Then, the fourth and fifth terms in Eq. (2.39) are rewritten as

\[
\delta\langle q \rangle \frac{1}{B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_B] - \frac{1}{2B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_B]
\]

\[
- \frac{1}{2B} \partial_q V [\hat{H}_M, \hat{Q}_B], \hat{Q}_A] - \frac{1}{2B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_B] |\phi(q)\rangle
\]

\[
= - \delta\langle q \rangle \frac{1}{2B} \partial_q V \left( [[\hat{Q}_A, \hat{Q}_B], \hat{H}_M] + [[\hat{H}_M, \hat{Q}_A], \hat{Q}_A] \right) |\phi(q)\rangle
\]

\[
= \delta\langle q \rangle \left( - \frac{1}{2B} \partial_q V [\hat{H}_M, \hat{Q}_A], \hat{Q}_A]
\]

\[
+ \frac{1}{2B} \partial_q V [\hat{H} - \lambda \hat{N}, [\hat{Q}_A, \hat{Q}_B]] - \frac{1}{2B} (\partial_q V)^2 [[\hat{Q}_B, \hat{Q}_A], \hat{Q}_B] |\phi(q)\rangle. \quad (2.42)
\]

In the second equality, we have used the Jacobi identity.

Finally we obtain the moving-frame QRPA equation of $O(p^2)$ as follows.

\[
\delta\langle q \rangle [\hat{H} - \lambda \hat{N} - \partial_q V \hat{Q}_A, \frac{1}{i} \hat{P}] - C(q) \hat{Q}_A - \partial_q \lambda \hat{N}
\]

\[
- \frac{1}{2B} \partial_q V \left( [\hat{H}_M, \hat{Q}_A], \hat{Q}_A] - [\hat{H} - \lambda \hat{N}, [\hat{Q}_A, \hat{Q}_B]]
\]

\[
+ \partial_q V [[\hat{Q}_B, \hat{Q}_A], \hat{Q}_B] \right) |\phi(q)\rangle = 0. \quad (2.43)
\]

It may be noteworthy that, in the derivation of this equation, we have used the moving-frame QRPA equation of $O(p)$ (2.17), which implies that this equation was derived with all the expansions of $O(1), O(p)$, and $O(p^2)$ of the equation of collective submanifold (2.12).
We compare Eq. (2.43) with Eq. (2.15) and find
\[ \hat{Q}^{(3)} - \frac{i}{2}[\hat{Q}^{(1)}, \hat{Q}^{(2)}] \leftrightarrow [[\hat{Q}_B, \hat{Q}_A], \hat{Q}_B]. \]  
(2.44)

Because \([\hat{Q}^{(1)}, \hat{Q}^{(2)}]\) is a B-term and does not contribute, we obtain
\[ \hat{Q}^{(3)} \leftrightarrow [[\hat{Q}_B, \hat{Q}_A], \hat{Q}_B] = -[\hat{Q}_B, [\hat{Q}_B, \hat{Q}_A]]. \]  
(2.45)

Again in this case, one can see the same correspondence as we have seen above
\[ \hat{Q}^{(2)} \leftrightarrow i[\hat{Q}_B, \hat{Q}_A]. \]  
(2.46)

3. Correspondence between higher-order operators and the B-part of the first-order operator

3.1. The case without pairing correlation

In the previous section, we have found some correspondence between the higher-order operators \(\hat{Q}^{(i)}\) \((i = 2, 3)\) in Approach A and the commutators of the first-order operators \(\hat{Q}_A\) and \(\hat{Q}_B\) in Approach B. It implies that it is equivalent to introduce the B-part of \(\hat{Q}\) to introducing the higher-order operators given by this correspondence, at least, at the level of the equations of motion, i.e., the moving-frame HFB & QRPA equations. In this section, we directly derive the correspondence between the B-part of the first-order operator and the higher-order operators by rewriting the state vector in Approach B. First, we consider the case where there is no pairing correlation to illustrate how to derive the relation of \(\hat{Q}_B\) to the higher-order operators. The state vectors in the no-pairing case are obtained by setting \(n = 0\) and \(\varphi = 0\) in Eq. (2.1) with \(\hat{G}\) (2.4). The case with pairing correlation is treated in a later subsection.

In Lemma 2 in Ref. [2], it is proven, in the case of no pairing, that the unitary operator \(e^{i\hat{G}}\) can be decomposed in the form of
\[ e^{i\hat{G}} = e^{i\hat{G}_A} e^{i\hat{G}_B}, \]  
(3.1)

where the Hermitian operators \(\hat{G}_A\) and \(\hat{G}_B\) consist of only A-terms and B-terms, respectively. In the no-pairing case, the \(a^\dagger a^\dagger (aa)\) terms correspond to the particle-hole pair creation (annihilation) operators, and the \(a^\dagger a\) terms correspond to the particle-scattering and hole-scattering terms. In Ref. [2], no explicit expressions of \(\hat{G}_A\) and \(\hat{G}_B\) are given. We shall give explicit expressions for \(\hat{G}_B\) below.

In the following, we denote \((i\hat{Q}_A, i\hat{Q}_B) := (A, B)\) and \((i\hat{G}_A, i\hat{G}_B) := (G_A, G_B)\) to simplify the notation, and then the state vector is written as
\[ e^{p(A+B)}|\phi\rangle = e^{G_A} e^{G_B}|\phi\rangle \]  
(3.2)

Here, \(G_{A(B)}\) contains only A(B)-terms. We shall see below that \(G_B\) consists of the \(a^\dagger a\) part and a constant \(\theta\). The \(a^\dagger a\) part does not contribute to the state vector because \(a^\dagger a|\phi(q)\rangle = 0\). Note that the constant term \(\theta\) can not be ignored, however. It depends on \(A\) and \(B\) as well as \(p\), that is, \(\theta = \theta(A, B, p)\). Actually, it is easily shown that, if we omit the constant term (and hence \(e^{G_B}\)) as below
\[ e^{p(A+B)}|\phi\rangle = e^{pA + \frac{3}{2}p^2A^{(2)} + \frac{3}{4}p^3A^{(3)} + \cdots}|\phi\rangle, \]  
(3.3)

expand in powers of \(p\) and compare the both sides order by order, \(A^{(3)}\) must contain a B-part.
We first show some formulae (Ref. [30]) we use below.

**Baker-Campbell-Hausdorff (BCH) formula:**

\[
e^{tA}e^{tB} = \exp \left\{ t(A + B) + \frac{t^2}{2}[A, B] \\
+ \frac{t^3}{12} ([A, [B, A]] + [A, [A, B]]) + \frac{t^4}{24} [[[B, A], A], B] + \cdots \right\}. \tag{3.4}
\]

**Zassenhaus formula:**

\[
e^{t(A+B)} = e^{tA}e^{tB}e^{-\frac{t^2}{2}[A,B]}e^{\frac{t^3}{3!}[2[B,[A,B]]+[A,[A,B]]]}
\times e^{-\frac{t^4}{4!}([[[B,A],A]+3[[A,B],A]+3[[A,B],[B,B]]] / 2 + [(A + B), [(A + B), [A, B]]])} \cdots . \tag{3.5}
\]

**Lie group commutator:**

\[
e^{tA}e^{tB}e^{-tA}e^{-tB} = e^{\mathcal{U}} \tag{3.6}
\]

\[
\mathcal{U}(t, A, B) = -\mathcal{U}(t, B, A) \\
= t^2[A, B] + \frac{t^3}{2}((A + B), [A, B]) \\
+ \frac{t^4}{3!}([[B, A], A)] / 2 + [(A + B), [(A + B), [A, B]]]) \cdots , \tag{3.7}
\]

from which we obtain

\[
e^{tA}e^{tB} = e^{tB}e^{tA}e^{\mathcal{U}(-t,A,B)} \\
= e^{tB}e^{tA} \exp \left\{ t^2 [A, B] - \frac{t^3}{2}((A + B), [A, B]) \\
+ \frac{t^4}{3!}([[B, A], A)] / 2 + [(A + B), [(A + B), [A, B]]]) \cdots \right\}. \tag{3.8}
\]

The formula (3.7) is derived from the BCH formula (3.4). By using these formulae, we rewrite \( e^{p(A+B)}|\phi\rangle \) to derive the expressions of \( G_A \) and \( G_B \). The basic strategy for the derivation is as follows.

(1) Using the Zassenhaus formula (3.5), transform a sum of Lie algebra elements into a product of Lie group elements.

(2) Change the order of a product of Lie group elements using the formula of Lie group commutator (3.8). (Shift a B-term to the right and an A-term to the left.)

(3) With the BCH formula (3.4), transform a product of Lie group elements into a sum of Lie algebra elements. In the sum, there appears B-terms, and then go back to (1).
We repeat these steps until we obtain the expression up to the order we need. Below we take up to $O(p^4)$ and omit the higher-order terms. We shift $e^{eB}$ to the right as below.

\[
e^{p(A+B)}|\phi\rangle = e^{pA} e^{eB} e^{-\frac{p^2}{2}[A,B]} e^{\frac{p^4}{4}[2[B,[A,B]]+[A,[A,B]]]}
\times e^{-\frac{p^2}{2}([A,B],[A]+3[[A,B],[B]]+3[[A,B],[B]])} \cdots |\phi\rangle
\]

\[
= e^{pA} e^{eB} \exp \left\{ -\frac{p^2}{2}[B,[A,B]] + \frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{\frac{p^2}{2}([A,B],[A+B])} \exp \left\{ -\frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{eB} \exp \left\{ -\frac{p^4}{2}[B,[B,[A,B]]] \right\}
\times e^{-\frac{p^2}{2}([A,B],[A]+3[[A,B],[B]]+3[[A,B],[B]])} \cdots |\phi\rangle
\]

\[
= e^{pA} e^{eB} \exp \left\{ -\frac{p^2}{2}[B,[A,B]] + \frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{\frac{p^2}{2}([A,B],[A+B])} \exp \left\{ -\frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{eB} \exp \left\{ -\frac{p^4}{6}[2[B,[A,B]]+4[B,[B,[A,B]]]] \right\}
\times e^{-\frac{p^2}{2}([A,B],[A]+3[[A,B],[B]]+3[[A,B],[B]])} \cdots |\phi\rangle
\]

\[
= e^{pA} e^{eB} \exp \left\{ -\frac{p^2}{2}[B,[A,B]] + \frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{\frac{p^2}{2}([A,B],[A+B])} \exp \left\{ -\frac{p^4}{4}[B,[B,[A,B]]] \right\}
\times e^{eB} \exp \left\{ -\frac{p^4}{6}[2[B,[A,B]]+4[B,[B,[A,B]]]] \right\}
\times e^{-\frac{p^2}{2}([A,B],[A]+3[[A,B],[B]]+3[[A,B],[B]])} \cdots |\phi\rangle.
\]

Noting that

\begin{align}
&[[[A,B],[B],[B]] = -[[B,[A,B]],B] = [B,[B,[A,B]]], \quad \text{(3.10)} \\
&[[A,B],[A],[B]] = -[[A,[A,B]],B] = [B,[A,[A,B]]], \quad \text{(3.11)} \\
&[[[A,B],[A],[A]] = -[[A,[A,B]],A] = [A,[A,[A,B]]], \quad \text{(3.12)}
\end{align}

and with the BCH formula (3.4), one can rewrite the state vector as

\[
e^{p(A+B)}|\phi\rangle = \exp \left\{ pA + \frac{p^2}{2}[B,A] + \frac{p^3}{6}[B,[B,A]] - \frac{p^4}{12}[A,[A,B]]
\right.
\left.
+ \frac{p^4}{24}[B,[B,[A,B]]] - \frac{p^4}{24}[B,[A,[B,A]]] + \frac{p^4}{12}[A,[B,[B,A]]] \right\} e^{pB} \cdots |\phi\rangle
\]

\[
= \exp \left\{ pA + \frac{p^2}{2}[B,A] + \frac{p^3}{6}[B,[B,A]] - \frac{p^4}{12}[A,[A,B]]
\right.
\left.
+ \frac{p^4}{24}[B,[B,[A,B]]] + \frac{p^4}{24}[B,[A,[B,A]]] \right\} e^{pB} \cdots |\phi\rangle.
\]

(3.13)
We have used that
\[ [A, [B, [B, A]]] = -[[B, A], A] - [[B, A], [B, A]] = [B, [A, [B, A]]]. \quad (3.14) \]
The exponent of the first factor contains B-terms in Eq. (3.13), so we decompose it using the Zassenhaus formula (3.5).

\[
e^{p(A+B)}|\phi\rangle = \exp \left\{ pA + \frac{p^2}{2} [B, A] + \frac{p^3}{6} [B, [B, A]] + \frac{p^4}{24} [B, [B, [B, A]]] - \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] \right\} e^{pB} \cdots |\phi\rangle
\]
\[
= \exp \left\{ pA + \frac{p^2}{2} [B, A] + \frac{p^3}{6} [B, [B, A]] + \frac{p^4}{24} [B, [B, [B, A]]] \right\} \exp \left\{ \frac{p^4}{24} [A, [A, [B, A]]] \right\} e^{pB} \cdots |\phi\rangle
\]
\[
= \exp \left\{ pA + \frac{p^2}{2} [B, A] + \frac{p^3}{6} [B, [B, A]] + \frac{p^4}{24} ([B, [B, [B, A]]] + [A, [A, [B, A]]]) \right\} \exp \left\{ \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] \right\} e^{pB} |\phi\rangle + O(p^5). \quad (3.15)\]

Note that
\[
e^{pB} |\phi\rangle = |\phi\rangle, \quad (3.16)\]
when B does not contain a constant term and consists of only \(a^\dagger a\) terms. (As mentioned above, it follows from the zeroth-order canonical-variable condition that \(B = i\hat{Q}_B\) consists of only \(a^\dagger a\) terms in the case of the ASCC method.) Omitting \(e^{pB}\), the state vector reads
\[
e^{p(A+B)}|\phi\rangle
\]
\[
= \exp \left\{ pA + \frac{p^2}{2} [B, A] + \frac{p^3}{6} [B, [B, A]] + \frac{p^4}{24} ([B, [B, [B, A]]] + [A, [A, [B, A]]]) \right\} \exp \left\{ \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] \right\} |\phi\rangle + O(p^5). \quad (3.17)\]
The exponent of the second exponential factor is B-terms and corresponds to \(G_B\). Note that \(G_B\) starts from the order of \(p^3\). The \(O(p^3)\) term of \(G_A\) does contribute to the moving-frame QRPA equation of \(O(p^3)\) because the first-order differential operator \(\partial_p\) is involved in the equation of collective submanifold (2.12). On the other hand, as \(\frac{p^3}{12} [A, [B, A]]\) is a B-term, it does not contribute to the moving-frame QRPA equation of \(O(p^2)\). (It contributes to the second-order canonical-variable conditions.) If there were a term of \(O(p^2)\) in \(G_B\), it would be involved in the moving-frame QRPA of \(O(p^2)\) in the form of a product with \(ip\hat{Q}_A\). However, in the case where the collective coordinate is one-dimensional and there is no pairing correlation, there can not be \(O(p^2)\) terms in \(G_B\) for the following reason. What makes B-terms at the second order is a combination of \([A\text{-term},A\text{-term}]\) or \([B\text{-term},B\text{-term}]\). The operators we have in this case are \(\hat{Q}_A\) and \(\hat{Q}_B\) only. B-terms made of them are \([\hat{Q}_A, \hat{Q}_A]\) and \([\hat{Q}_B, \hat{Q}_B]\), and they vanish. Therefore, it is trivial that there appears no \(O(p^2)\) term in
In the next subsection, we shall show that $G_B$ starts from the third order in general, also in the case with pairing correlation and/or the multi-dimensional collective coordinates.

The two factors including B-terms in Eq. (3.15) can be also rewritten as follows.

\[
\exp \left\{ \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] \right\} e^{pB} \\
= \exp \left\{ pB + \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] + \frac{1}{2} \left[ \frac{p^3}{12} [A, [B, A]], pB \right] + O(p^5) \right\} \\
= \exp \left\{ pB + \frac{p^3}{12} [A, [B, A]] + \frac{p^4}{24} [B, [A, [B, A]]] + \frac{p^5}{24} [[A, [B, A]], B] + O(p^5) \right\} \\
= \exp \left\{ pB + \frac{p^3}{12} [A, [B, A]] + O(p^5) \right\},
\]

(3.18)

Thus we can rewrite Eq. (3.17) as

\[
e^{(A+B)} |\phi\rangle \\
= \exp \left\{ pA + \frac{p^2}{2} [B, A] + \frac{p^3}{6} [B, [B, A]] + \frac{p^4}{24} ([B, [B, [B, A]]] + [A, [A, [B, A]]]) \right\} \\
\times \exp \left\{ pB + \frac{p^3}{12} [A, [B, A]] \right\} |\phi\rangle + O(p^5).
\]

(3.19)

The fifth- or even higher-order expression can be obtained similarly with use of the formulae (3.4)–(3.8). Also in that case, $G_B$ is written in terms of (multiple) commutators of $A$ and $B$ and can be rewritten as sum of $a^i a$ and constant terms. As $e^{G_B}$ gives just a phase factor, which depends on $p$ as mentioned above, it does not affect the correspondence between the higher-order operators in Approach A and commutators in Approach B listed below.

Finally we find

\[
A^{(1)} = i\hat{Q}^{(1)} = A = i\hat{Q}_A,
\]

(3.20)

\[
A^{(2)} = i\hat{Q}^{(2)} = [B, A] = [i\hat{Q}_B, i\hat{Q}_A],
\]

(3.21)

\[
A^{(3)} = i\hat{Q}^{(3)} = [B, [B, A]] = [i\hat{Q}_B, [i\hat{Q}_B, i\hat{Q}_A]],
\]

(3.22)

\[
A^{(4)} = i\hat{Q}^{(4)} = [B, [B, [B, A]]] + [A, [A, [A, B]]] \\
= [i\hat{Q}_B, [i\hat{Q}_B, [i\hat{Q}_B, i\hat{Q}_A]]] + [i\hat{Q}_A, [i\hat{Q}_A, [i\hat{Q}_A, i\hat{Q}_B]]],
\]

(3.23)

that is,

\[
\hat{Q}^{(1)} = \hat{Q}_A,
\]

(3.24)

\[
\hat{Q}^{(2)} = i[\hat{Q}_B, \hat{Q}_A],
\]

(3.25)

\[
\hat{Q}^{(3)} = [\hat{Q}_B, [\hat{Q}_A, \hat{Q}_B]],
\]

(3.26)

\[
\hat{Q}^{(4)} = -i([\hat{Q}_B, [\hat{Q}_B, [\hat{Q}_B, \hat{Q}_A]]] + [\hat{Q}_A, [\hat{Q}_A, [\hat{Q}_A, \hat{Q}_B]]]).
\]

(3.27)

Eqs. (3.25)–(3.27) can be regarded as a prescription to determine the higher-order operators. Once the B-part of $\hat{Q}$ is given, the higher-order operators are determined by the above correspondence. One prescription to determine $\hat{Q}_B$ is given in Ref. [9]. Note that the inclusion of higher-order operators in $\hat{G}$ is not equivalent to that of the B-part of the first-order operator. The B-part of the first-order operator can be always replaced by the higher-order

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A-terms defined by the above correspondence, but not vice versa. In general, the high-order operators cannot be expressed by a single operator $\hat{Q}_B$. It is easily understood by counting the numbers of degrees of freedom to identify $\hat{Q}_B$ and $\hat{Q}^{(i)}$ ($i = 1, 2, 3, \cdots$).

3.2. The case with pairing correlation
The case with pairing correlation can be treated similarly. Let us denote $(A^1, A^2) := (i\hat{Q}_A, i\hat{\Theta}_A)$, $(B^1, B^2) := (i\hat{Q}_B, i\hat{\Theta}_B)$, and $(p_1, p_2) := (p, n)$, and use the Einstein summation convention to simplify the notation below. Let us derive the expression up to $O(p^4)$. The state vector in Approach A is given by $e^{i\hat{G}(q,p,n)|\phi(q)}$ with $\hat{G}(q,p,n)$ expanded to the third order as shown in Eq. (2.2):

$$
\hat{G}(q,p,n) = p\hat{Q}^{(1)}(q) + n\hat{\Theta}^{(1)}(q) + \frac{1}{2}p^2\hat{Q}^{(2)}(q) + \frac{1}{2}n^2\hat{\Theta}^{(2)}(q) + pm\hat{X}
$$
$$
+ \frac{1}{3!}p^3\hat{Q}^{(3)}(q) + \frac{1}{3!}n^3\hat{\Theta}^{(3)}(q) + \frac{1}{2}p^2n\hat{Q}^{(2,1)}(q) + \frac{1}{2}pn^2\hat{Q}^{(1,2)}(q). \tag{2.2}
$$

We shall transform the state vector in Approach B and compare $\hat{G}_A$ with $\hat{G}$ (2.2) as we did in the previous subsection. Similarly to the previous subsection, we obtain

$$
e^{ip(\hat{Q}_A+\hat{\Theta}_A)+in(\hat{\Theta}_A+\hat{\Theta}_B)|\phi(q)} = e^{p A^i + p B^i}|\phi(q)\rangle
$$
$$
= \exp\{p_i A^i + \frac{1}{2}[p_i B^i, p_j A^j] + \frac{1}{6}[p_i B^i, [p_j B^j, p_k A^k]]\}
$$
$$
\times \exp\{-\frac{1}{12}[p_i A^i, [p_j A^j, p_k B^k]]\}e^{p_i B^i}|\phi\rangle + O(p^4)
$$
$$
= \exp\{p_i A^i + \frac{1}{2}[p_i B^i, p_j A^j] + \frac{1}{6}[p_i B^i, [p_j B^j, p_k A^k]]\}
$$
$$
\times \exp\{p_i B^i - \frac{1}{12}[p_i A^i, [p_j A^j, p_k B^k]]\}e^{ip\hat{Q}_A}|\phi\rangle + O(p^4)
$$
$$
= \exp\left\{ip\hat{Q}_A + in\hat{\Theta}_A - \frac{1}{2}p^2[\hat{Q}_B, \hat{Q}_A] - \frac{1}{2}n^2[\hat{\Theta}_B, \hat{\Theta}_A] - \frac{1}{2}pm([\hat{\Theta}_B, \hat{Q}_A] + [\hat{Q}_B, \hat{\Theta}_A])
$$
$$
- \frac{i}{6}p^3[\hat{Q}_B, [\hat{Q}_B, \hat{Q}_A]] - \frac{i}{6}n^3[\hat{\Theta}_B, [\hat{\Theta}_B, \hat{\Theta}_A]]
$$
$$
- \frac{i}{6}p^2n([\hat{Q}_B, [\hat{Q}_B, \hat{\Theta}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{Q}_A]] + [\hat{Q}_B, [\hat{\Theta}_B, \hat{Q}_A]])
$$
$$
- \frac{i}{6}pn^2([\hat{\Theta}_B, [\hat{\Theta}_B, \hat{Q}_A]] + [\hat{Q}_B, [\hat{\Theta}_B, \hat{\Theta}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{\Theta}_A]])\right\}
$$
$$
\times \exp\{-\frac{1}{12}[p_i A^i, [p_j A^j, p_k B^k]]\}e^{i(p\hat{Q}_A+n\hat{\Theta}_B)}|\phi\rangle + O(p^4)
$$

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\begin{align}
&= \exp \left\{ i p \hat{Q}_A + in \hat{\Theta}_A - \frac{1}{2} p^2 [\hat{Q}_B, \hat{Q}_A] - \frac{1}{2} n^2 [\hat{\Theta}_B, \hat{\Theta}_A] - \frac{1}{2} p n ([\hat{\Theta}_B, \hat{Q}_A] + [\hat{Q}_B, \hat{\Theta}_A]) \\
&\quad - \frac{i}{6} p^3 [\hat{Q}_B, [\hat{Q}_B, \hat{Q}_A]] - \frac{i}{6} n^3 [\hat{\Theta}_B, [\hat{\Theta}_B, \hat{\Theta}_A]] \\
&\quad - \frac{i}{6} p n^2 \left( [\hat{Q}_B, [\hat{Q}_B, \hat{\Theta}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{Q}_A]] + [\hat{Q}_B, [\hat{\Theta}_B, \hat{Q}_A]] \right) \\
&\quad - \frac{i}{6} n p^2 \left( [\hat{\Theta}_B, [\hat{\Theta}_B, \hat{Q}_A]] + [\hat{Q}_B, [\hat{\Theta}_B, \hat{\Theta}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{\Theta}_A]] \right) \right\} \\
&\quad \times \exp \{i (n \hat{Q}_B + p \hat{\Theta}_B) - \frac{1}{12} [p_i A^i, [p_j A^j, p_k B^k]] \} |\phi\rangle + O(p^4). \tag{3.28}
\end{align}

One can easily see that the exponents of the first and second factors are A-terms and B-terms, and correspond to \( i \hat{G}_A \) and to \( i \hat{G}_B \), respectively. By comparing \( \hat{G} \) \eqref{2.2} with \( \hat{G}_A \) in \eqref{3.28}, we read

\begin{align}
\hat{Q}^{(2)} &= i [\hat{Q}_B, \hat{Q}_A], \tag{3.29} \\
\hat{\Theta}^{(2)} &= i [\hat{\Theta}_B, \hat{\Theta}_A], \tag{3.30} \\
\hat{X} &= \frac{i}{2} \left( [\hat{Q}_B, \hat{\Theta}_A] + [\hat{\Theta}_B, \hat{Q}_A] \right), \tag{3.31} \\
\hat{Q}^{(3)} &= [\hat{Q}_B, [\hat{Q}_A, \hat{Q}_B]], \tag{3.32} \\
\hat{\Theta}^{(3)} &= [\hat{\Theta}_B, [\hat{\Theta}_A, \hat{\Theta}_B]], \tag{3.33} \\
\hat{Q}^{(2,1)} &= -\frac{1}{2} \left( [\hat{Q}_B, [\hat{Q}_B, \hat{\Theta}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{Q}_A]] + [\hat{Q}_B, [\hat{\Theta}_B, \hat{Q}_A]] \right), \tag{3.34} \\
\hat{Q}^{(1,2)} &= -\frac{1}{2} \left( [\hat{Q}_B, [\hat{\Theta}_B, \hat{Q}_A]] + [\hat{\Theta}_B, [\hat{Q}_B, \hat{Q}_A]] + [\hat{\Theta}_B, [\hat{\Theta}_B, \hat{Q}_A]] \right). \tag{3.35}
\end{align}

The part of \( e^{G_B} |\phi(q)\rangle \) can be rewritten as

\begin{align}
\exp \{i (p \hat{Q}_B + n \hat{\Theta}_B) - \frac{1}{12} [p_i A^i, [p_j A^j, p_k B^k]] \} |\phi\rangle \\
= \exp \left\{ -\frac{1}{12} [p_i A^i, [p_j A^j, p_k B^k]] \right\} \exp \{i (p \hat{Q}_B + n \hat{\Theta}_B) \} |\phi\rangle + O(p^4) \\
= \exp \left\{ -\frac{1}{12} [p_i A^i, [p_j A^j, p_k B^k]] \right\} |\phi\rangle + O(p^4), \tag{3.36}
\end{align}

and thus \( G_B \) is actually \( O(p_1^2) \). Above we have used that \( \hat{\Theta}_B \) does not contain a constant term, which follows from the zeroth-order canonical-variable condition,

\begin{align}
\langle \phi(q) | \hat{\Theta}(q) |\phi(q)\rangle = \langle \phi(q) | \hat{\Theta}_B(q) |\phi(q)\rangle = 0. \tag{3.37}
\end{align}

Here we have considered the case where the collective coordinate is one-dimensional. One can easily see that \( G_B \) is \( O(p^3) \) also in the multi-dimensional case. Hence, \( G_B \) does not contribute to the moving-frame HFB & QRPA equations up to \( O(p^2) \).
4. Inertial mass

As shown in Ref. [6], when the higher-order operators are included, the collective Hamiltonian is given by

\[ \mathcal{H}(q, p, n) = V(q) + \frac{1}{2}B(q)p^2 + \lambda n + \frac{1}{2}D(q)n^2, \]  

(4.1)

\[ V(q) = \langle \phi(q)|\hat{H}|\phi(q)\rangle, \]  

(4.2)

\[ B(q) = \langle \phi(q)|[\hat{H}, i\hat{Q}^{(2)}]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}^{(1)}], \hat{Q}^{(1)}]|\phi(q)\rangle, \]  

(4.3)

\[ \lambda(q) = \langle \phi(q)|[\hat{H}, i\hat{\Theta}^{(1)}]|\phi(q)\rangle, \]  

(4.4)

\[ D(q) = \langle \phi(q)|[\hat{H}, i\hat{Q}^{(2)}]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{\Theta}^{(1)}], \hat{\Theta}^{(1)}]|\phi(q)\rangle. \]  

(4.5)

The second-order operators \( \hat{Q}^{(2)} \) and \( \hat{\Theta}^{(2)} \) contribute to the inertial functions \( B(q) \) and \( D(q) \), respectively.

We compare the inertial mass \( B(q) \) in the two approaches: one is Approach A with the second-order operators defined by (3.29), and the other Approach B. We confirm that the inertial masses obtained in the two approaches coincide with each other. Substituting Eq. (3.29) into Eq. (4.8), we obtain the inertial mass \( B(q) \) as

\[ B(q) = -\langle \phi(q)|[\hat{H}, [\hat{Q}_B, \hat{Q}_A]]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_A]|\phi(q)\rangle \]

\[ = \langle \phi(q)|[\hat{Q}_B, [\hat{Q}_A, \hat{H}]]|\phi(q)\rangle + \langle \phi(q)|[\hat{Q}_A, [\hat{H}, \hat{Q}_B]]|\phi(q)\rangle \]

\[ - \langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_A]|\phi(q)\rangle \]

\[ = -\langle \phi(q)|[[\hat{H}, \hat{Q}_B], \hat{Q}_A]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_A]|\phi(q)\rangle \]

\[ + \langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_B]|\phi(q)\rangle, \]  

(4.6)

where we denoted \( \hat{Q}^{(1)} \) by \( \hat{Q}_A \) and used the Jacobi identity.

Next, in Approach B, the inertial mass \( B(q) \) is given by

\[ B(q) = -\langle \phi(q)|[[\hat{H}, \hat{Q}_A + \hat{Q}_B], \hat{Q}_A + \hat{Q}_B]|\phi(q)\rangle \]

\[ = -\langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_A]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}_B], \hat{Q}_B]|\phi(q)\rangle \]

\[ - \langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_B]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}_B], \hat{Q}_B]|\phi(q)\rangle \]  

(4.7)

Noting that \( \hat{Q}_B|\phi\rangle = 0 \), we find that both of the two approaches give the same result,

\[ B(q) = -\langle \phi(q)|[[\hat{H}, \hat{Q}_A], \hat{Q}_A]|\phi(q)\rangle - \langle \phi(q)|[[\hat{H}, \hat{Q}_B], \hat{Q}_B]|\phi(q)\rangle. \]  

(4.8)

One can easily see that such is the case with the inertial function \( D(q) \). The second term is the contribution from the second-order collective coordinate operator \( \hat{Q}^{(2)} \) in Approach A and that from the B-part of the first-order operator \( \hat{Q}_B \) in Approach B.

When the ASCC method without pairing correlation is applied to the translational motion, the second term in Eq. (4.8) vanishes for the following reason. For the translational motion, \( \partial_q V(q) = 0 \) and the moving-frame Hamiltonian \( \hat{H}_M \) reduces to the Hamiltonian \( \hat{H} \). Then, \( \hat{H}_M = \hat{H} \) does not contain A-terms in the quasiparticle representation, and the expectation value \( \langle \phi(q)|[[\hat{H}, \hat{Q}_B], \hat{Q}_A]|\phi(q)\rangle \) vanishes because \( \hat{H}, \hat{Q}_B \) consists of B-terms and normally ordered fourth-order terms. This can be understood as the reason why the correct mass was obtained without including the B-part of \( \hat{Q} \) in Ref. [27].
5. Concluding remarks

In this paper, we studied the role of $a^\dagger a$ terms in $\hat{G}$ of the state vector $e^{i\hat{G}}|\phi\rangle$ in the context of the ASCC method. We have shown that the B-part of the first-order collective coordinate operator can be rewritten as the higher-order operators consisting of only A-terms in the adiabatic expansion of $\hat{G}$. We have given the explicit expressions of the corresponding higher-order operators, which are written in terms of (multiple) commutators of the A-part and B-part of the first-order collective operators. Once the B-part of the first-order operator is given, the corresponding higher-order operators are automatically determined. Thus, this correspondence serves as a prescription to determine the higher-order collective operators in the adiabatic expansion.

As mentioned above, it is not equivalent including the B-part at the first order to including the higher-order operators of the adiabatic expansion. As shown in Ref. [6], the gauge symmetry in the ASCC method is (partially) broken by two sources, i.e., the decomposition of the equation of motion depending on the order of $p$ and the truncation of the adiabatic expansion. The gauge symmetry broken by the truncation can be conserved by including higher-order operators up to sufficiently high order. However, in the case where only the first-order operators are taken into account, the gauge symmetry of the canonical-variable conditions is broken, even if the B-part of the first-order operator is introduced.

As discussed in Ref. [6] and this paper, the higher-order operators contribute to the moving-frame QRPA equations and the inertial function, and thus they may affect the low-lying states physically. So far, we have considered the moving-frame equations up to $O(p^2)$ in the formulation of the ASCC method. When the higher-order operators are taken into account, one may need to solve the moving-frame equation(s) of $O(p^i)$ ($i \geq 3$) to determine them. However, in general, it may not be easy to solve such higher-order moving-frame equations self-consistently, and one may need an alternative way to determine the higher-order operators without solving the higher-order moving-frame equations. The correspondence we have seen in this paper gives one prescription. With this prescription, what one has to do is to give the B-part of the first-order collective operator. One prescription to determine the B-part is already given by Hinohara et al (Refs. [9–11]), and the B-part of the collective coordinate operator $\hat{Q}_B(q)$ is determined by requiring $[\hat{Q}, \hat{N}] = 0$ for the gauge symmetry of the moving-frame HFB & QRPA equations to be conserved. (In this case, the gauge symmetry of the canonical-variable conditions is not completely conserved. This should be regarded as an approximate way to conserve the gauge symmetry.)

In the case without pairing correlation, there exists no gauge symmetry (Ref. [26]). Therefore, one does not need to introduce the B-part in order to retain the gauge symmetry. However, with the B-part included, one can take into account in an effective way the contribution from the higher-order operators, which do contribute to the moving-frame QRPA equations and inertial mass. When there is no pairing correlation, $[\hat{Q}, \hat{N}] = 0$ and a prescription other than that by Hinohara et al is necessary. It would be interesting to investigate other possible prescriptions and how meaningful the contribution from the higher-order operators is. A possible prescription will be studied in a future publication. As discussed in Sect. 4, for the translational motion without pairing correlation, the correct mass can be reproduced with neither B-terms nor higher-order terms (Ref. [27]). However, for large-amplitude
collective motion in general, the higher-order terms or B-terms contribute to the inertial mass and the moving-frame (Q)RPA equations.

Acknowledgment
The author thanks K. Matsuyanagi, T. Nakatsukasa, N. Hinohara, and M. Matsuo for fruitful discussions and comments.

A. Some commutators of fermion operators
Here we show some formulae of commutators involving the second- and forth-order fermion operators, which are useful for understanding of the derivation in this paper.

\[
[a_\alpha a_\beta, a_\gamma^\dagger a_\delta^\dagger] = \delta_\alpha_\delta \delta_\beta_\gamma - \delta_\alpha_\gamma \delta_\beta_\delta - \delta_\beta_\gamma a_\delta^\dagger a_\alpha + \delta_\beta_\delta a_\gamma^\dagger a_\alpha + \delta_\alpha_\gamma a_\delta^\dagger a_\beta - \delta_\alpha_\delta a_\gamma^\dagger a_\beta, \tag{A1}
\]

\[
[a_\alpha^\dagger a_\beta, a_\gamma^\dagger a_\delta^\dagger] = \delta_\beta_\gamma a_\alpha^\dagger a_\delta^\dagger - \delta_\beta_\delta a_\alpha^\dagger a_\gamma^\dagger, \tag{A2}
\]

\[
[a_\alpha^\dagger a_\beta, a_\delta a_\gamma] = \delta_\alpha_\gamma a_\beta a_\delta - \delta_\alpha_\delta a_\beta a_\gamma, \tag{A3}
\]

\[
[a_\alpha^\dagger a_\beta, a_\gamma^\dagger a_\delta] = \delta_\delta_\gamma a_\alpha a_\beta^\dagger - \delta_\gamma_\alpha a_\beta a_\delta^\dagger. \tag{A4}
\]

\[
[a_\alpha^\dagger a_\beta a_\delta a_\gamma^\dagger a_\alpha, a_\beta^\dagger a_\nu] = -\delta_\nu_\alpha a_\mu a_\beta a_\delta a_\gamma a_\mu^\dagger - \delta_\nu_\beta a_\mu a_\alpha a_\delta a_\gamma a_\mu^\dagger - \delta_\nu_\beta a_\mu a_\gamma a_\delta a_\alpha a_\mu^\dagger - \delta_\nu_\gamma a_\mu a_\beta a_\delta a_\alpha a_\mu^\dagger, \tag{A5}
\]

\[
[a_\alpha^\dagger a_\beta a_\delta a_\gamma^\dagger a_\alpha, a_\gamma^\dagger a_\nu] = \delta_\nu_\gamma a_\mu a_\beta a_\delta a_\alpha a_\mu^\dagger + \delta_\nu_\beta a_\mu a_\gamma a_\delta a_\alpha a_\mu^\dagger - \delta_\nu_\gamma a_\mu a_\beta a_\delta a_\alpha a_\mu^\dagger + \delta_\nu_\beta a_\mu a_\gamma a_\delta a_\alpha a_\mu^\dagger, \tag{A6}
\]

\[
[a_\alpha^\dagger a_\beta a_\delta a_\gamma^\dagger a_\alpha, a_\nu^\dagger a_\gamma] = \delta_\nu_\delta a_\mu a_\beta a_\gamma a_\alpha a_\mu^\dagger + \delta_\nu_\gamma a_\mu a_\beta a_\delta a_\alpha a_\mu^\dagger - \delta_\nu_\delta a_\mu a_\gamma a_\delta a_\alpha a_\mu^\dagger - \delta_\nu_\gamma a_\mu a_\beta a_\delta a_\alpha a_\mu^\dagger, \tag{A7}
\]

From Eqs. (A5)–(A7) and their Hermitian conjugates, it is easily seen that the commutators between normally ordered forth-order terms with \(a^\dagger a\) terms give normally ordered forth-order terms.

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