Microscopic derivation of the Bohr–Mottelson collective Hamiltonian and its application to quadrupole shape dynamics

Invited Comment

Microscopic derivation of the Bohr–Mottelson collective Hamiltonian and its application to quadrupole shape dynamics

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Abstract

We discuss the nature of the low-frequency quadrupole vibrations from small-amplitude to large-amplitude regimes. We consider full five-dimensional quadrupole dynamics including three-dimensional rotations restoring the broken symmetries as well as axially symmetric and asymmetric shape fluctuations. Assuming that the time evolution of the self-consistent mean field is determined by five pairs of collective coordinates and collective momenta, we microscopically derive the collective Hamiltonian of Bohr and Mottelson, which describes low-frequency quadrupole dynamics. We show that the five-dimensional collective Schrödinger equation is capable of describing large-amplitude quadrupole shape dynamics seen as shape coexistence/mixing phenomena. We summarize the modern concepts of microscopic theory of large-amplitude collective motion, which is underlying the microscopic derivation of the Bohr-Mottelson collective Hamiltonian.

(Some figures may appear in colour only in the online journal)

1. Introduction

The subject of this review has a long history of more than 50 years. Instead of describing the whole history, we mainly discuss the recent progress in the microscopic derivation of the Bohr–Mottelson collective Hamiltonian from a viewpoint of microscopic theory of large-amplitude collective motion.

Special emphasis will be put on the development of fundamental concepts underlying the collective model. It is intended to motivate future studies by younger generations on the open problems suggested in this review.

Progress in fundamental concepts of the collective model

Vibrational and rotational motions of a nucleus can be described as time evolutions of a self-consistent mean field. This is the key idea of the collective model of Bohr and Mottelson, which opened up a new field of contemporary

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physics, *quantum many-body theory of nuclear collective dynamics*. The central theme in this field is to describe the single-particle and collective motions in finite quantum systems in a unified manner. After the first paper in 1952 [1], the basic concepts underlying the unified model of Bohr and Mottelson have been greatly developed. The progress achieved until 1975 is summarized in their textbook [2, 3] and Nobel lectures in 1975 [4, 5].

The unified description of complementary concepts such as the collective and single-particle motions in nuclei possess a great conceptual significance in theoretical physics in general. Needless to say, understanding the coexistence of complementary concepts (such as particle-wave duality) constitutes a central theme in theoretical physics. The physics underlying the Bohr-Mottelson unified model is deep and wide. Among the rich subjects pertinent to this model, we select and focus on the subject of microscopic derivation of the Bohr–Mottelson collective Hamiltonian: that is, we concentrate on the collective Hamiltonian H_{coll} in the unified model Hamiltonian

$$H_{uni} = H_{part} + H_{coll} + H_{coupl}, \tag{1}$$

where H_{part} describes the single-particle motions in a self-consistent mean field and H_{coupl} is the coupling Hamiltonian generating the interplay between the single-particle motions and collective motions. Specifically, we focus on the low-frequency quadrupole collective motions and call the quadrupole collective Hamiltonian *the Bohr–Mottelson collective Hamiltonian*. We discuss its generalized form as described in their textbook, where the mass parameters (collective inertial masses) appearing in the collective Hamiltonian are not constant but functions of deformation variables. In our point of view, it is desirable to adopt this general definition of the Bohr–Mottelson collective Hamiltonian in order to respect the conceptual progress achieved by collaborative efforts of many researchers worldwide during 1952 to 1975. In this connection, we would like to quote a sentence from their Nobel lectures: 'The viewpoints that I shall try to summarize gradually emerged in this prolonged period' [4].

Brief remarks about the history

Soon after the introduction of the collective model by Bohr and Mottelson in 1952–1953, attempts to formulate a microscopic theory of the collective model started. This became one of the major subjects of theoretical physics in the 1950's and greatly stimulated to open up a new fertile field, the nuclear many-body theory, to derive the collective phenomena starting from the nucleon degrees of freedom constituting the nucleus.

The major approach at that time was to introduce collective coordinates explicitly as functions of coordinates of individual nucleons and separate collective shape degrees of freedom from the rest. From among numerous papers, we refer Tomonaga theory [6, 7] and a similar work by Marumori *et al* [8] as representative examples. In spite of their conceptual significance, however, it turned out that these approaches fail for description of low-energy modes of shape fluctuations. The main reasons of this failure are 1) the assumption that the collective coordinates are given by local one-body operators (such as mass-quadrupole operators) leads to the inertial masses of irrotational fluids [3], in contradiction to experimental data which suggest that the inertial masses of the first excited quadrupole vibrational states are much larger than the irrotational masses, and, as we shall discuss in this review, 2) the quantum shell structure of the single-particle motion in the self-consistent mean field and the pairing correlations among nucleons near the Fermi surface play essential roles in the emergence of the low-frequency quadrupole modes of excitation in nuclei. Interestingly, it became clear much later that the Tomonaga theory is applicable to high-frequency giant resonances, rather than the originally intended low-frequency quadrupole vibrations [9–12]. One of the important lessons we learned from these early attempts is that, it is not trivial at all to define microscopic structure of collective coordinates appropriate to low-energy shape vibrations.

In 1960, the quasiparticle random-phase approximation (QRPA) based on the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity was introduced in nuclear structure theory [13, 14]. This was a starting point of the modern approach to determine, on the basis of the time-dependent mean-field picture, the microscopic structures of the collective coordinates and their conjugate momenta without postulating them by physical intuition.

After the initial success of the BCS+QRPA approach for small amplitude oscillations in the 1960's and its extensions by boson expansion methods [15] in succeeding years, attempts to construct a microscopic theory of large-amplitude collective motion (LACM) started in mid 1970's [16]. At that time, time-dependent Hartree-Fock (TDHF) calculations for heavy-ion collisions also started [17]. These attempts introduced collective coordinates as parameters specifying the time evolution of the self-consistent mean field, instead of explicitly defining them as functions of coordinates of individual nucleons. *This was a historical turning point in the basic concept of collective coordinate theory*: in these new approaches, it is unnecessary to define *global* collective operators as functions of coordinates of individual nucleons. In this paper, we shall discuss the basic ideas of such modern approaches and describe how to derive, in a microscopic way, the quadrupole collective Hamiltonian of Bohr and Mottelson on the basis of the moving self-consistent mean-field picture.

Contents of this review

Our major aim is to review the progress in the fundamental concept of '*collective motion, collective coordinates, and collective momenta*' which have been acquired during the long-term efforts of many researchers to give a *microscopic foundation* of the Bohr–Mottelson collective model. Special emphasis will be put on the developments during the 40 years after the Nobel Prize of 1975 to Bohr, Mottelson, and Rainwater [4, 5, 18]. Although we focus on the quadrupole collective motions, the techniques and underlying concepts are general and applicable to other collective motions at zero temperature as well, including octupole collective motions

[19] and various kinds of many-body tunneling phenomena of finite quantum systems, such as spontaneous fissions [20] and subbarrier fusion reactions [21].

In section 2, we summarize the basic properties of the low-frequency quadrupole collective excitations.

In section 3, the Bohr–Mottelson collective Hamiltonian is recapitulated.

In section 4, we discuss the basics of the microscopic theory of nuclear collective motion. We start from the QRPA as a small amplitude approximation of the time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory, which is an extension of the TDHF to superfluid (superconducting) systems taking into account the pairing correlations. (We use the terms, superfluidity and superconductivity, in the same meaning.) We then discuss how to extend the basic ideas of the QRPA to treat LACM as seen in shape coexistence/mixing phenomena widely observed in nuclear chart.

In section 5, we introduce the *local* QRPA method and describe how to derive the Bohr–Mottelson collective Hamiltonian in a microscopic way on the basis of the TDHFB theory.

In section 6, we present an illustrative example of numerical calculation for a shape coexistence/mixing phenomenon.

In section 7, we briefly remark on other microscopic approaches to derive the Bohr–Mottelson collective Hamiltonian.

In section 8, we review fundamentals of the microscopic theory of LACM. The basic concepts underlying the adiabatic self-consistent coordinate (ASCC) method and the local QRPA method will be summarized.

In section 9, we discuss future outlook. Possible extensions to new regions of nuclear structure dynamics will be suggested.

In section 10, we conclude this review emphasizing future subjects awaiting applications and further extensions of the collective Hamiltonian approach.

This review is an extended version of the short article published quite recently [22][9] and provides more detailed discussions on the basic ideas and fundamental concepts in the microscopic derivation of the Bohr–Motteson collective Hamiltonian. As we develop the basic concepts of collective motion on the basis of the time-dependent self-consistent mean-field theory, we refer to the review by Próchniak and Rohoziński [23] for other microscopic approaches and a detailed account of the techniques of treating the Bohr–Motteson collective Hamiltonian. For the analysis of a wide variety of quadrupole collective phenomena in terms of various models related to the Bohr–Motteson collective Hamiltonian, we refer to the recent review by Frauendorf [24]. Because our major aim is the microscopic derivation of the collective inertial masses, we leave out discussions on phenomenological models reviewed by Cejnar, Jolie, and Casten [25], where the inertial masses are treated as parameters.

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[9] Accordingly, there is some similarity between sections 2.3, 4.3, 7.1, 7.2 and 8.1, and reference [22].

2. Low-frequency quadrupole collective motions

In this section, we first summarize the basic properties of the low-frequency quadrupole collective excitations and then introduce the Bohr–Mottelson collective Hamiltonian.

2.1. Nature of the first excited 2^+ modes

Except for doubly magic nuclei in the spherical *j-j* coupling shell-model picture, the first excited states in almost all even-even nuclei (consisting of even numbers of neutrons and protons) have angular momentum two with positive parity ($I^\pi = 2^+$). Systematics of experimental data for these first 2^+ states shows that their excitation energies are very low in comparison to the energy gap 2Δ that characterizes nuclei with superfluidity (superconductivity), and that their electric quadrupole ($E2$) transition probabilities to the 0^+ ground states are very large compared to those associated with single-particle transitions. For nuclei whose mean fields are spherical, the first excited 2^+ states can be characterized as collective vibrations of finite quantum systems with superfluidity [26]. They are genuine quantum vibrations that are essentially different from surface oscillations of a classical liquid drop. In other words, the superfluidity and shell structure play indispensable roles in their emergence.

In axially deformed nuclei, whose mean fields break the rotational symmetry but conserve the axial symmetry, the first excited 2^+ state can be interpreted as quantum rotational states whose mean fields are uniformly rotating about an axis perpendicular to the symmetry axis. Regular rotational spectra appear when the amplitudes of quantum shape fluctuation are smaller than the magnitude of equilibrium deformation. Nuclei that have very small ratios, $E(2^+)/2\Delta$, of the 2^+ excitation energies to the energy gaps, (less than, as a rule of thumb, 0.1) belong to this category. The rotational moments of inertia evaluated from $E(2^+)$ are found to be about half of the rigid-body value. This deviation of the moment of inertia from the rigid-body value is one of the most clear evidences that the ground states of nuclei are in a superfluid phase. Large portion of nuclei exhibiting regular rotational spectra have the prolate (elongated spheroidal) shape. Origin of prolate shape dominance over oblate (flattened spheroidal) shape is an interesting fundamental problem (prolate-oblate asymmetry) [27, 28].

When the mean field of the ground state conserves the rotational symmetry, the first excited 2^+ state have been regarded as quadrupole vibrational excitation of a spherical shape with frequencies lower than the energy gap. They are more lowered as the numbers of neutrons and/or protons deviate from the spherical magic numbers. Eventually the vibrational 2^+ states turn into the rotational 2^+ states discussed above. Thus, one may regard low-lying quadrupole vibrations as soft modes of the quantum phase transition that breaks the spherical symmetry of the mean field. In finite quantum systems such as nuclei, however, this phase transition takes place rather gradually for a change of nucleon number, creating a wide transitional region in the nuclear chart. Low-energy excitation spectra of these nuclei exhibit

intermediate characters between the vibrational and rotational ones. Softer the mean field toward the quadrupole deformation, larger the amplitude and stronger the nonlinearity of the vibration.

2.2. Quantum shape transitions in nuclei

Why are nuclei deformed?

As is well known, the equilibrium shape of the classical liquid drop is spherical. When it rotates, it becomes oblate due to the effect of the centrifugal force. In contrast, most nuclei favor the prolate shape, except for nuclei situated near the closed shells of the j-j coupling shell model (whose proton number Z and/or neutron number N are near the spherical magic numbers). As we shall discuss later, even such nuclei whose ground state are spherical, deformed states appear in their excited states. The appearance of the deformed shapes in nuclei is due to quantum-mechanical shell effects associated with the single-particle motions in the mean field. Let us first start with what this means.

Deformable mean field and deformed shell structure

It is well known from the success of the j-j coupling shell model [29] that the concept of *single-particle motion in a mean field* holds in nuclear structure. Differently from electrons in an atom, the shell-model potential is collectively generated by all nucleons constituting the nucleus. In other words, the single-particle picture of the shell model emerges as a result of collective effects of all nucleons generating the self-consistent mean field. It implies that the single-particle potential of the nucleus is a deformable quantum object [4, 5, 18]. In fact, as we shall discuss below, the self-consistent mean field possesses *collective predisposition* to generate a variety of vibrational and rotational modes of excitation.

Because the nucleus is a finite quantum system, the single-particle states form a shell structure. The spherical shell structure in the j-j coupling shell model gradually changes with the growth of deformation in the mean field and generates *deformed shell structures* and *deformed magic numbers* at certain deformed shapes [30, 31]. The gain of binding energies associated with deformed magic numbers appearing at various deformed shapes for certain combinations of (Z, N) stabilizes the deformed shape. For instance, for a nucleus whose (Z, N) are far from the spherical magic numbers but near the deformed magic numbers associated with a certain prolate shape, it is energetically favorable for this nucleus to take the prolate shape. This is the major origin of the appearance of a rich variety of deformed shapes in nuclei. The deformed shell structure effects are clearly seen in the appearance of superdeformed nuclei having prolate shapes with the axis ratio about 2:1 [32, 33].

The shell structures can be defined, in a general concept, as regularly oscillating gross structures in the distribution of single-particle-energy eigenvalues [3, 20, 34]. It is very important to notice that those structures are quite sensitive to
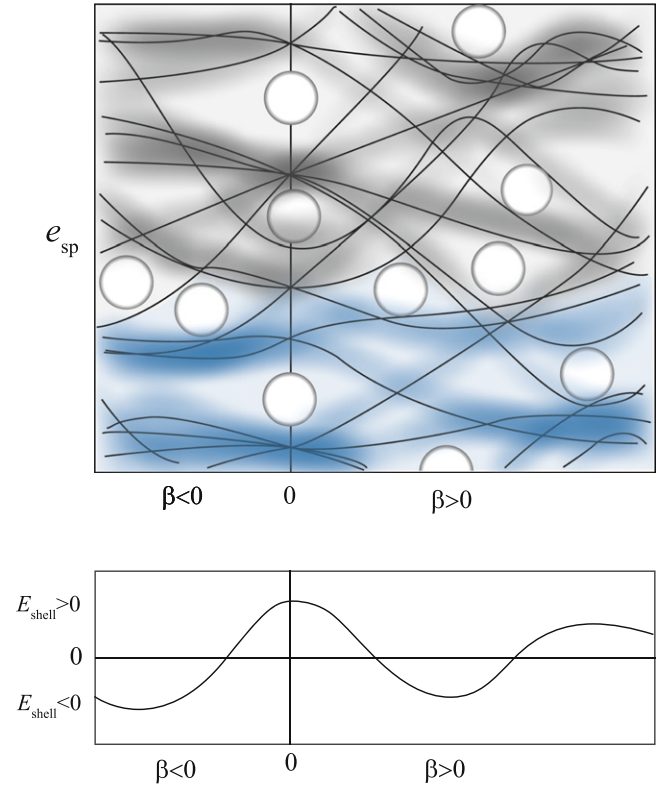
Figure 1. Illustration of shell structure and its change with increasing deformation. The level densities are drawn as functions of the single-particle energy e_{sp} and the deformation parameter β. Positive and negative β corresponds to the prolate and oblate shapes, respectively. Regions with high- and low-level densities are shown by shading (shade for high and light for low). Occupied and unoccupied regions are indicated by blue and gray shades, respectively. The circles indicate appearance of (spherical and deformed) magic numbers. The contribution of the shell structure to the binding energy (shell structure energy) for a fixed neutron (or proton) number changes as a function of β. Generally, it exhibits an oscillating pattern. This conceptual figure is drawn on the basis of the realistic calculation [35] by using the deformed Wood-Saxon potential for ^{80}Sr.

the shape of the mean-field potential. The oscillation pattern changes following the variation of the deformation parameter. Figure 1 illustrates this concept.

Although one can easily calculate single-particle-energy eigenvalues for a given shape of the mean field, such a quantum-mechanical calculation does not explain the origins of the appearance of such gross structures. For a deeper understanding of the origins, one can make use of the semi-classical theory of (deformed) shell structure. For further discussions on this subject, we refer to the textbook by Brack and Bhaduri [34] and the review by Arita [28].

Emergence of collective rotational motions restoring broken symmetries

The central concept of the BCS theory of superconductivity is spontaneous gauge-symmetry breaking and emergence of associated collective modes. The massless collective modes that restore the broken symmetry are called Anderson–

Nambu–Goldstone (ANG) modes [26, 36, 37]. Nuclear rotations are manifestations of this dynamics in finite quantum systems, as pointed out by Bohr and Mottelson [3, 4]; they are ANG modes restoring the spherical symmetry broken by the self-consistently generated mean field.

The spontaneous breaking of the spherical symmetry (deformation) in the self-consistent mean field enables us to define the orientation degrees of freedom that specify the orientation of the body-fixed (intrinsic) frame relative to the laboratory frame. The body-fixed frame can be defined as a principal-axis frame of the deformed self-consistent mean field generated by all nucleons constituting the nucleus. It is important to keep in mind that *the spontaneous breaking of symmetry can be hidden in finite quantum systems such as nuclei*; that is, the experimental measurements probe the states in the laboratory frame, which preserves the symmetries of the original Hamiltonian. Thus, nuclear rotations may be viewed as rotational motions of the self-consistent mean field relative to the laboratory frame.

'The spontaneous breaking of the rotational symmetry in the self-consistent mean field' is the key concept to a unified description of the single-particle motion and the collective rotational motion. With this concept we can generalize the notion of the single-particle motion in a spherical mean field to that in a deformed mean field. At the same time the deformed mean field is rotating to restore the broken symmetry. Thus, extension of the concept of single-particle excitation with spontaneous breaking of the symmetry and appearance of new collective excitation restoring the broken symmetry are *dual concepts* that underline the quantum many-body theory of nuclear structure. We shall discuss in section 8 how to generalize this concept of *particle-collective duality* to slowly vibrating mean fields where the time scales of the single-particle and vibrational motions are separated in a good approximation.

Excitation spectra in the transitional region

The low-frequency quadrupole vibrations can be regarded as soft modes of the quantum phase transition generating equilibrium deformations in the mean field. In nuclei situated in the transitional region from spherical to deformed, the amplitudes of quantum shape fluctuation about the equilibrium shape increase significantly. The large shape fluctuations occur also in weakly deformed nuclei where the binding-energy gains due to the symmetry breaking are comparable in magnitude to the vibrational zero-point energies. Such transitional situations are abundant in nuclear chart and those transitional nuclei show quite rich excitation spectra (see e.g., [38]). Existence of wide transitional regions is a characteristic feature of finite quantum systems and provides an invaluable opportunity to investigate the process of the quantum phase transition through the change of quantum spectra with nucleon number. A detailed account of instability phenomena and strong anharmonicity effects in the transitional region is given in chapter 6 of [3].

2.3. Quadrupole collective dynamics

Before introducing the Bohr–Mottelson collective Hamiltonian, we add some remarks on quadrupole collective phenomena that await its application.

Interplay of low-frequency shape fluctuations and rotational motions

In finite quantum systems such as nuclei, the rotational ANG modes may couple with quantum shape-fluctuation modes rather strongly. For example, even when the self-consistent mean field acquires a deep local minimum at a finite value of β in this direction, the deformation energy surface may be flat in the γ direction. In this case, the nucleus may exhibit a large-amplitude shape fluctuation in the γ degree of freedom. (Here, β and γ represent the magnitudes of axial and triaxial quadrupole deformations.) Actually, such a situation, called γ soft, is widely observed in experiments. In nuclei which preserve the axial symmetry, the quantum-mechanical collective rotation about the symmetry axis is forbidden. Once the axial symmetry is dynamically broken by quantum shape fluctuations, however, the rotational degrees of freedom about three principal axes are all activated. As a consequence, the rotational spectra in such γ-soft nuclei do not exhibit a simple $I(I + 1)$ pattern of an axial rotor. Such an interplay of the shape-fluctuation and rotational modes may be regarded as a characteristic feature of finite quantum systems and provides an invaluable opportunity to investigate the process of the quantum phase transition through analysis of quantum spectra.

Thus, we need to treat the two kinds of collective modes (symmetry-restoring ANG modes and quantum shape fluctuation modes) in a unified manner to describe low-energy excitation spectra of nuclei.

Quantum shape fluctuations and shape coexistence

When different kinds of quantum eigenstates associated with different shapes coexist in the same energy region, we call them '*shape coexistence phenomena*.' This situation is realized when shape mixing due to tunneling motion is weak and collective wave functions retain their localizations about different equilibrium shapes. In contrast, when the shape mixing is strong, large-amplitude shape fluctuations (*delocalization* of the collective wave functions) extending to different local minima may occur.

When a few local minima of the mean field with different shapes appear in the same energy region, LACM tunneling through potential barriers and extending between local minima may take place. These phenomena may be regarded as a kind of macroscopic quantum tunneling. Note that the barriers are not given by external fields but are self-consistently generated as a consequence of quantum dynamics of the many-body system. Quantum spectra of low-energy excitation that needs such concepts have been observed in almost all regions of the nuclear chart [39–41].

3. Bohr–Mottelson collective Hamiltonian

Bohr and Mottelson introduced the five-dimensional (5D) quadrupole collective Hamiltonian describing the quadrupole vibrations and rotations in a unified manner [3]. It is written as

$$H_{\text{coll}} = T_{\text{vib}} + T_{\text{rot}} + V(\beta, \gamma), \tag{2}$$

$$T_{\text{vib}} = \frac{1}{2} D_{\beta\beta}(\beta, \gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta, \gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2}D_{\gamma\gamma}(\beta, \gamma)\dot{\gamma}^2, \tag{3}$$

$$T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} \mathcal{J}_k(\beta, \gamma)\dot{\varphi}_k^2. \tag{4}$$

Here, φ_k are components of the rotational angle on the three intrinsic axes. The quadrupole deformations (β, γ) and the rotational angles φ_k are treated as dynamical variables, and $(\dot{\beta}, \dot{\gamma})$ and $\dot{\varphi}_k$ represent their time derivatives. The $\dot{\varphi}_k$ are called angular velocities. We shall define in section 5 the (β, γ) deformations through the expectation values of the quadrupole operators with respect to the time-dependent mean-field states. The quantities $(D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma})$ appearing in the kinetic energies of vibrational motion, T_{vib}, represent inertial masses of the vibrational motion. They are functions of β and γ. The quantities $\mathcal{J}_k(\beta, \gamma)$ in the rotational energy T_{rot} represent the moments of inertia with respect to the intrinsic (body-fixed) axes. The intrinsic axes may be defined by the principal axes of the body-fixed frame that is attached to the instantaneous shape of the time-dependent mean field. The term, $V(\beta, \gamma)$, represents the potential energy as a function of β and γ.

The Bohr–Mottelson collective Hamiltonian (2) is often referred to in relation to the liquid drop model. It should be emphasized, however, that, the analogy with the *classical* liquid drop is irrelevant to low-frequency quadrupole collective motions. Already in the 1950's, it was recognized that the nucleus is 'an unusual idealized *quantum* fluid' and 'one is dealing with a most interesting new form of matter' [42]. Indeed, as discussed in section 2, most of nuclei may be regarded as a superfluid of extremely small size (with a radius of a few femtometer), and the nature of nuclear deformation is essentially different from that of surface shape oscillations of the classical liquid drop; that is, the nuclear deformation is associated with quantum shell structure and spontaneous breaking of the spherical symmetry in the self-consistent mean field.

The form of the collective Hamiltonian (2) is quite general and applicable to various finite many-body systems, but the specific dynamical properties of the system of interest are revealed by the values and the (β, γ)-dependence of the collective inertia masses $(D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma}, \mathcal{J}_k)$ as well as the potential energy $V(\beta, \gamma)$. For understanding the dynamical properties of the nucleus, therefore, it is imperative to derive these quantities in a microscopic way and compare with what experimental data indicate. We shall show in this review that the collective Hamiltonian (2) with the collective inertial masses and the potential energy microscopically evaluated on the basis of the moving superfluid mean-field picture

describes very well the low-frequency quadrupole collective dynamics of the nucleus. Furthermore, quantum correlations beyond the mean field are nicely described by quantizing the collective variables that govern the time evolution of the self-consistent mean field.

The classical Hamiltonian (2) is given in terms of the five curvilinear coordinates (β, γ, and the three Euler angles which are connected with φ_k by a linear transformation) and their time derivatives. For quantization in curvilinear coordinates, we can adopt the so-called Pauli prescription [43]. (For convenience of readers, we recapitulate this prescription in appendix A.) We shall discuss on its foundation in section 5 describing the microscopic derivation of the Bohr–Mottelson collective Hamiltonian. The quantized 5D quadrupole collective Hamiltonian takes the following form:

$$\hat{H}_{\text{coll}} = \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + V(\beta, \gamma). \tag{5}$$

Here, the vibrational kinetic energy term $\hat{T}_{\text{vib}}$ is given by

$$\hat{T}_{\text{vib}} = -\frac{1}{2\sqrt{WR}} \left\{ \frac{1}{\beta^4} \left[\frac{\partial}{\partial\beta} \left(\beta^2 \sqrt{\frac{R}{W}} D_{\gamma\gamma} \frac{\partial}{\partial\beta} \right) \right. \right.$$
$$\left. - \frac{\partial}{\partial\beta} \left(\beta^2 \sqrt{\frac{R}{W}} D_{\beta\gamma} \frac{\partial}{\partial\gamma} \right) \right]$$
$$+ \frac{1}{\beta^2 \sin 3\gamma} \left[-\frac{\partial}{\partial\gamma} \left(\sqrt{\frac{R}{W}} \sin 3\gamma D_{\beta\gamma} \frac{\partial}{\partial\beta} \right) \right.$$
$$\left. \left. + \frac{\partial}{\partial\gamma} \left(\sqrt{\frac{R}{W}} \sin 3\gamma D_{\beta\beta} \frac{\partial}{\partial\gamma} \right) \right] \right\}, \tag{6}$$

and the rotational energy term $\hat{T}_{\text{rot}}$ is given by

$$\hat{T}_{\text{rot}} = \sum_{k=1,2,3} \frac{\hat{I}_k^2}{2\mathcal{J}_k(\beta, \gamma)} \tag{7}$$

with $\hat{I}_k$ denoting three components of the angular momentum operator with respect to the intrinsic axes. In this paper, we use the unit with $\hbar = 1$. In the above equations,

$$\beta^2 W(\beta, \gamma) = D_{\beta\beta}(\beta, \gamma)D_{\gamma\gamma}(\beta, \gamma) - D_{\beta\gamma}^2(\beta, \gamma), \tag{8}$$

$$R(\beta, \gamma) = D_1(\beta, \gamma)D_2(\beta, \gamma)D_3(\beta, \gamma), \tag{9}$$

and $D_k(\beta, \gamma)$ ($k = 1, 2, 3$) are the rotational inertial functions related to the moments of inertia by

$$\mathcal{J}_k(\beta, \gamma) = 4\beta^2 D_k(\beta, \gamma)\sin^2(\gamma - 2\pi k/3). \tag{10}$$

If all inertial masses ($D_{\beta\beta}, D_{\gamma\gamma}\beta^{-2}, D_1, D_2, D_3$) are replaced by a common constant D and $D_{\beta\gamma}$ is ignored, the above $\hat{T}_{\text{vib}}$ is reduced to

$$\hat{T}_{\text{vib}} = -\frac{1}{2D} \left(\frac{1}{\beta^4} \frac{\partial}{\partial\beta} \beta^4 \frac{\partial}{\partial\beta} + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial\gamma} \sin 3\gamma \frac{\partial}{\partial\gamma} \right). \tag{11}$$

Such a drastic approximation may be valid only for small-amplitude vibrations about a spherical HFB equilibrium. The need to go beyond this simplest approximation for the inertia masses has been pointed out [3]. For recent experimental data

and phenomenological analyses of this problem, we refer [44, 45] and references therein.

The collective Schrödinger equation is

$$[\hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + V(\beta, \gamma)]\Psi_{\alpha IM}(\beta, \gamma, \Omega) = E_{\alpha I}\Psi_{\alpha IM}(\beta, \gamma, \Omega). \tag{12}$$

The collective wave function in the laboratory frame, $\Psi_{\alpha IM}(\beta, \gamma, \Omega)$, is a function of β, γ, and a set of three Euler angles Ω. It is specified by the total angular momentum I, its projection onto the z-axis in the laboratory frame M, and α that distinguishes the eigenstates possessing the same values of I and M. With the rotational wave function $\mathcal{D}^I_{MK}(\Omega)$, they are written as

$$\Psi_{\alpha IM}(\beta, \gamma, \Omega) = \sum_{K=\text{even}} \Phi_{\alpha IK}(\beta, \gamma)\langle\Omega|IMK\rangle, \tag{13}$$

where

$$\langle\Omega|IMK\rangle = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}}[\mathcal{D}^I_{MK}(\Omega) + (-)^I\mathcal{D}^I_{M,-K}(\Omega)]. \tag{14}$$

The vibrational wave functions in the body-fixed frame, $\Phi_{\alpha IK}(\beta, \gamma)$, are normalized as

$$\int d\beta d\gamma \sqrt{G(\beta, \gamma)}|\Phi_{\alpha I}(\beta, \gamma)|^2 = 1, \tag{15}$$

where

$$|\Phi_{\alpha I}(\beta, \gamma)|^2 \equiv \sum_{K=\text{even}} |\Phi_{\alpha IK}(\beta, \gamma)|^2, \tag{16}$$

and the volume element is given by $\sqrt{G(\beta, \gamma)}\,d\beta d\gamma$ with

$$G(\beta, \gamma) = 4\beta^8 W(\beta, \gamma)R(\beta, \gamma)\sin^2 3\gamma. \tag{17}$$

Thorough discussions of symmetries of the collective wave functions and the boundary conditions for solving the collective Schrödinger equation are given in [3, 23, 46, 47].

Inserting (13) into the collective Schrödinger equation (12), we obtain the eigenvalue equation for vibrational wave functions

$$[\hat{T}_{\text{vib}} + V(\beta, \gamma)]\Phi_{\alpha IK}(\beta, \gamma)$$
$$+ \sum_{K'=\text{even}} \langle IMK|\,\hat{T}_{\text{rot}}\,|IMK'\rangle\Phi_{\alpha IK'}(\beta, \gamma)$$
$$= E_{\alpha I}\Phi_{\alpha IK}(\beta, \gamma). \tag{18}$$

Solving this equation, we obtain quantum spectra and collective wave functions. It is then straightforward to calculate electromagnetic transition probabilities among collective excited states. We recapitulate some basic formulae in appendix B.

Historical note

The simple expression (11) with a constant mass parameter D for the vibrational kinetic energy is valid for harmonic vibrations about a spherical equilibrium point of the mean field, as derived in the 1952 paper [1] by transforming the collective Hamiltonian for harmonic shape vibrations to the body-fixed frame defined as the instantaneous principal axis frame of the vibrating density distribution. Combined with the

irrotational mass parameter D_{irrot} resulting from modeling the vibrational flow by that of the irrotational fluid, it is sometimes referred to the Bohr liquid drop Hamiltonian. It should be emphasized, however, that the inadequacy of the irrotational fluid model for the low-frequency quadrupole excitations was recognized from early on.

In the preface to the second edition (March 1, 1957) of the 1953 paper [48], Bohr and Mottelson wrote: 'As a first orientation, one attempted to employ for these parameters obtained from a liquid drop model, but already the early analysis of various nuclear properties showed the limitation of this comparison. The inadequacy of the liquid drop estimates was especially clearly brought out by the comparison of the nuclear moment of inertia with the deformations deduced from the rate of the electric quadrupole rotational transitions.' 'An improved understanding of the collective nuclear properties has come from the efforts to derive these directly from the motion of the nucleons; this analysis has revealed the important influence of the nuclear shell structure on the collective motion.' 'The inadequacy of the liquid drop model with irrotational flow implies that the collective coordinates considered as functions of the nucleonic variables are of more general form than (II.2) , ...' ((II.2) is the famous definition of the collective parameters $\alpha_{\lambda,\mu}$ in terms of the polar coordinates of individual particles).

Indeed, if we assume that a collective coordinate corresponds to a *local* one-body operator in the coordinate space (such as the mass-multipole operator), we obtain a collective mass parameter associated with an irrotational velocity field (see p. 510 of [3] and [49]).

Illustration of typical situations

Figure 2 illustrates typical patterns of the collective potential energy surface $V(\beta, \gamma)$; these are classified according to the location of the local minimum. In the case that the potential energy $V(\beta, \gamma)$ has a deep minimum at a finite value of β and $\gamma = 0°$ (or $\gamma = 60°$), a regular rotational spectrum with the $I(I+1)$ pattern may appear. In addition to the ground band, we can expect the β and γ bands to appear, where vibrational quanta with respect to the β and γ degrees of freedom are excited. Detailed investigations on the γ-vibrational bands over many nuclei have revealed, however, that they usually exhibit significant anharmonicities (non-linearlities) [50]. Situations for the β-vibrational bands are quite mysterious. Recent experimental data indicate the need for a radical review of their characters [41]. We shall discuss on this problem in section 9. The coexistence of two local minima at oblate and prolate shapes is a typical example of shape coexistence. Experimental data indicate that the potential barrier between the two minima is, in many cases, low and the collective wave functions extend over the oblate and prolate regions through quantum tunneling (shape mixing). Also, there are many nuclei exhibiting intermediate features between the large-amplitude collective vibrations associated with the oblate-prolate shape coexistence and the rotational motions associated with the triaxial shape. We present in appendix C a simple model that may be useful to understand several interesting limits of triaxial deformation dynamics in a
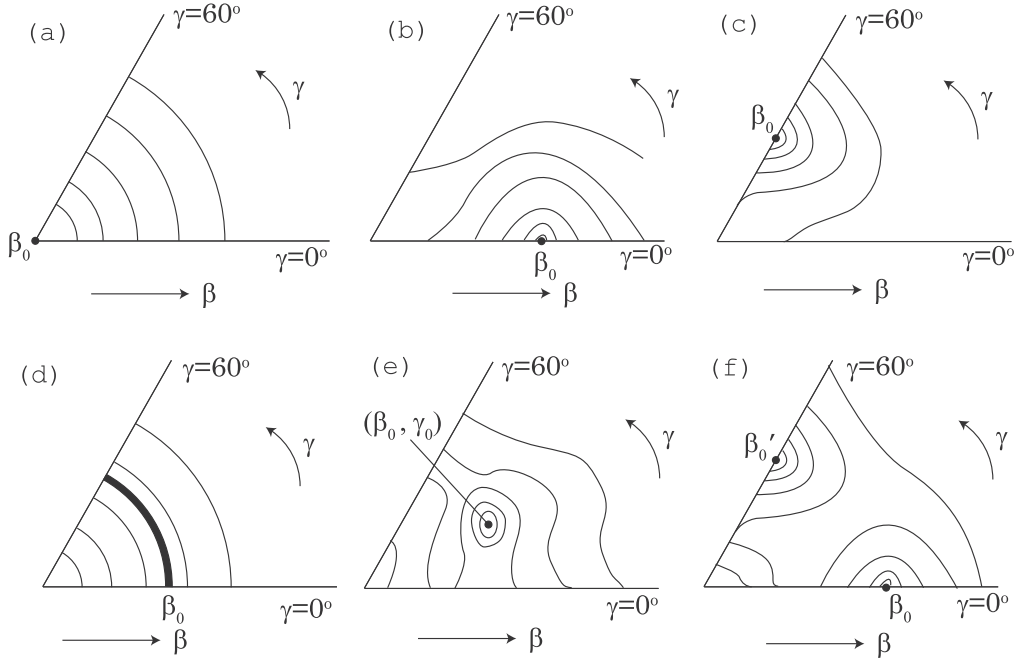
Figure 2. Illustration of typical patterns of the collective potential-energy surface $V(\beta, \gamma)$, classified according to the location of the local minimum point(s) (β_0, γ_0): (a) spherical, (b) prolate, (c) oblate, (d) $\beta_0 \neq 0$ in the β direction but the potential is flat with respect to γ (so-called γ-unstable situation [51]), (e) triaxial, and (f) coexistence of the oblate and prolate minima.

unified perspective, including the axially symmetric rotor model, the γ-unstable model [51], the triaxial rigid rotor model [52], and an ideal situation of the oblate-prolate shape coexistence.

4. QRPA and its extensions

In this section, we summarize the elementary concepts in microscopic theory of nuclear collective motion [53–57]. We adopt the time-dependent mean-field picture. The main reason is that it provides a basis for a clear understanding of the correspondence between the quantum and classical aspects of the nuclear collective motions. Furthermore, this approach enables us to microscopically derive the collective coordinates and momenta on the basis of the time-dependent variational principle.

We shall start from small-amplitude vibrations about the spherical equilibrium shape and then go to large-amplitude regime, where we need to consider full 5D quadrupole collective dynamics including three-dimensional (3D) rotations restoring the broken symmetries as well as axially symmetric and asymmetric shape fluctuations.

4.1. Collective motion as moving self-consistent mean field

Let us consider even-even nuclei whose ground states consist of correlated nucleon pairs occupying time-reversal conjugate single-particle states. The Hartree–Fock–Bogoliubov (HFB) method is a generalized mean-field theory treating the formation of the HF mean field and superfluidity (nucleon pair condensate) in a self-consistent manner [54, 55, 57, 58], and

yields the concept of quasiparticles as single-particle excitation modes in the presence of the pair condensate. Bohr and Mottelson opened the way to a unified understanding of single-particle and collective modes of motion of nuclei by introducing the concept of moving self-consistent mean field [3–5]. The time-dependent extension of the HFB mean field, called the time-dependent HFB (TDHFB) theory, is suitable to formulate their ideas [47, 54, 55, 57].

It is well known that the time evolution of the TDHF state vectors can be written as time-dependent unitary transformations (see e.g., [59, 60]). It is called the generalized Thouless theorem. Adapting this theorem for nuclei with superfluidity, the TDHFB state vector $|\phi(t)\rangle$ may be written as [61]:

$$|\phi(t)\rangle = e^{i\hat{G}(t)}|\phi(t=0)\rangle = e^{i\hat{G}(t)}|\phi_0\rangle, \quad (19)$$

$$i\hat{G}(t) = \sum_{(kl)} \{g_{kl}(t)a_k^\dagger a_l^\dagger - g_{kl}^*(t)a_l a_k\}, \quad (20)$$

where the HFB ground state $|\phi_0\rangle$ is a vacuum for quasiparticles $(a_k^\dagger, a_l)$,

$$a_k|\phi_0\rangle = 0, \quad (21)$$

with the suffix k distinguishing different quasiparticle states. (See appendix D for more details.) The functions $g_{kl}(t)$ in the one-body operator $\hat{G}(t)$ is determined by the time-dependent variational principle

$$\delta \langle \phi(t)| \left(i\frac{\partial}{\partial t} - \hat{H} \right) |\phi(t)\rangle = 0. \quad (22)$$

The TDHFB states can be regarded as generalized coherent states, which are a kind of wave packets and cover the whole Hilbert space of a given Fermion many-body system [62, 63].

We call this space 'the TDHFB phase space.' It may also be called 'the TDHFB symplectic manifold' [63, 64]. This semiclassical concept is quite important because it provides a clear physical picture of collective dynamics. We shall see below that the unitary representation (19) is very convenient to develop a microscopic theory of nuclear collective motions.

4.2. Small-amplitude approximation (QRPA)

For small-amplitude vibrations around an HFB equilibrium point, one can make the linear approximation to the TDHFB equations and obtain the quasiparticle random phase approximation (QRPA). This is a starting point of microscopic theory of collective motion [13, 14]. Expanding equation (19) in a power series of $\hat{G}(t)$ and taking only the linear order, we obtain

$$\delta \langle \phi_0 | [\hat{H}, \, i\hat{G}] + \frac{\partial \hat{G}}{\partial t} | \phi_0 \rangle = 0. \tag{23}$$

In place of the functions $g_{kl}(t)$ and $g_{kl}^*(t)$ in equation (20), let us introduce normal coordinates $q(t) = \{q^1(t), \, q^2(t), \cdots, q^f(t)\}$ and conjugate momenta $p(t) = \{p_1(t), \, p_2(t), \cdots, p_f(t)\}$, and represent $\hat{G}(t)$ in terms of the infinitesimal generators $(\hat{Q}^i, \hat{P}_i)$ of $(p_i(t), q^i(t))$ as

$$\hat{G}(t) = \sum_{i=1}^{f} (p_i(t)\hat{Q}^i - q^i(t)\hat{P}_i). \tag{24}$$

Here it is important to distinguish the *classical* dynamical variables $(q_i(t), p^i(t))$ from the *quantum* infinitesimal generators $(\hat{Q}^i, \hat{P}_i)$. This representation is equivalent to equation (20) if the number of normal coordinates, f, is equal to the number of independent two-quasiparticle configurations (kl). In reality, we shall be interested in only a few collective modes among the f normal modes. For small-amplitude vibrations under consideration, the harmonic approximation holds; that is, time dependence of $q^i(t)$ and $p_i(t)$ is given by

$$\dot{p}_i(t) = B_i \ddot{q}^i(t) = -C_i q^i(t), \tag{25}$$

where the $\dot{p}_i(t)$, C_i, and B_i denote time-derivative of $p_i(t)$, the stiffness (restoring force) parameter, and the inertial mass for the normal mode (specified by the suffix i), respectively. Inserting (24) into (23) and using (25), we obtain the QRPA equation

$$[\hat{H}, \, \hat{Q}^i] = -iB^i\hat{P}_i, \tag{26}$$

$$[\hat{H}, \, \hat{P}_i] = iC_i\hat{Q}^i. \tag{27}$$

where B^i denotes the reciprocal of B_i, i.e., $B^i = 1/B_i$. These equations determine the microscopic structure of $\hat{Q}^i$ and $\hat{P}_i$ as coherent superpositions of many two-quasiparticle excitations: expressing them as sums over independent two-quasiparticles states (kl),

$$\hat{Q}^i = \sum_{(kl)} q_{kl}^i (a_k^\dagger a_l^\dagger + a_l a_k), \tag{28}$$

$$\hat{P}_i = i \sum_{(kl)} p_{kl}^i (a_k^\dagger a_l^\dagger - a_l a_k), \tag{29}$$

and inserting these into (26) and (27), we obtain linear eigenvalue equations determining the frequency squared, $\omega_i^2 = B^i C_i$, and the amplitudes (q_{kl}^i, p_{kl}^i). Actually, we have to choose appropriate solutions among large number of solutions (the number of independent two-quasiparticle configurations). It is not difficult to identify them, however, because the solutions corresponding to low-frequency quadrupole vibrations appear much lower than twice the pairing gap, 2Δ, (or the lowest two-quasiparticle excitation energy) and they are formed by coherent superpositions of many two-quasiparticle excitations. Because the time evolution of the TDHFB state $|\phi(t)\rangle$ is determined by the normal coordinates and momenta $(q^i(t), p_i(t))$, we can write it as $|\phi(q, p)\rangle$. Using equations (26), (27), and (35) below, we can easily calculate the expectation value of the microscopic Hamiltonian with respect to $|\phi(q, p)\rangle$:

$$\langle \phi(q, p) | \, \hat{H} \, | \phi(q, p) \rangle = \langle \phi_0 | \, \hat{H} \, | \phi_0 \rangle$$
$$+ \frac{1}{2} \sum_{i=1}^{f} (B^i p_i^2 + C_i q^{i2}). \tag{30}$$

The increase of the total energy due to the vibrational motion,

$$\mathcal{H}(q, p) \equiv \langle \phi(q, p) | \, \hat{H} \, | \phi(q, p) \rangle - \langle \phi_0 | \, \hat{H} \, | \phi_0 \rangle, \tag{31}$$

may be identified as the classical vibrational Hamiltonian. Below we shall not consider the ground-state energy (the second term in the r.h.s.), because it does not affect the equations of motion for $(q^i(t), p_i(t))$.

For vibrational modes whose frequencies, $\omega_i = \sqrt{B^i C_i}$, are positive, we can define the creation and annihilation operators $(\Gamma_i^\dagger, \Gamma_i)$ of the excitation mode as

$$\Gamma_i^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{\omega_i}{B^i}} \hat{Q}^i - i\sqrt{\frac{B^i}{\omega_i}} \hat{P}_i \right) \tag{32}$$

and their Hermitian conjugates Γ_i. As is well known, they are written in terms of the quasiparticle operators as

$$\Gamma_i^\dagger = \sum_{(kl)} (x_{kl}^i a_k^\dagger a_l^\dagger - y_{kl}^i a_l a_k), \tag{33}$$

and obey the QRPA equation of motion,

$$[\hat{H}, \, \Gamma_i^\dagger] = \omega_i \Gamma_i^\dagger. \tag{34}$$

It is worth noting that the $(\hat{Q}^i, \hat{P}_i)$ representation possesses a wider applicability than the $(\Gamma_i^\dagger, \Gamma_i)$ representation. First, for the ANG modes with $\omega_i = 0$, the former is valid while the latter is undefined. Note that their inertial masses, B_i (inverse of B^i), are positive, whereas their frequencies ω_i become to zero because the restoring-force parameters C^i vanish. Second, the $(\hat{Q}^i, \hat{P}_i)$ representation is valid also for unstable HFB equilibria where C_i is negative and ω_i is imaginary. Obviously, we cannot define the creation and annihilation operators $(\Gamma_i^\dagger, \Gamma_i)$ for imaginary ω_i. We shall see that this is one of the key points when we try to extend the QRPA approach to non-equilibrium points far from the HFB local minima.

Merits of the QRPA

One of the beauties of the QRPA is that it is able to determine the microscopic structures of collective coordinates and momenta in terms of a large number of microscopic (particle-hole, particle-particle, hole-hole) degrees of freedom. We can thus learn how collective vibrations are generated as coherent superpositions of many two-quasiparticle excitations. It is well known that two kinds of isoscalar quadrupole vibration appear exhibiting quite different characteristics; the low- (usually first excited 2^+) and high-frequency (giant resonance) modes. Examining the microscopic structure of the low-frequency quadrupole vibrations, we see that the weights of two-quasiparticle excitations near the Fermi surface are much larger than those in the mass quadrupole operators (see, e.g., [65]). This example clearly shows the importance of describing collective modes in a microscopic way.

Another merit of the QRPA is that it yields the ANG modes as self-consistent solutions and determines their collective inertial masses. With use of the QRPA, we can restore the symmetries broken by the mean-field approximation. Furthermore, the QRPA fulfills the energy-weighted sum rules [66].

Quantization condition

In the QRPA, the following condition is customarily imposed to ortho-normalize the amplitudes (q_{kl}^i, p_{kl}^i) or (x_{kl}^i, y_{kl}^i).

$$\langle \phi_0 | [\hat{Q}^i, \hat{P}_j] | \phi_0 \rangle = i\delta_{ij}, \tag{35}$$

or

$$\langle \phi_0 | [\Gamma_i, \Gamma_j^\dagger] | \phi_0 \rangle = \delta_{ij}. \tag{36}$$

We shall call this condition *canonical-variable condition*. It should be emphasized that, differently from the time-independent approaches, e.g. [13], these conditions cannot be derived within the standard framework of the TDHFB theory. For the derivation and justification of the canonical-variable conditions, we need to clarify the canonical structure of the TDHFB theory. We shall discuss on this point in section 8.

In this connection, we note that the inertial masses are not uniquely determined by (26) and (27), because the QRPA equations are invariant against the scale transformations $\hat{Q}^i \rightarrow s^i \hat{Q}^i$ and $\hat{P}_i \rightarrow \hat{P}_i/s^i$ with arbitrary values of s^i. It is therefore possible to adopt the values of s^i such that the collective inertial masses become unity. This arbitrariness is related to the freedom of scale transformations of the normal coordinates and momenta (q^i, p_i).

Because (q^i, p_i) are canonical variables, we can make canonical quantization and obtain the quantum collective Hamiltonian,

$$\hat{H}_{\text{QRPA}} = \frac{1}{2} \sum_{i=1}^{f} (B^i (\hat{p}_i)^2 + C_i (\hat{q}^i)^2). \tag{37}$$

Here, the collective coordinates and momenta, $\hat{p}_i$ and $\hat{q}^i$, are quantum operators. It is important to note that the QRPA

ground state after the quantization is different from the HFB ground state due to the quantum zero-point fluctuations.

The necessity of canonical quantization in order to derive QRPA from the TDHFB theory, discussed above, is not necessarily emphasized in standard textbooks on theoretical nuclear physics. We shall see in section 8, however, that the recognition of this point is essential to extend the basic ideas of the QRPA for small amplitude vibrations to LACM.

Effective interactions for QRPA calculations

In the investigation of low-energy excitation spectra, the pairing-plus-quadrupole (P + Q) model [67–69] and its extension [70] have been playing the major roles. This phenomenological effective interaction represents the competition between the pairing correlations favoring the spherical symmetry and the quadrupole (particle-hole) correlations leading to the quadrupole deformation of the mean field [3, 71].

In recent years, QRPA calculations using density-dependent effective interactions [72–76] have become possible. Density-dependent contact interactions such as the Skyrme interactions [72, 73, 76] may be founded on the density functional theory (DFT) [58]. From this point of view, the Skyrme interactions may be better called the Skyrme *energy density functionals* (EDFs). Accordingly, the self-consistent calculations that use the same density-dependent contact interactions in solving the HFB equations for the ground state and the QRPA for excited states may be regarded as small-amplitude approximations of the time-dependent DFT (TDDFT) [77]. A number of good textbooks on DFT and TDDFT are available, e.g., [78, 79]. Note, however, there are conceptual differences between those for condensed-matter and those for nuclei, since the nucleus is a self-bound system without an external potential [77].

For spherical mean fields, the QRPA matrix is block-diagonal with respect to the angular momentum (J) and the parity (π) of two-quasiparticle configurations. Usually, the $J^\pi = 2^+$ solution with lowest positive ω_i corresponds to the first excited quadrupole vibrational state. In this case, many calculations were performed [58, 80]. For axially symmetric deformed mean fields, the QRPA matrix is block-diagonal with respect to the K quantum number (projection of angular momentum on the symmetry axis) and the parity of two-quasiparticle configurations. The $K^\pi = 2^+ (0^+)$ solution with lowest positive ω_i may correspond to the first excited γ (β)-vibrational state. It is well known, however, that the lowest $K^\pi = 0^+$ solution contains an appreciable mixture of the pairing vibrational modes of protons and/or neutrons (sensitively depending on the deformed shell structure around the Fermi surface) [3]. Moreover, as we shall discuss in section 9, recent experiments reveal mysterious characters of the lowest $K^\pi = 0^+$ excitations. Although the dimension of the QRPA matrix is much larger than that in the spherical case, large scale QRPA calculations with modern EDFs have been carried out also for deformed nuclei in recent years [81–89]. In this way, it becomes one of the modern subjects in nuclear structure physics to carry out fully self-consistent

QRPA calculations on the basis of DFT for superfluid (spherical and deformed) nuclei and treat low- and high-frequency vibrations (giant resonances) as well as the ground states in a unified way for all nuclei from the proton-drip line to the neutron-drip line.

For triaxial mean fields breaking the axial symmetry, the dimension of the QRPA matrix further increases and it becomes computationally too heavy to diagonalize it at the present time. To overcome this problem, a new method of solving the QRPA equations without recourse to diagonalization of the QRPA matrix has been developed in recent years [90–92]. It is called the *finite-amplitude method*, and applied mainly to calculate strength functions for giant resonances [93–97]. We shall suggest in section 5 that this method may be useful also for solving the *local* QRPA equations.

Relations to spherical shell-model calculations

The lowest 2^+ vibrational states are obtained in the spherical shell model as coherent superpositions of many configurations. The *coherence* is indirectly confirmed by, e.g. the enhancements of the electric-quadrupole (E2) transition probabilities $B(E2; 2_1^+ \to 0_1^+)$. In the QRPA, we can directly see the coherence in the QRPA amplitudes, x_{kl}^i and y_{kl}^i (or q_{kl}^i and p_{kl}^i). In the time-dependent mean-field picture, *this coherence represents the correlations generating the self-consistent deformed mean field*. In this way, the TDHFB theory provides a transparent physical interpretation on the microscopic mechanism of emergence of nuclear collective motions.

4.3. Beyond the QRPA

Boson expansion method

The boson expansion method is well known as a useful microscopic method for describing anharmonic (non-linear) vibrations going beyond the harmonic approximation of the QRPA. In this approach, we first construct a collective subspace spanned by many-phonon states of vibrational quanta (determined by the QRPA) in the huge-dimensional shell-model space, and then map these many-phonon states one-to-one to many-boson states in an ideal boson space. Anharmonic effects neglected in the QRPA are treated as higher-order terms in the power-series expansion with respect to the boson creation and annihilation operators. Starting from the QRPA about a spherical shape, one can thus derive the 5D quadrupole collective Hamiltonian in a fully quantum mechanical manner. The boson expansion method has been successfully applied to low-energy quadrupole excitation spectra in a wide range of nuclei including those lying in regions of quantum phase transitions from spherical to deformed [15, 98].

Non-perturbative approaches to LACM

The boson expansion about a single HFB local minimum is not suitable for treating a situation where a few local minima in the potential-energy surface $V(\beta, \gamma)$ compete in energy. In such situations the collective wave functions are not necessarily localized around a single minimum but tunnel through the potential barrier. We frequently encounter such situations, called 'shape coexistence/mixing phenomena' in low-energy excitation spectra. The need to develop non-perturbative approaches capable of treating quantum many-body barrier penetrations is high also for treating large-amplitude collective motions in low-energy regions, such as spontaneous fissions and sub-barrier fusion reactions. It has been one of the longstanding fundamental subjects in nuclear structure physics to construct a microscopic theory of LACM by extending the QRPA concepts to arbitrary points in the $V(\beta, \gamma)$ plane far from the HFB minima [77, 99, 100].

State vectors of time-dependent mean field are kinds of generalized coherent states, and we can rigorously formulate the TDHFB as a theory of classical Hamiltonian dynamical system of large dimension [63, 101]. Because time evolution of the mean field is determined by the classical Hamilton equations, we cannot describe, within the framework of the TDHFB, quantum spectra of low-lying states and macroscopic quantum tunneling phenomena such as spontaneous fissions and sub-barrier fusions. To describe these genuine quantum phenomena, we need to introduce a few collective variables determining the time evolution of the mean field and quantize them. Succeeding and developing the ideas in microscopic theories of LACM acquired during 1970's-1990's, we have developed a new method, called the ASCC method [102], and shown its usefulness by applying it to shape coexistence/mixing phenomena [103, 104].

Introduction to the ASCC method

Here we very briefly describe the basic ideas of the ASCC method [102]. It will be presented in section 8 in a more systematic way. In this approach, assuming that the time evolution of the TDHFB state is determined by a few collective coordinates $q = (q^1, q^2, \cdots, q^f)$ and collective momenta $p = (p_1, p_2, \cdots, p_f)$, we write the TDHFB state as $|\phi(t)\rangle = |\phi(q(t), p(t))\rangle$. The TDHFB states $|\phi(q, p)\rangle$ constitute the $2f$-dimensional submanifold in the TDHFB phase space, which is called *collective submanifold*. In the ASCC method, we further assume that $|\phi(q, p)\rangle$ can be written in a form

$$|\phi(q, p)\rangle = \exp\left\{ i \sum_{i=1}^{f} p_i \hat{Q}^i(q) \right\} |\phi(q)\rangle, \qquad (38)$$

where $\hat{Q}^i(q)$ are one-body operators corresponding to infinitesimal generators of p_i locally defined at the state $|\phi(q)\rangle$ which represents a TDHFB state $|\phi(q, p)\rangle$ at $p \to 0$. This state $|\phi(q)\rangle$ is called a *moving-frame HFB state*. Inserting (38) into the time-dependent variational principle, equation (22), and considering that the time dependence is determined by the collective coordinates and momenta (q, p),

we obtain

$$\delta \langle \phi(q, p)| \left\{ i \sum_{i=1}^{f} \left(\dot{q}^i \frac{\partial}{\partial q^i} + \dot{p}_i \frac{\partial}{\partial p_i} \right) - \hat{H} \right\} |\phi(q, p)\rangle = 0. \quad (39)$$

We shall give a rigorous formulation to determine the microscopic structures of the infinitesimal generator $\hat{Q}^i(q)$ of p_i on the basis of the time-dependent variational principle (39). We shall also introduce infinitesimal generators $\hat{P}_i(q)$ of q^i and determine their microscopic structures. Furthermore, we shall formulate the theory such that the collective variables (q, p) can be treated as canonical variables.

Quite recently, we have proposed a practical approximation scheme to the ASCC method. It is called the *local QRPA* (LQRPA) method [105–110]. Here, the adjective '*local*' means that it is locally defined around a point in the (β, γ) deformation space. More rigorously speaking, it is defined around a point on the collective submanifold embedded in the TDHFB phase space, and this point is mapped onto the (β, γ) space. The infinitesimal generators appearing in this method are nonlocal in the coordinate space. It may be regarded as an extension of the ordinary QRPA to non-equilibrium states, where the moving-frame HFB states $|\phi(q)\rangle$ play a role analogous to the static HFB ground state $|\phi_0\rangle$. Because of this analogy it may be easy to understand the LQRPA method. In the next section, we show how this method is used for a microscopic derivation of the Bohr-Mottelson collective Hamiltonian. Fundamentals and validity of the LQRPA method will be discussed later in section 8.

5. Microscopic derivation of the Bohr–Mottelson collective Hamiltonian

In this section, we derive the quadrupole collective Hamiltonian making use of the LQRPA method. We also discuss fundamental problems related to the microscopic derivation of the collective Hamiltonian.

5.1. Procedure for the microscopic derivation

Instead of treating the 5D collective coordinates simultaneously, we first calculate the collective inertial masses for two-dimensional (2D) vibrational motions corresponding to the (β, γ) deformation degree of freedom, and subsequently calculate the moments of inertia for 3D rotational motions at each point of (β, γ). We then derive the collective Hamiltonian for the 5D quadrupole collective dynamics and quantize it.

Microscopic calculation of the vibrational inertial masses

We first derive two canonical coordinates (q^1, q^2) that correspond to the (β, γ) vibrational degrees of freedom in the Bohr–Mottelson collective model. In this section we use the notation q to represent (q^1, q^2) and write the moving-frame HFB state as $|\phi(q)\rangle$.

First, we solve the moving-frame HFB equations,

$$\delta \langle \phi(q)| \, \hat{H}_{\mathrm{M}}(q) |\phi(q)\rangle = 0, \quad (40)$$

$$\hat{H}_{\mathrm{M}}(q) = \hat{H} - \sum_{\tau} \lambda^{(\tau)}(q) \tilde{N}^{(\tau)} - \sum_{m=0,2} \mu_m(q) \hat{D}_{2m}^{(+)}, \quad (41)$$

where $\hat{D}_{2m}^{(+)}$ and $\tilde{N}^{(\tau)} \equiv \hat{N}^{(\tau)} - N_0^{(\tau)}$ are the mass quadrupole operators and the number operators (measured from the expectation values at the ground state) for protons and neutrons ($\tau = $ p, n), respectively. The quadrupole-deformation variables (β, γ) are defined through the expectation values of $\hat{D}_{2m}^{(+)}$ with respect to $|\phi(q)\rangle$:

$$\beta \cos \gamma = \eta D_{20}^{(+)}(q) = \eta \langle \phi(q)| \, \hat{D}_{20}^{(+)} \, |\phi(q)\rangle, \quad (42)$$

$$\frac{1}{\sqrt{2}} \beta \sin \gamma = \eta D_{22}^{(+)}(q) = \eta \langle \phi(q)| \, \hat{D}_{22}^{(+)} \, |\phi(q)\rangle, \quad (43)$$

where η is a scaling factor with the dimension of L^{-2}.

Through the above definitions of (β, γ) we can make a one-to-one correspondence between (q^1, q^2) and (β, γ). As illustrated in figure 3, this correspondence may be viewed as a mapping of the collective coordinates (q^1, q^2) onto the (β, γ) plane of the Bohr–Mottelson collective model. For our purpose, it is sufficient to assume that this correspondence is one-to-one in the neighborhood of an arbitrary point (q^1, q^2), because the collective inertial masses represent the inertia of the LACM for infinitesimal variation in time of the collective coordinates. Thus, the moving-frame HFB state $|\phi(q)\rangle$ may also be written as $|\phi(\beta, \gamma)\rangle$. The solutions of equation (40) for every point on the (q^1, q^2) plane provide the moving-frame HFB states $|\phi(\beta, \gamma)\rangle$ off the HFB ground state $|\phi(\beta_0, \gamma_0)\rangle$ at the local minimum (β_0, γ_0) on the potential energy surface $V(\beta, \gamma)$.

Next, we consider the TDHFB states of the form, equation (38), with $f = 2$. Assuming that the collective motion is slow, we expand it in powers of p and consider up to the second order in p. Then, under certain approximations explained in section 8, we obtain the following set of equations of motion for $\hat{Q}^i(q)$ and $\hat{P}_i(q)$,

$$\delta \langle \phi(q)| [\hat{H}_{\mathrm{M}}(q), \hat{Q}^i(q)] + iB^i(q) \hat{P}_i(q) |\phi(q)\rangle = 0, \quad (44)$$

$$\delta \langle \phi(q)| [\hat{H}_{\mathrm{M}}(q), \hat{P}_i(q)] - iC_i(q) \hat{Q}^i(q) |\phi(q)\rangle = 0, \quad (45)$$

with the 'weakly' canonical commutation relations,

$$\langle \phi(q)| [\hat{Q}^i(q), \hat{P}_j(q)] |\phi(q)\rangle = i\delta_{ij}, \quad (46)$$

meaning that the canonical commutation relations hold only for their expectation values with respect to $|\phi(q)\rangle$. The equations (44) and (45) are called the LQRPA equations and may be regarded as generalizations of the QRPA equations (26) and (27) about the HFB ground state to those for a moving-frame HFB state $|\phi(q)\rangle$.

Analogously to the $(\hat{Q}^i, \hat{P}_i)$ operators in the ordinary QRPA, the one-body operators $\hat{Q}^i(q)$ and $\hat{P}_i(q)$, called infinitesimal generators of collective motion, can be written as linear combinations of bilinear products of the local quasi-particle operators $(a_k^\dagger, a_l)$ that are defined with respect to the
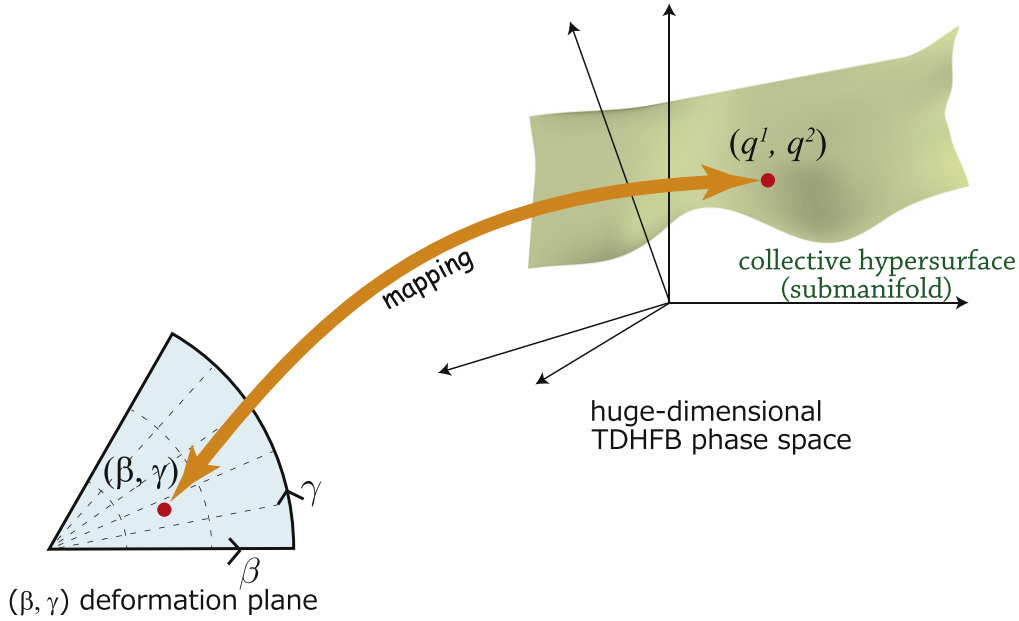
Figure 3. Illustration of the mapping of (q^1, q^2) defined on the collective submanifold onto the (β, γ) deformation plane of the Bohr-Mottelson collective model. The collective submanifold is illustrated as a hypersurface in the huge-dimensional TDHFB phase space.

moving-frame HFB state $|\phi(q)\rangle$ by $a_k\ |\phi(q)\rangle = 0$:

$$\hat{Q}^i(q) = \sum_{(kl)} q_{kl}^i(q)(a_k^\dagger a_l^\dagger + a_l a_k), \qquad (47)$$

$$\hat{P}_i(q) = i \sum_{(kl)} p_{kl}^i(q)(a_k^\dagger a_l^\dagger - a_l a_k). \qquad (48)$$

Because the collective coordinates (q^1, q^2) corresponding to (β, γ) and their conjugate momenta (p_1, p_2) are canonical variables, it is possible to make a scale transformation such that the collective masses relating (p_1, p_2) to the time derivatives $(\dot{q}^1, \dot{q}^2)$ of (q^1, q^2) become unity. Thus, we can write the kinetic energy of vibrational motions as

$$T_{\mathrm{vib}} = \frac{1}{2}\sum_{i=1,2}(p_i)^2 = \frac{1}{2}\sum_{i=1,2}(\dot{q}^i)^2 \qquad (49)$$

without loss of generality.

Microscopic calculation of the rotational moments of inertia

In a manner similar to the calculation of the vibrational inertial masses described above, we calculate, at every point on the (β, γ) plane, the rotational moments of inertia $\mathcal{J}_k$ for 3D rotational motions ($k = 1, 2, 3$). To treat the 3D rotational motions, we write rotating TDHFB states in the following form:

$$|\phi(q, \varphi, \dot{\varphi})\rangle = \exp\left[i \sum_{k=1}^{3} \{\mathcal{J}_k(q)\dot{\varphi}_k \hat{\Psi}^k(q) - \varphi_k \hat{I}_k\} \right] |\phi(q)\rangle. \qquad (50)$$

Here $\hat{\Psi}^k(q)$ are local angle operators conjugate to the angular-momentum operators $\hat{I}_k$ and satisfy the 'weak' canonical commutation relations,

$$\langle \phi(q)|[\hat{\Psi}^k(q), \hat{I}_l]|\phi(q)\rangle = i\delta_{kl}. \qquad (51)$$

The set $(\hat{\Psi}^k(q), \hat{I}_k)$ corresponds to the infinitesimal generators $(\hat{Q}^i(q), \hat{P}_i(q))$ for vibrational motions considered above. The variables φ_k and $\dot{\varphi}_k$ denote the rotational angles and their time derivatives. The set $(\varphi_k, \mathcal{J}_k(q)\dot{\varphi}_k)$ corresponds to the set of collective coordinates and momenta (q^i, p_i). The inverse of $B^i(q)$ corresponds to $\mathcal{J}_k(q)$. Needless to say, in contrast to $\hat{P}_i(q)$ for vibrational motions, the infinitesimal generators for rotational motions are the angular-momentum operators $\hat{I}_k$ *independent of* q, and the restoring-force parameters $C_k(q)$ are zero for rotational motions.

Inserting equation (50) for $|\phi(t)\rangle$ in the time-dependent variational principle equation (22) and considering only the linear-order terms with respect to $\hat{\Psi}^k(q)$ and $\hat{I}_k$, we obtain the LQRPA equations for 3D rotational motions:

$$\delta \langle \phi(q)|[\hat{H}_{\mathrm{M}}(q), \hat{\Psi}^k(q)] + i\frac{\hat{I}_k}{\mathcal{J}_k(q)}\ |\phi(q)\rangle = 0. \qquad (52)$$

These equations are the same as the Thouless–Valatin equations [111], except that we solve these equations not only at the equilibrium deformation (β_0, γ_0) but also at every points on the (β, γ) plane off the equilibrium.

Solving equations (52) at every point on the (q^1, q^2) plane and make a one-to-one mapping to the (β, γ) plane, we obtain the three moments of inertia $\mathcal{J}_k(\beta, \gamma)$, which determine the rotational masses $D_k(\beta, \gamma)$ through equation (10), and the rotational energy,

$$T_{\mathrm{rot}} = \frac{1}{2}\sum_{k=1,2,3} \mathcal{J}_k(\beta, \gamma)\dot{\varphi}_k^2, \qquad (53)$$

in the collective Hamiltonian (2). If $D_k(\beta, \gamma)$ are replaced with a constant, $D_k(\beta, \gamma) = D$, then $\mathcal{J}_k(\beta, \gamma)$ reduce to the moments of inertia for irrotational fluid. As mentioned in section 2, this approximation may be valid only for harmonic vibrations about the spherical shape.

Derivation of the quadrupole collective Hamiltonian and its quantization

Displacements of (q^1, q^2) are related to variations of the expectation values $D_{2m}^{(+)}$ of the mass quadrupole operators by

$$\mathrm{d}D_{2m}^{(+)} = \sum_{i=1,2} \frac{\partial D_{2m}^{(+)}}{\partial q^i}\mathrm{d}q^i, \qquad m = 0, 2. \tag{54}$$

This relation leads to the kinetic energy of vibrational motions given in terms of time derivatives of the quadrupole deformation,

$$T_{\mathrm{vib}} = \frac{1}{2}\sum_{m,m'=0,2} M_{mm'}\dot{D}_{2m}^{(+)}\dot{D}_{2m'}^{(+)}, \tag{55}$$

where

$$M_{mm'}(\beta, \gamma) = \sum_{i=1,2} \frac{\partial q^i}{\partial D_{2m}^{(+)}}\frac{\partial q^i}{\partial D_{2m'}^{(+)}}. \tag{56}$$

Taking time derivatives of equations (42) and (43), we can straightforwardly transform the expression (55) to the form in terms of $(\dot{\beta}, \dot{\gamma})$. The vibrational masses $(D_{\beta\beta}, D_{\beta\gamma}, D_{\gamma\gamma})$ are then obtained from (M_{00}, M_{02}, M_{22}) through the following relations:

$$D_{\beta\beta} = \eta^{-2}\Big(M_{00}\cos^2\gamma + \sqrt{2}M_{02}\sin\gamma\cos\gamma$$
$$+ \frac{1}{2}M_{22}\sin^2\gamma\Big), \tag{57}$$

$$D_{\beta\gamma} = \beta\eta^{-2}\Big[-M_{00}\sin\gamma\cos\gamma$$
$$+ \frac{1}{\sqrt{2}}M_{02}(\cos^2\gamma - \sin^2\gamma) + \frac{1}{2}M_{22}\sin\gamma\cos\gamma\Big], \tag{58}$$

$$D_{\gamma\gamma} = \beta^2\eta^{-2}\Big(M_{00}\sin^2\gamma - \sqrt{2}M_{02}\sin\gamma\cos\gamma$$
$$+ \frac{1}{2}M_{22}\cos^2\gamma\Big). \tag{59}$$

In this way, we can calculate, in a microscopic way, all the collective inertial masses appearing in the Bohr–Mottelson collective Hamiltonian (2). For quantization, we can apply the quantization scheme for the 5D curvilinear coordinates (so-called Pauli prescription, see appendix A). After a somewhat lengthy but straightforward calculation, we obtain the quantized collective Hamiltonian (5).

5.2. Discussions

Let us discuss some fundamental problems related to the microscopic derivation of the quadrupole collective Hamiltonian.

Applicability of the Pauli prescription for quantization

In the pioneering work of Baranger and Kumar toward microscopic derivation of the Bohr–Motttelson collective

Hamiltonian, they wrote [46]: 'The next problem is that of quantizing Hamiltonian H. There is no unique way of doing this. Bohr uses the Pauli prescription, which is designed to give the right answer when the variables can be transformed to Cartesian coordinates. But this is not the case here and therefore the Pauli prescription loses its only justification.'

In the 50 years since their work, we now have good prospects of justifying the use of the Pauli prescription. Because it is just the transformation of the Laplacian in Cartesian coordinates to that in the curvilinear coordinates, as Baranger and Kumar pointed out, the crucial question is whether or not we can derive the 5D collective coordinates which are Cartesian. As we have shown above, we have derived a local 5D canonical coordinate system on the collective submanifold embedded in the large-dimensional TDHFB phase space. (This concept will be further discussed in section 8.) In our view, to derive the kinetic energy term and the inertial masses, it is enough to define *a local coordinate system* at each point of the collective submanifold; that is, it is unnecessary to define a *global* canonical coordinate system. It remains, however, as an interesting subject to develop a firm theoretical formulation to clarify the validity and limitation of the use of the Pauli prescription for quantization of collective coordinates.

Treatment of 3D rotational motions

It should be emphasized that we can define the local angle operators $\hat{\Psi}^k(q)$, although the global angle operators canonically conjugate to $\hat{I}_k$ do not exist. For the microscopic calculation of the moments of inertia $\mathcal{J}_k$, it is sufficient to determine the microscopic structure of the local angle operators $\hat{\Psi}^k(q)$. This is because, similarly to the vibrational inertial masses, $\mathcal{J}_k(q)$ represents the inertia for an infinitesimal change of the rotational angles of the moving-frame HFB state $|\phi(q)\rangle$. It should be kept in mind that we use the expression (50) for rotating TDHFB states only for infinitesimal rotations, i.e., for very small rotational angles φ_k. For large φ_k, we have to consider higher-order effects associated with the non-Abelian nature of the angular momentum operators [112]. Fortunately, it is unnecessary to consider such higher-order effects for our aim of evaluating the inertial masses for rotational motions.

Effective interaction in the microscopic Hamiltonian

The LQRPA method is quite general and it can be used for any microscopic Hamiltonian $\hat{H}$. Inserting equations (47) and (48) into equations (44) and (45), we obtain linear eigenvalue equations for the amplitudes q_{kl}^i and p_{kl}^i. For effective interactions of separable type such as the P + Q force model, we can rewrite these equations into a form of dispersion equation determining the frequencies squared $\omega_i^2 = B^i C_i$ and the amplitudes, q_{kl}^i and p_{kl}^i (see e.g., [113]). It is then easy to find the solutions satisfying the dispersion equation. For effective interactions of the Skyrme type or modern density functionals, we have to diagonalize the QRPA matrix of very large dimension. This is the case for deformed HFB states,

especially for triaxial deformations, and the computation becomes heavy. Although a large-scale calculation is required, such an application of the LQRPA method with realistic interactions/functionals is a challenging future subject. A step toward this goal has recently been carried out for axially symmetric cases [108]. To overcome this computational problem, the finite-amplitude method [90–92] may be utilized. In particular, the recently developed technique [114–117] may be useful to find a few low-frequency solutions possessing strong collectivities. It is a great challenge to develop the LQRPA approach on the basis of the TDDFT and nuclear EDFs.

Physical meaning of the collective inertial masses

The pairing correlation plays a crucial role in determining the inertial masses of collective motion. The reason may be understood microscopically as follows.

The single-particle energies and wave functions are determined by the nuclear mean field. The time evolution of the mean field changes them and causes a number of single-particle level crossings. The level crossing near the Fermi surface induces the change of the lowest-energy configuration. Without the pairing, it is difficult for the system to rearrange to more energetically favorable configurations at the level crossing. In the presence of the pairing correlation, however, the nucleon pairs can make a hopping from up-sloping levels to down-sloping levels at the level crossing [118]. Such easiness/hardness of the configuration rearrangements at level crossings determines the adiabaticity/diabaticity of the collective motion. The collective inertia represents a property of the system trying to keep a definite configuration during the collective motion. Thus, the inertia becomes smaller for stronger pairing.

In spherical mean fields, the pairing correlation acts for monopole nucleon pairs that couples to an angular momentum $J = 0$. In deformed mean fields, the nucleon pair becomes a superposition of multiple angular momenta J because of the rotational symmetry breaking. In particular, the quadrupole $J = 2$ pairing correlation plays an important role. The reason is understood as follows. When a mean field develops toward a larger prolate deformation, single-particle levels favoring the prolate deformation are pushed down, while those that favor the oblate deformation are pushed up. At the level crossing, the easiness/hardness of the rearrangement depends on the magnitude of the pairing matrix elements between the crossing single-particle levels. The spacial overlaps between the single-particle wave functions of the up-sloping and down-sloping levels are smaller than those at the spherical limit. Such reductions of the pairing matrix elements between the prolate-favoring and the oblate favoring levels are well described by taking into account the quadrupole pairing (in addition to the monopole pairing) [26]. The Galilean invariance provides a link between the monopole and quadrupole pairing strengths [119]. It is shown with the use of the ASCC and LQRPA methods [105, 120] that the quadrupole pairing induces time-odd components (that change sign under time reversal) in the moving mean field and enhances the inertial

masses. This indicates that the the collective dynamics associated with the pairing correlations is well described by these microscopic methods. More detailed investigation on the roles of the pairing in level crossing dynamics will prove fruitful for a deeper understanding of the microscopic mechanism determining the inertial masses.

5.3. Remarks on microscopic derivation of the particle-collective coupling Hamiltonian

In this review, we concentrate on the collective Hamiltonian H_{coll} in the unified model Hamiltonian (1) of Bohr and Mottelson. Needless to say, it is a great challenge to develop a microscopic theory capable of treating the single-particle and collective motions in a unified manner. The particle-collective coupling Hamiltonian H_{coupl} in the unified model Hamiltonian may be derived by using the same concept of time-dependent self-consistent mean field which has been used in the microscopic derivation of the collective Hamiltonian H_{coll}. As is well known, properties of single-particle motions are determined by the mean fields which are collectively generated by all nucleons constituting the nucleus. This implies that the dynamical time evolution of the mean field affects the single-particle motion and generates the particle-collective couplings.

For small-amplitude vibrations about an equilibrium point of the HFB mean field, we can expand the single-particle Hamiltonian associated with mean field of the moving HFB state $|\phi(\beta, \gamma)\rangle$ in terms of the vibrational amplitudes. We then obtain the particle-vibration coupling Hamiltonian in the linear order [3, 121]. To overcome the problem of over-completeness and non-orthogonality that arises from the use of the basis states consisting of both the single-particle modes (defined at the HFB minimum point) and the elementary modes of vibrations, the 'Nuclear Field Theory (NFT)' has been developed since 1970's [122]. The NFT has been used for microscopic analyses of anharmonicities of vibrational motions as well as the 'dressing' of single-particle motions due to the particle-vibration couplings. For these applications and recent achievements of the NFT, we refer the contribution by Broglia *et al* to this Special Edition [123].

A promising approach to derive the particle-vibration coupling Hamiltonian beyond the linear order is to derive the single-particle Hamiltonian in the moving self-consistent mean field and expand it in powers of collective variables. An interesting attempt in this direction was done by Yamada [124] using the self-consistent collective coordinate (SCC) method with the (η, η^*) expansion (described in section 8.2). It is interesting to further develop this approach. Looking for future, it will certainly become an important fundamental subject in nuclear structure theory to derive the particle-vibration coupling Hamiltonian starting from the TDDFT.

We should also remark the longstanding problem of deriving the particle-rotation coupling Hamiltonian starting from a microscopic many-body theory. In [125], the single-particle motions in rapidly rotating mean field are described by means of the SCC method with a power-series expansion in the rotational frequency, and the alignments of single-

quasiparticle and the rotational angular momenta are studied. Developing this line of approach, the SCC method may be used also for deriving the particle-rotation coupling Hamiltonian, but this subject remains for future. In our view, construction of a microscopic theory capable of treating the single-particle and collective motions in a unified manner, initiated by Bohr and Mottelson, still remains as the most fundamental and principal subject in nuclear structure dynamics.

Historical note

The construction of a self-consistent microscopic theory of collective motion capable of deriving the unified-model Hamiltonian of Bohr and Mottelson is a longstanding and difficult subject which always inspires the development of fundamental new concepts. Let us quote some remarks by Villars, which may be worthwhile to keep in mind:

'Although such a synthesis of the collective and the particle aspect of nuclear dynamics is rather easily achieved in words, by simply combining results borrowed from various models, a decent mathematical formulation of the same programme is far from easy.' in 1967 [126].

'It always appeared to this author that the proper formulation of a microscopic theory of nuclear collective motion is a strangely difficult subject.' 'Much is to be learned yet in the problem of formulating a consistent quantum theory of collective motion.' in 1982 [127].

6. Illustrative examples

We here present some applications of the LQRPA method for deriving the 5D collective Hamiltonian. In the numerical examples below, the $P + Q$ model Hamiltonian [69] (including the quadrupole-pairing interaction) is employed in solving the LQRPA equations. The single-particle energies and the $P + Q$ interaction strengths are determined such that the results of the Skyrme-HFB calculation for the ground states are best reproduced within the $P + Q$ model (see [106, 107] for details). More examples can be found for $^{68-72}$Se [104, 105], ^{72,74,76}Kr [106], the ^{26}Mg region [128], $^{30-34}$Mg [107], $^{58-68}$Cr [108], $^{58-66}$Cr [109], and $^{128-132}$Xe, $^{130-134}$Ba [129].

Oblate-prolate shape coexistence and fluctuations in ^{74}Kr

The collective potential $V(\beta, \gamma)$ depicted in figure 4 exhibits two local minima. The prolate minimum is lower than the oblate minimum, and the spherical shape is a local maximum. This figure also shows that the valley runs in the triaxially deformed region and the barrier connecting the oblate and prolate minima is low. Accordingly, one may expect large-amplitude quantum shape fluctuations to occur along the triaxial valley. In fact, the vibrational wave function of the ground 0_1^+ state has bumps around the two potential minima,

but the wave function spreads over the entire γ region along the potential valley. It is interesting to notice that, as the angular momentum increases, the localization of the vibrational wave functions in the (β, γ) deformation plane develops; namely, the rotational effect plays an important role for the emergence of the shape coexistence character. This development of localization results from the $\beta - \gamma$ dependence of the rotational moments of inertia. One can clearly see the oblate-prolate asymmerty of the moment of inertia $\mathcal{J}_1$ shown in figure 4(c). Due to this asymmetry, the localization on the prolate side develops in the ground band. In the yrare band, although the vibrational wave functions have a two-peak structure, the localization on the oblate side develops due to the orthogonality to the yrast states.

We note that the rotational inertial functions (D_1, D_2, D_3) and the pairing gaps significantly change as functions of (β, γ), as well as the vibrational inertial masses $(D_{\beta\beta}, D_{\gamma\gamma}, D_{\beta\gamma})$. Due to the time-odd contributions of the moving HFB self-consistent field, the collective inertial masses calculated with the LQRPA method are 20%–50% larger than those evaluated with the Inglis-Belyaev cranking formula. Their ratios also change as functions of (β, γ) [106]. As a consequence, as shown in Figure 5(a), the excitation spectrum calculated with the LQRPA masses is in much better agreement with experimental data than that with the Inglis-Belyaev cranking masses. Figure 5(b) shows the spectroscopic quadrupole moments calculated with the LQRPA masses for ^{74}Kr. One sees that, aside from a minor deviation for the 2_3^+ state, the calculated spectroscopic quadrupole moments are in excellent agreement with the experimental data. In particular, the signs and the increasing tendency of the magnitudes with angular momentum in the ground band are well reproduced.

7. Some remarks on other approaches

In this section, we give short remarks on other methods widely used for microscopic calculation of collective inertial masses.

7.1. Constrained HFB + adiabatic perturbation

This method is convenient and widely used in the microscopic description of LACM [131–135]. It is based on the adiabatic assumption that the collective motion is much slower than the single-particle motion. In this approach, we first postulate a few one-body operators $\hat{F}_i$ corresponding to collective coordinates α^i, and solve the constrained HFB (or constrained HF + BCS) equation,

$$\delta \langle \phi_0(\alpha)| \hat{H} - \sum_i \mu^i(\alpha)\hat{F}_i |\phi_0(\alpha)\rangle = 0, \qquad (60)$$

to find the constrained HFB states $|\phi_0(\alpha)\rangle$. Here, $\mu^i(\alpha)$ are the Lagrange multipliers whose values are determined to fulfill the constraining conditions,

$$\alpha^i = \langle \phi_0(\alpha)| \hat{F}_i |\phi_0(\alpha)\rangle. \qquad (61)$$
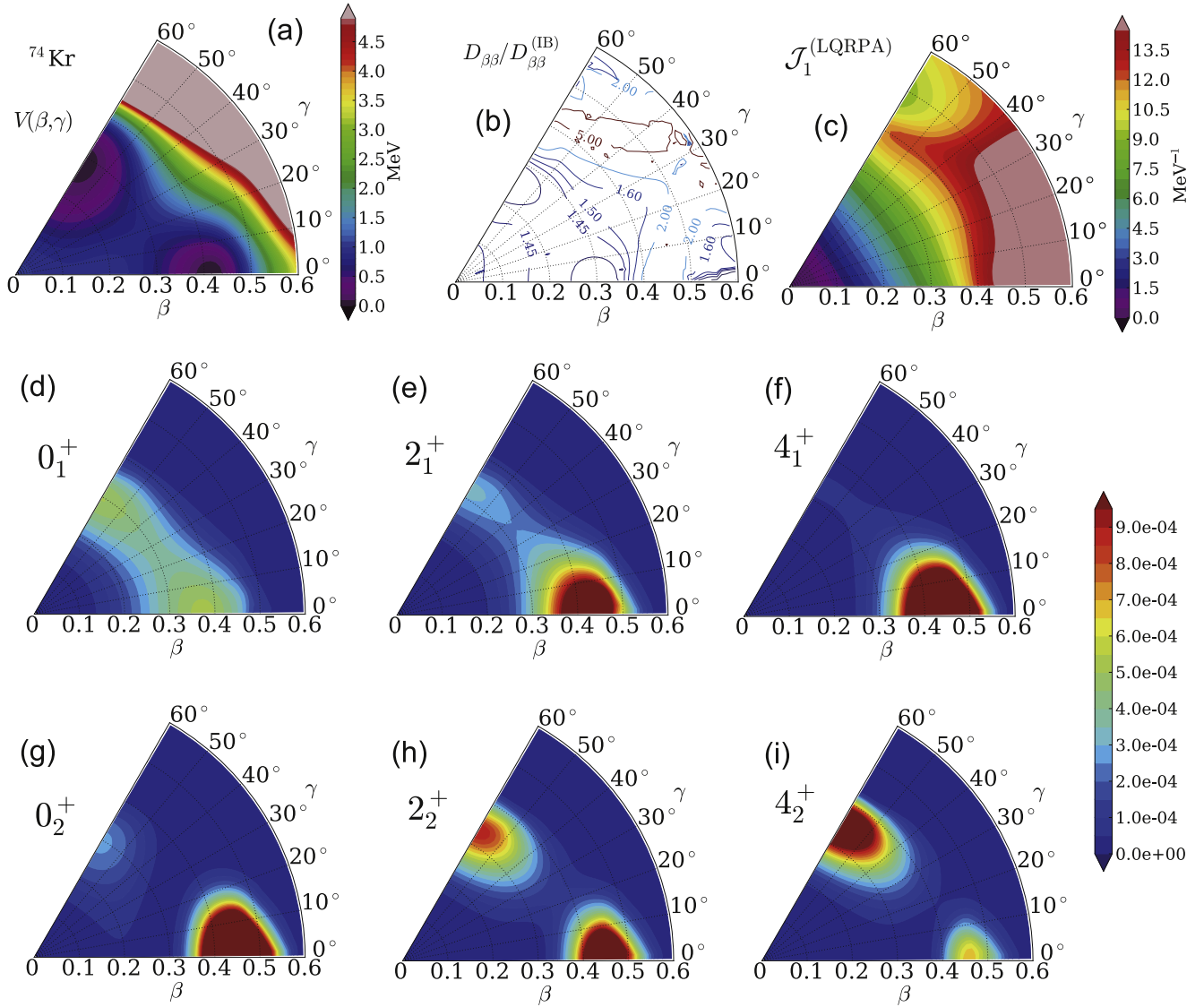
Figure 4. Application of the LQRPA method to the oblate-prolate shape coexistence/fluctuation phenomenon in ^{74}Kr (from [106]). Reproduced with permission. Copyright Elsevier 2011. (a) Collective potential $V(\beta, \gamma)$, (b) Ratio of the collective inertial mass $D_{\beta\beta}(\beta, \gamma)$ to the Inglis-Belyaev cranking mass. (c) The LQRPA moment of inertia $\mathcal{J}_1$ for rotation about the $x-$ axis. Vibrational wave functions squared, $\sum_K \beta^4 |\Phi_{\alpha lK}(\beta, \gamma)|^2$, for (d) the 0_1^+ state, (e) the 2_1^+ state, (f) the 4_1^+ state, (g) the 0_2^+ state, (h) the 2_2^+ state, and (i) the 4_2^+ state. For the β^4 factor, see the text.

Assuming that the frequencies of the collective motion are much smaller than those of non-collective two-quasiparticle excitation, we then calculate the collective kinetic energy T_{coll} using the adiabatic perturbation theory:

$$T_{\text{coll}} = \frac{1}{2} \sum_{ij} D_{ij}(\alpha) \dot{\alpha}^{i*} \dot{\alpha}^j, \tag{62}$$

where

$$\begin{aligned}
&D_{ij}(\alpha) \\
&= 2 \sum_n \frac{\langle \phi_0(\alpha)| \frac{\partial}{\partial \alpha^{i*}} |\phi_n(\alpha)\rangle \langle \phi_n(\alpha)| \frac{\partial}{\partial \alpha^j} |\phi_0(\alpha)\rangle}{E_n(\alpha) - E_0(\alpha)}
\end{aligned} \tag{63}$$

are called Inglis-Belyaev cranking masses [54]. Here $|\phi_0(\alpha)\rangle$ and $|\phi_n(\alpha)\rangle$ represent the ground and two-quasiparticle excited states for a given set of values $\alpha = \{\alpha^i\}$. In most of

applications it is simplified furthermore by introducing an assumption that the derivatives of the constrained HFB Hamiltonian with respect to α^i is proportional to $\hat{F}_i$. Equation (63) then reduces to

$$D_{ij}(\alpha) = \frac{1}{2} [\mathcal{M}_1^{-1}(\alpha) \mathcal{M}_3(\alpha) \mathcal{M}_1^{-1}(\alpha)]_{ij} \tag{64}$$

with

$$\mathcal{M}_k(\alpha)_{ij} = \sum_n \frac{\langle \phi_0(\alpha)| \hat{F}_i^{\dagger} |\phi_n(\alpha)\rangle \langle \phi_n(\alpha)| \hat{F}_j |\phi_0(\alpha)\rangle}{(E_n(\alpha) - E_0(\alpha))^k}. \tag{65}$$

In recent years, a systematic investigation on low-lying quadrupole spectra has been carried out in terms of the quadrupole collective Hamiltonian by using the Inglis-
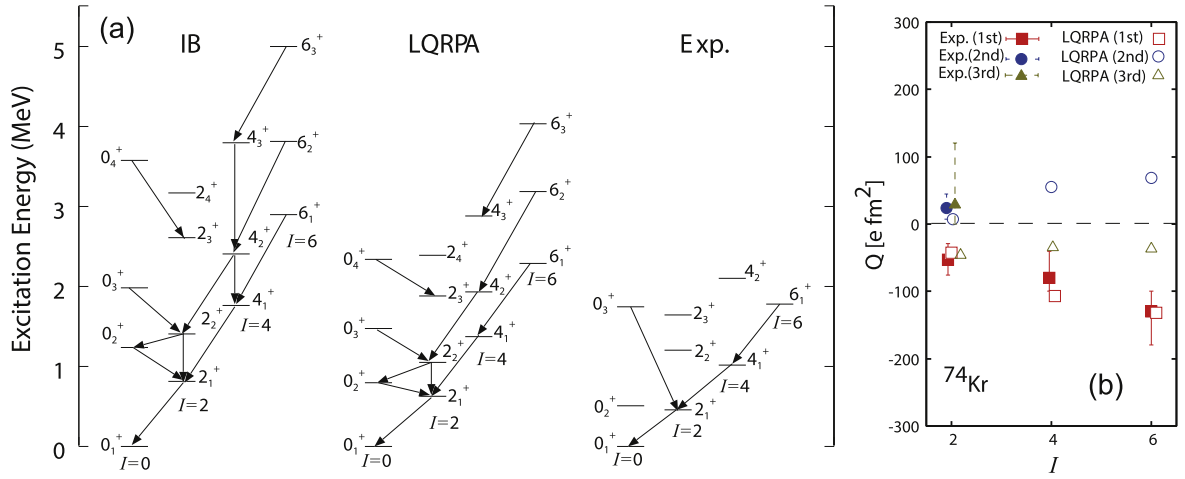
Figure 5. (a) Partial excitation spectrum calculated for ^{74}Kr by means of the LQRPA method [106] and experimental data [130]. For comparison, the results calculated using the Inglis-Belyaev cranking masses (denoted by IB) are also shown. Only the levels with even angular momentum are shown (see [106] for the whole spectrum.) The $E2$ transitions with $B(E2)$ larger than 50 Weisskopf units are indicated by arrows. (b) Spectroscopic quadrupole moments in unit of $e$fm^2 of the first (square), second (circle) and third (triangle) states for each angular momentum in ^{74}Kr (from [106]). Calculated values are shown by open symbols, while experimental data [130] are indicated by filled symbols.

Belyaev cranking formula and the collective potential energies derived from the relativistic (covariant) density functionals [136–142].

A problem of the Inglis–Belyaev cranking formula is that the collective inertial masses are underestimated [143]. Moving mean fields induce time-odd components that change sign under time reversal. However, the Inglis–Belyaev cranking formula ignores their effects on the collective inertial masses. By taking into account such time-odd corrections to the cranking masses, one can better reproduce low-lying spectra [129]. For rotational moments of inertia, we may estimate the time-odd corrections taking the limit of $\omega_{\text{rot}} \to 0$ for the solution of the HFB equation in the rotating frame, that is defined by adding the cranking term $-\omega_{\text{rot}}\hat{J}_x$ to the constrained HFB Hamiltonian. Since this provides about 20%–40% enhancement from the Inglis–Belyaev formula, the similar enhancement factors of 1.2–1.4 have been often utilized for vibrational inertial masses without solid justification.

7.2. Adiabatic TDHF theory

In the 1960's, Belyaev, Baranger, and Kumar began efforts to self-consistently derive the collective Hamiltonian using adiabatic approximation to time evolution of mean fields [47, 69]. In these pioneer works, they derived the quadrupole collective Hamiltonian using the P + Q force model [67]. During the 1970's, the time-dependent mean-field approach with the use of the P + Q force model was generalized to be applicable to any effective interaction. This advanced approach is called adiabatic TDHF (ATDHF) [144–146].

In the ATDHF theory of Baranger and Vénéroni [144], the density matrix $\rho(t)$ is written in the following form and expanded as a power series with respect to $\chi(t)$.

$$\rho(t) = e^{i\chi(t)}\rho_0(t)e^{-i\chi(t)} \tag{66}$$

$$= \rho_0(t) + i[\chi(t), \rho_0(t)] - \frac{1}{2}[\chi(t), [\chi(t), \rho_0(t)]] + \cdots. \tag{67}$$

Here the matrix elements $\rho_{ij}(t)$ of $\rho(t)$ are defined by $\rho_{ij}(t) = \langle\phi_{\text{HF}}(t)|\, c_j^\dagger c_i\, |\phi_{\text{HF}}(t)\rangle$ with the time-dependent HF state $|\phi_{\text{HF}}(t)\rangle$ and the nucleon creation and annihilation operators, $c_i^\dagger$ and c_j, in the single-particle states i and j. The above expansion is regarded as an adiabatic expansion with respect to $\chi(t)$ which plays the role of the collective momentum associated with the time-even density matrix $\rho_0(t)$. Baranger and Vénéroni suggested a possibility of introducing collective coordinates as parameters that describe the time evolution of the density matrix $\rho_0(t)$. They discussed an iterative procedure to solve the ATDHF equations. This idea has not been realized until now, however. We note that the ATDHF does not reduce to the RPA in the small-amplitude limit if a few collective coordinates are introduced by hand. In fact it gives a collective mass different from the RPA [147].

Villars developed another ATDHF theory with the aim of self-consistently determining the optimum collective coordinates on the basis of the time-dependent variational principle [148]. In the same way as in the ASCC method described in section 8, the TDHFB states are written in the form of equation (38). Villars encountered a difficulty, however, that he could not get unique solutions of the basic equations determining the collective path. This problem was later solved by treating the second-order terms of the momentum expansion in a self-consistent manner (see Mukherjee and Pal [149], and Klein *et al* [150, 151]). It was shown that, when the number of collective coordinate is only one, a collective path maximally decoupled from non-collective degrees of freedom runs along a valley in the multi-dimensional potential-energy surface associated with the TDHF states.

To describe low-frequency collective motions, it is necessary to take into account the pairing correlations. In other words, we need to develop the adiabatic TDHFB (ATDHFB) theory. This is one of the reasons why applications of the ATDHF have been restricted to collective phenomena where pairing correlations play minor roles such as low-energy collisions between spherical closed-shell nuclei [152] and giant resonances [147]. As discussed in section 5.2, when large-amplitude shape fluctuations take place, single-particle level crossings often occur. To follow the adiabatic configuration across the level crossing points, the pairing correlation plays an essential role. Therefore, we need to develop the ATDHFB theory to describe low-frequency collective excitations.

In the past, Dobaczewski and Skalski [153] tried to develop the ATDHFB theory assuming the axially symmetric quadrupole deformation parameter β as the collective coordinate. Quite recently, Li *et al* [154] tried to derive the 5D quadrupole collective Hamiltonian on the basis of the ATDHFB. The extension of ATDHF to ATDHFB is not straightforward, however. This is because, as will be discussed in section 8, we need to decouple the number-fluctuation degrees of freedom from the LACM of interest, respecting the gauge invariance with respect the pairing rotational angles.

7.3. Generator coordinate method

The generator coordinate method (GCM) has been used for a wide variety of nuclear collective phenomena [155–157]. Using the angular-momentum projector $\hat{P}_{IMK}$ and the neutron (proton)-number projector $\hat{P}_N$ ($\hat{P}_Z$), we write the state vector as a superposition of the projected mean-field states with different deformation parameters (β, γ),

$$|\Psi^i_{NZIM}\rangle = \int d\beta d\gamma \sum_K f^i_{NZIK}(\beta, \gamma) \hat{P}_N \hat{P}_Z \hat{P}_{IMK} |\phi(\beta, \gamma)\rangle.$$
(68)

Because the projection operators contain integrations, it has been a difficult task to carry out such high-dimensional numerical integrations in solving the Hill–Wheeler equation for the states $|\phi(\beta, \gamma)\rangle$ obtained by the constrained HFB method. In recent years, however, remarkable progress has been taking place, which makes it possible to carry out such large-scale numerical computations [158–163]. The HFB calculations with use of density-dependent effective interactions are better founded on density functional theory (DFT). Accordingly, the modern GCM calculation is referred to as 'multi-reference DFT' [158].

We can derive a collective Schrödinger equation by making the gaussian overlap approximation (GOA) to the Hill–Wheeler equation [164–167]. There is no guarantee, however, that dynamical effects associated with time-odd components of moving mean field are sufficiently taken into account in the collective inertial masses obtained through this procedure. It is well known for the case of center of mass

motion that we need to use complex generator coordinates to obtain the correct mass. This fact indicates that collective momenta conjugate to collective coordinates should also be treated as generator coordinates [54, 168].

A fundamental question is how to choose the optimal generator coordinates. With the variational principle, Holzwarth and Yukawa [169] proved that the mean-field states parametrized by a single optimal generator coordinate run along a valley of the collective potential energy surface. This line of investigation stimulated the challenge toward constructing a microscopic theory of LACM [170]. In this connection, we note that conventional GCM calculations parametrized by a few real generator coordinates do not reduce to the (Q)RPA in the small-amplitude limit. It should be distinguished from the case that all two-quasiparticle (particle-hole) degrees of freedom are treated as complex generator coordinates [171].

It is very important to distinguish the 5D collective Hamiltonian obtained by making use of the GOA to the GCM from that derived in the preceding section by using the LQRPA to the ASCC method. In the latter, the canonical conjugate pairs of collective coordinate and momentum are self-consistently derived on the basis of the time-dependent variational principle. The canonical formulation enables us to adopt the standard canonical quantization procedure. Furthermore, effects of the time-odd components of the moving mean field are automatically taken into account in the collective inertial masses. It is therefore misleading to say as if the 5D collective Hamiltonian approach is an approximation to the full 5D (three Euler angles, β, and γ) GCM calculation.

Additional remarks

In view of the above points, it is desirable to carry out a systematic comparison of collective inertial masses evaluated by different approximations including the LQRPA (based on the ASCC method summarized in the next section), the adiabatic cranking methods, the ATDHFB, and the GCM + GOA for a better understanding of their physical implications. In this connection, we notice that the results of the recent GCM calculation for ^{76}Kr [162], using the particle-number and angular-momentum projected basis, equation (68), are rather similar to those obtained by use of the Bohr–Mottelson collective Hamiltonian with the Inglis–Belyaev cranking masses, except for an overall overestimation of the excitation energies by about 20%. This work casts an interesting question as to why the two different approaches yield rather similar results.

8. Fundamentals of microscopic theory of LACM

In this section, we review the modern concept of LACM and the fundamental theory underling the LQRPA method used in section 5 to derive the Bohr–Mottelson collective Hamiltonian.

8.1. Extraction of collective submanifold

It is possible to formulate the TDHFB dynamics as the classical Hamilton equations for canonical variables in the TDHFB phase space [63, 75, 101]. The dimension of this phase space is very large; twice of the number of all the two-quasiparticle pairs. The TDHFB state vector $|\phi(t)\rangle$ can be regarded as a generalized coherent state moving on a trajectory in the large-dimensional TDHFB phase space. For low-frequency collective motions, however, we assume that the time evolution is governed by a few collective variables.

During the attempts to construct microscopic theory of LACM since the latter half of the 1970's, significant progress has been achieved in the fundamental concepts of collective motion. Especially important is the recognition that microscopic derivation of the collective Hamiltonian is equivalent to extraction of a collective submanifold embedded in the TDHFB phase space, which is approximately decoupled from other 'non-collective' degrees of freedom. From this point of view we can say that collective variables are nothing but *local canonical variables* which can be flexibly chosen on this submanifold. Here, we recapitulate recent developments achieved on the basis of such concepts.

Attempts to formulate a LACM theory without assuming adiabaticity of large-amplitude collective motion were initiated by Rowe and Bassermann [172] and Marumori [173] and led to the formulation of the SCC method by Marumori, Maskawa, Sakata, and Kuriyama [59]. In these approaches, collective coordinates and collective momenta are treated on the same footing. In the SCC method, basic equations determining the collective submanifold are derived by requiring *maximal decoupling* of the collective motion of interest from other non-collective degrees of freedom. The collective submanifold is invariant with respect to the choice of the coordinate system, whereas the collective coordinates depend on it. The idea of coordinate-independent theory of collective motion was developed also by Rowe [174], and Yamamura and Kuriyama [63]. This idea had a significant impact on the fundamental question, '*what are the collective variables?*'. The SCC method was first formulated on the basis of the TDHF theory without pairing. Later, it is extended to treat pairing correlations in superfluid nuclei on the basis of the TDHFB theory [61].

In the SCC method, the TDHFB state $|\phi(t)\rangle$ is written as $|\phi(q, p)\rangle$ under the assumption that the time evolution is governed by a few collective coordinates $q = (q^1, q^2, \cdots, q^f)$ and collective momenta $p = (p_1, p_2, \cdots, p_f)$. The parametrization of the TDHFB state with the $2f$-degrees of freedom (q, p) means that we define a submanifold inside the TDHFB phase space, which is called '*collective submanifold.*' Below, we summarize the basic equations that determine the collective submanifold on which the TDHFB state $|\phi(q, p)\rangle$ evolves in time. (For simplicity, we here omit the terms arising from the pairing-rotational degrees of freedom, which will be discussed in section 8.4.)

8.1.1. Invariance principle of the TDHFB equation
We require that the TDHFB equation of motion is invariant in the collective submanifold. In a variational form, this requirement can be written as

$$\delta \langle \phi(q, p)| \left(i\frac{\partial}{\partial t} - \hat{H} \right) |\phi(q, p)\rangle = 0. \quad (69)$$

Here, the variation δ is given by $\delta |\phi(q, p)\rangle = a_i^\dagger a_j^\dagger |\phi(q, p)\rangle$ in terms of the quasiparticle operators $(a_i^\dagger, a_j)$, which satisfy the vacuum condition, $a_i |\phi(q, p)\rangle = 0$. Under the basic assumption, we can replace the time derivative with

$$\frac{\partial}{\partial t} = \sum_{i=1}^{f} \left(\dot{q}^i \frac{\partial}{\partial q^i} + \dot{p}_i \frac{\partial}{\partial p_i} \right) = \dot{q}^i \frac{\partial}{\partial q^i} + \dot{p}_i \frac{\partial}{\partial p_i}. \quad (70)$$

Hereafter, to simplify the notation, we adopt the Einstein summation convention and remove $\sum_{i=1}^{f}$. Accordingly, we can rewrite equation (69) as

$$\delta \langle \phi(q, p)| \{ \dot{q}^i \mathring{P}_i(q, p) - \dot{p}_i \mathring{Q}^i(q, p) - \hat{H} \} |\phi(q, p)\rangle = 0, \quad (71)$$

where the local infinitesimal generators are defined by

$$\mathring{P}_i(q, p)|\phi(q, p)\rangle = i\frac{\partial}{\partial q^i} |\phi(q, p)\rangle, \quad (72)$$

$$\mathring{Q}^i(q, p)|\phi(q, p)\rangle = -i\frac{\partial}{\partial p_i} |\phi(q, p)\rangle. \quad (73)$$

These are one-body operators which can be written as linear combinations of bilinear products $\{a_i^\dagger a_j^\dagger, a_j a_i\}$ of the quasiparticle operators defined with respect to $|\phi(q, p)\rangle$.

8.1.2. Canonicity conditions.
We require q and p to be canonical variables. According to the Frobenius-Darboux theorem [175], pairs of canonical variables (q, p) exist for the TDHFB states $|\phi(q, p)\rangle$ satisfying the following *canonicity conditions*,

$$\langle \phi(q, p)| \mathring{P}_i(q, p) |\phi(q, p)\rangle = p_i + \frac{\partial S}{\partial q^i}, \quad (74)$$

$$\langle \phi(q, p)| \mathring{Q}^i(q, p) |\phi(q, p)\rangle = -\frac{\partial S}{\partial p_i}, \quad (75)$$

where S is an arbitrary differentiable function of q and p [59, 63, 64]. By specifying the functional form of $S(q, p)$ and $S'(q', p')$ and demanding that the form of these equations be preserved, we can fix the type of allowed canonical transformations, $(q, p) \rightarrow (q', p')$ among the collective variables. We shall discuss typical examples in sections 8.2 and 8.3, and call the canonicity conditions with a specified function $S(q, p)$ '*canonical-variable conditions.*' Taking derivatives of equations (74) and (75) with respect to p_i and q^i, respectively, we can easily confirm that the local infinitesimal generators satisfy the 'weakly' canonical commutation relations,

$$\langle \phi(q, p)| [\mathring{Q}^i(q, p), \mathring{P}_j(q, p)] |\phi(q, p)\rangle = i\delta_{ij}. \quad (76)$$

Taking variations of equation (71) in the direction of the collective variables, q and p, generated by $\mathring{P}_i$ and $\mathring{Q}^i$, we

obtain the Hamilton equations of motion,

$$\frac{\mathrm{d}q^i}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial q^i}. \quad (77)$$

Here, the total energy $\mathcal{H}(q, p) \equiv \langle \phi(q, p)| \hat{H} |\phi(q, p)\rangle$ plays the role of the classical collective Hamiltonian.

8.1.3. Equation of collective submanifold. The variational principle (71) and equation (77) lead to the equation of collective submanifold:

$$\delta \langle \phi(q, p)| \left\{ \hat{H} - \frac{\partial \mathcal{H}}{\partial p_i} \mathring{P}_i(q, p) \right.$$
$$\left. - \frac{\partial \mathcal{H}}{\partial q^i} \mathring{Q}^i(q, p) \right\} |\phi(q, p)\rangle = 0. \quad (78)$$

Taking variations $\delta_\perp$ in the directions orthogonal to q and p, we see that

$$\delta_\perp \langle \phi(q, p)| \hat{H} |\phi(q, p)\rangle = 0. \quad (79)$$

This implies that the energy expectation value is stationary with respect to all variations except for those along directions tangent to the collective submanifold. In other words, the large-amplitude collective motion is decoupled from other modes of excitation.

8.2. Solution with (η, η^*) expansion

In the original paper of the SCC method [59], the TDHFB state $|\phi(q, p)\rangle$ is written as

$$|\phi(q, p)\rangle = U(q, p)|\phi_0\rangle = \mathrm{e}^{\mathrm{i}\hat{G}(q, p)}|\phi_0\rangle. \quad (80)$$

Here, $U(q, p)$ is a time-dependent unitary transformation written in terms of an Hermitian one-body operator $\hat{G}(q, p)$. The HFB ground state $|\phi_0\rangle$ is taken as an initial state; $U(q, p) = 1$ at $(q, p) = (0, 0)$.

Using complex variables $\eta = (\eta_1, \eta_2, \cdots, \eta_f)$ defined by

$$\eta_i = \frac{1}{\sqrt{2}}(q^i + \mathrm{i}p_i), \quad \eta_i^* = \frac{1}{\sqrt{2}}(q^i - \mathrm{i}p_i), \quad (81)$$

we can rewrite the TDHFB state as

$$|\phi(\eta, \eta^*)\rangle = U(\eta, \eta^*)|\phi_0\rangle = \mathrm{e}^{\mathrm{i}\hat{G}(\eta, \eta^*)}|\phi_0\rangle. \quad (82)$$

Correspondingly, we define local infinitesimal generators, $\mathring{O}_i^\dagger(\eta, \eta^*)$ and $\mathring{O}_i(\eta, \eta^*)$, by

$$\mathring{O}_i^\dagger(\eta, \eta^*)|\phi(\eta, \eta^*)\rangle = \frac{\partial}{\partial \eta_i} |\phi(\eta, \eta^*)\rangle, \quad (83)$$

$$\mathring{O}_i(\eta, \eta^*)|\phi(\eta, \eta^*)\rangle = -\frac{\partial}{\partial \eta_i^*} |\phi(\eta, \eta^*)\rangle. \quad (84)$$

Replacing (q, p) by (η, η^*), the equation of collective submanifold (78) is rewritten as

$$\delta \langle \phi_0| U^\dagger(\eta, \eta^*) \left\{ \hat{H} - \frac{\partial \mathcal{H}}{\partial \eta_i^*} \mathring{O}_i^\dagger(\eta, \eta^*) \right.$$
$$\left. - \frac{\partial \mathcal{H}}{\partial \eta_i} \mathring{O}_i(\eta, \eta^*) \right\} U(\eta, \eta^*)|\phi_0\rangle = 0. \quad (85)$$

Here, the variation is to be performed only for the HFB ground state $|\phi_0\rangle$.

Let us consider the following canonical-variable conditions,

$$\langle \phi(\eta, \eta^*)| \mathring{O}_i^\dagger(\eta, \eta^*)|\phi(\eta, \eta^*)\rangle = \frac{1}{2}\eta_i^*, \quad (86)$$

$$\langle \phi(\eta, \eta^*)| \mathring{O}_i(\eta, \eta^*)|\phi(\eta, \eta^*)\rangle = \frac{1}{2}\eta_i, \quad (87)$$

which are obtained by a specific choice of $S = -\frac{1}{2}\sum_i q^i p_i$ in the canonicity conditions, (74) and (75). From equations (86) and (87), we can easily obtain the 'weak' boson commutation relations,

$$\langle \phi(\eta, \eta^*)|[\mathring{O}_i(\eta, \eta^*), \mathring{O}_j^\dagger(\eta, \eta^*)]|\phi(\eta, \eta^*)\rangle = \delta_{ij}. \quad (88)$$

We note that only linear canonical transformations among η and η^*, which do not change the power of (η, η^*), are allowed under the conditions, (86) and (87). Therefore, these canonical-variable conditions are suitable for solving the variational equation (85) by means of a power series expansion of $\hat{G}$ with respect to (η, η^*):

$$\hat{G}(\eta, \eta^*) = \hat{G}_i^{(10)}\eta_i^* + \hat{G}_i^{(01)}\eta_i + \hat{G}_{ij}^{(20)}\eta_i^*\eta_j^*$$
$$+ \hat{G}_{ij}^{(11)}\eta_i^*\eta_j + \hat{G}_{ij}^{(02)}\eta_i\eta_j + \cdots. \quad (89)$$

Requiring that the variational principle (85) holds for every power, we can successively determine the one-body operator $\hat{G}^{(m,n)}$ with $m + n = 1, 2, 3, \cdots$. This method of solution is called the '(η, η^*)-expansion method.' Because (η, η^*) are complex canonical variables, they are replaced by boson operators after the canonical quantization. The lowest linear order corresponds to the QRPA. Accordingly, the collective variables (η_i, η_i^*) correspond to a specific QRPA mode in the small-amplitude limit. In the higher orders, however, the microscopic structure of $\hat{G}$ changes as a function of (η, η^*) due to the mode-mode coupling effects among different QRPA modes. In this sense, the (η, η^*)-expansion method may be regarded as a dynamical extension of the boson expansion method [176]. Thus, it is a powerful method of treating anharmonic effects originating from mode-mode couplings, as shown in its application to the two-phonon states of anharmonic γ vibration [50, 177]. The SCC method was also used for derivation of the 5D collective Hamiltonian and analysis of the quantum phase transition from spherical to deformed shapes [178] and for constructing diabatic representation in the rotating shell model [125]. The validity of the canonical quantization procedure, including a treatment of the ordering ambiguity problem, was examined in [176]. Description of the 3D rotational motions by means of the

SCC method was discussed in [112] from a viewpoint of constrained dynamical system.

8.3. Solution with adiabatic expansion

The (η, η^*) expansion about a single HFB equilibrium point is not suitable for treating situations where a few local minima having different shapes energetically compete in the HFB potential-energy surface and large-amplitude shape-mixing vibrations occur. It is also difficult to apply the expansion method to a collective motion which goes far away from the equilibrium, such as nuclear fission. The time evolution of these low-energy LACM's in nuclei are usually slow (adiabatic) in comparison with the time scale of the single-particle motions. For describing adiabatic LACM extending over very far from the HFB equilibrium, a new method of solution has been proposed [102]. In this method, the basic equations of the SCC method are solved by an expansion with respect to the collective momenta, keeping full orders in the collective coordinates. It is called 'adiabatic SCC (ASCC) method.' Similar methods have been proposed also by Klein, Walet, and Do Dang [150], and Almehed and Walet [179], but the gauge invariance in the TDHFB theory (discussed in section 8.4 below) were not considered in these papers.

A microscopic theory for adiabatic LACM is constructed by the ASCC method in the following way. We assume that the TDHFB state $|\phi(q, p)\rangle$ can be written in a form

$$|\phi(q, p)\rangle = \exp\{ip_i \hat{Q}^i(q)\}|\phi(q)\rangle, \qquad (90)$$

where $\hat{Q}^i(q)$ are infinitesimal generators of p_i locally defined at the state $|\phi(q)\rangle$ that represents a TDHFB state $|\phi(q, p)\rangle$ at $p \to 0$. This state $|\phi(q)\rangle$ is called a 'moving-frame HFB state.'

We use the following canonical-variable conditions different from (86) and (87),

$$\langle\phi(q, p)|\, \mathring{P}_i(q, p)|\phi(q, p)\rangle = p_i, \qquad (91)$$

$$\langle\phi(q, p)|\, \mathring{Q}^i(q, p)|\phi(q, p)\rangle = 0, \qquad (92)$$

which are obtained by putting $S = \text{const.}$ in the canonicity conditions (74) and (75). These canonical-variable conditions are suitable for the adiabatic expansion with respect to the collective momenta p, because only point transformations, $q \to q'(q)$ (more generally, similarity transformations) which do not mix p and q, are allowed under the conditions, (91) and (92). We insert the above form of the TDHFB state (90) into the equation of collective submanifold (85) and the canonical-variable conditions, (91) and (92), and make a power-series expansion in p. We can determine the microscopic structures of $\hat{Q}^i(q)$ and $|\phi(q)\rangle$ by requiring that these equations hold for every power of p. We take into account up to the second order. The canonical variable conditions, (91) and (92), then yield the 'weakly' canonical commutation relations,

$$\langle\phi(q)|[\hat{Q}^i(q), \hat{P}_j(q)]|\phi(q)\rangle = i\delta_{ij}. \qquad (93)$$

Here, $\hat{P}_i(q)$ are infinitesimal generators of q^i, locally defined at the state $|\phi(q)\rangle$ by

$$\hat{P}_i(q)|\phi(q)\rangle = i\frac{\partial}{\partial q^i}|\phi(q)\rangle. \qquad (94)$$

We also obtain $\langle\phi(q)|\hat{Q}^i(q)|\phi(q)\rangle = 0$ and $\langle\phi(q)|\hat{P}_i(q)|\phi(q)\rangle = 0$, which are trivially satisfied. Note that $\hat{Q}^i(q)$ and $\hat{P}_i(q)$ operate on $|\phi(q)\rangle$, while $\mathring{Q}^i(q, p)$ and $\mathring{P}_i(q, p)$ on $|\phi(q, p)\rangle$.

The time derivatives, $\dot{q}^i$ and $\dot{p}_i$, are determined by the Hamilton equations of motion (77) with the classical collective Hamiltonian $\mathcal{H}(q, p)$ expanded with respect to p up to the second order,

$$\mathcal{H}(q, p) = V(q) + \frac{1}{2}B^{ij}(q)p_i p_j, \qquad (95)$$

where

$$V(q) = \mathcal{H}(q, p = 0), \quad B^{ij}(q) = \left.\frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}\right|_{p=0}. \qquad (96)$$

The collective inertial tensors $B_{ij}(q)$ are defined as the inverse matrix of $B^{ij}(q)$, $B^{ij}B_{jk} = \delta^i_k$. Under these preparations, the following equations, which constitute the core of the ASCC method, can be derived [102]. Here, to further simplify the expression, we show the case for normal systems with TDHF (see the next subsection about the extension to TDHFB).

1. *Moving-frame HF(B) equation*

$$\delta\langle\phi(q)|\hat{H}_M(q)|\phi(q)\rangle = 0, \qquad (97)$$

where $\hat{H}_M(q)$ represents the Hamiltonian in the frame attached to the moving mean field,

$$\hat{H}_M(q) = \hat{H} - \frac{\partial V}{\partial q^i}\hat{Q}^i(q), \qquad (98)$$

and is called 'moving-frame Hamiltonian.'

2. *Moving-frame (Q)RPA equations (or 'Local harmonic equations')*

$$\delta\langle\phi(q)|[\hat{H}_M(q), \hat{Q}^i(q)] - \frac{1}{i}B^{ij}(q)\hat{P}_j(q)$$
$$+ \frac{1}{2}\left[\frac{\partial V}{\partial q^j}\hat{Q}^j(q), \hat{Q}^i(q)\right]|\phi(q)\rangle = 0, \qquad (99)$$

$$\delta\langle\phi(q)|[\hat{H}_M(q), \frac{1}{i}\hat{P}_i(q)] - C_{ij}(q)\hat{Q}^j(q)$$
$$- \frac{1}{2}\left[\left[\hat{H}_M(q), \frac{\partial V}{\partial q^k}\hat{Q}^k(q)\right], B_{ij}(q)\hat{Q}^j(q)\right]|\phi(q)\rangle = 0, \qquad (100)$$

where

$$C_{ij}(q) = \frac{\partial^2 V}{\partial q^i \partial q^j} - \Gamma^k_{ij}\frac{\partial V}{\partial q^k}, \qquad (101)$$

$$\Gamma_{ij}^k(q) = \frac{1}{2}B^{kl}\left(\frac{\partial B_{li}}{\partial q^j} + \frac{\partial B_{lj}}{\partial q^i} - \frac{\partial B_{ij}}{\partial q^l}\right). \quad (102)$$

The double-commutator term in equation (100) arises from the q-derivative of the infinitesimal generators $\hat{Q}^i(q)$ and represents the curvatures of the collective submanifold. Diagonalizing the matrix, $B^{ik}C_{kj}$, at each point of q, we may identify the local normal modes and eigen-frequencies $\omega_i(q)$ of the moving-frame QRPA equations.

Extension from TDHF to TDHFB for superfluid nuclei can be achieved by introducing the number fluctuation $n \equiv N - N_0$ and their conjugate angle φ as additional collective variables [102] (see section 8.4).

Solving equations (97), (99), and (100) self-consistently, we can determine the microscopic expressions of the infinitesimal generators, $\hat{Q}^i(q)$ and $\hat{P}_i(q)$, in bilinear forms of the quasiparticle creation and annihilation operators defined locally with respect to $|\phi(q)\rangle$. These equations reduce to the HF(B) and (Q)RPA equations at the equilibrium point where $\partial V/\partial q^i = 0$. Therefore, they are regarded as natural extensions of the well-known HFB-QRPA equations to non-equilibrium states.

Some key points of the ASCC method are noted below:

i. *Meaning of adiabatic approximation.* The term 'adiabatic approximation' is frequently used for different meanings. In the present context, we use this term for the approximate solution of the variational equation (71) by taking into account up to the second order in an expansion with respect to the collective momenta p. It is important to note that the effects of finite frequency of the LACM are taken into account through the moving-frame QRPA equation. No assumption is made, such as that the kinetic energy of LACM is much smaller than the lowest two-quasiparticle excitation energy at every point of q.

ii. *Difference from the constrained HFB equations.* The moving-frame HFB equation (97) resembles the constrained HFB equation. An essential difference is that the infinitesimal generators $\hat{Q}^i(q)$ are here self-consistently determined together with $\hat{P}_i(q)$ as solutions of the moving-frame QRPA equations, (99) and (100), at every point of the collective coordinate q. Thus, contrary to constrained operators in the constrained HFB theory, their microscopic structure changes as functions of q. The optimal 'constraining' operators are locally determined at each q. The collective submanifold embedded in the TDHFB phase space is extracted in this way.

iii. *Canonical quantization.* The collective inertial tensors $B_{ij}(q)$ take a diagonal form when the classical collective Hamiltonian is represented in terms of the local normal modes of the moving-frame QRPA equations. We can then make a scale transformation of the collective coordinates q such that they become unity. The kinetic energy term in the resulting collective Hamiltonian depends only on p. Thus, there is no ordering ambiguity

between q and p in the canonical quantization procedure.

iv. *Collective inertial mass.* Although the collective submanifold is invariant against coordinate transformations, $q \to q'(q)$, the collective inertial tensors $B_{ij}(q)$ depends on the adopted coordinate system. The scale of the coordinates can be arbitrarily chosen as far as the canonical-variable conditions are satisfied. To obtain physical insights and to examine the effects of time-odd components in the mean field, however, it is convenient to adopt a conventional coordinate system, such as the quadrupole (β, γ) variables.

8.4. Inclusion of the pairing rotation and gauge invariance

In the QRPA at the HFB equilibrium, the ANG modes such as the number fluctuation (pairing rotational) modes are decoupled from other normal modes. Thereby, the QRPA restores the gauge invariance (number conservation) broken in the HFB mean field [26]. It is desirable to retain this merit of the QRPA beyond the small-amplitude regime. Otherwise, spurious number-fluctuation modes would heavily mix in the LACM of interest. It is possible to achieve this aim by using the SCC method for superfluid nuclei [61].

Introducing the number fluctuation $n = N - N_0$ and the gauge angle φ (conjugate to n) as additional collective variables, we generalize the TDHFB state (90) to

$$|\phi(q, p, \varphi, n)\rangle = \mathrm{e}^{-\mathrm{i}\varphi\hat{N}}|\phi(q, p, n)\rangle, \quad (103)$$

$$|\phi(q, p, n)\rangle = \mathrm{e}^{\mathrm{i}[p_i\hat{Q}^i(q)+n\hat{\Theta}(q)]}|\phi(q)\rangle. \quad (104)$$

Here $\hat{N}$ and $\hat{\Theta}(q)$ denote the nucleon-number operator and the infinitesimal generator of n, respectively, and N_0 is a reference value of the nucleon number N. In the generalized TDHFB state, (103), the number operator $\hat{N}$ and the state vector $|\phi(q, p, n)\rangle$ may be regarded as an infinitesimal generator of the gauge angle φ and an intrinsic state with respect to the pairing rotational motion, respectively. It is straightforward to extend the equation for the collective submanifold (71) as

$$\delta\langle\phi(q, p, \varphi, n)|\left\{\mathrm{i}\dot{q}^i\frac{\partial}{\partial q^i} + \mathrm{i}\dot{p}_i\frac{\partial}{\partial p_i}\right.$$
$$\left. + \mathrm{i}\dot{\varphi}\frac{\partial}{\partial\varphi} - \hat{H}\right\}|\phi(q, p, \varphi, n)\rangle = 0. \quad (105)$$

Note that $\dot{n} = 0$, because the Hamilton equations for the canonical conjugate pair (n, φ) are

$$\dot{\varphi} = \frac{\partial\mathcal{H}}{\partial n}, \quad \dot{n} = -\frac{\partial\mathcal{H}}{\partial\varphi}, \quad (106)$$

and the classical collective Hamiltonian $\mathcal{H}(q, p, \varphi, n) \equiv \langle\phi(q, p, \varphi, n)|\hat{H}|\phi(q, p, \varphi, n)\rangle$ does not depend on φ. Making a power-series expansion with respect to n as well as p and considering up to the second order, we can determine $\hat{\Theta}(q)$ simultaneously with $\hat{Q}^i(q)$ and $\hat{P}_i(q)$ such that the moving-frame equations become invariant against the rotation of the gauge angle φ. In fact, we introduce two sets of

$(\hat{N}, \hat{\Theta}(q))$ to describe the pairing rotations of neutrons and protons, separately.

Writing the time derivative $\dot{\varphi}$ of the gauge angle as λ, we can easily confirm that the term proportional to $\dot{\varphi}$ in (105) leads to an operator $\lambda\hat{N}$ on the intrinsic state $|\phi(q, p, n)\rangle$. In this form, $\dot{\varphi}$ corresponds to the chemical potential in the BCS theory of superconductivity. The term, $\lambda\hat{N}$, in the BCS theory is usually interpreted as a constraining term to impose the condition that $\langle\phi(q, p, n)| \hat{N} |\phi(q, p, n)\rangle = N$. It should be emphasized, however, that this term is naturally derived by introducing the concept that the moving-frame TDHFB state, $|\phi(q, p, n)\rangle$, is an intrinsic state with respect to the pairing-rotational motion of the gauge angle φ. In the microscopic approach under discussion, the 'chemical potential' λ plays a role analogous to the rotational velocities $\dot{\varphi}_k$ in equation (50) for the rotational motions in the 3D coordinate space; that is, they are not introduced as Lagrange multipliers but dynamical variables.

Hinohara *et al* investigated the gauge-invariance properties of the ASCC equations and extended the infinitesimal generators $\hat{Q}^i(q)$ to include quasiparticle creation-annihilation ($a_i^\dagger a_j$) parts in addition to two-quasiparticle creation ($a_i^\dagger a_j^\dagger$) and annihilation ($a_j a_i$) parts [180]. This is the reason why equations (99) and (100) are written in a more general form than those originally given in [102]. The gauge invariance of the ASCC method implies that we need to fix the gauge in numerical applications. A convenient procedure for the gauge fixing is given in [180]. A more general consideration on the gauge symmetry of the ASCC method is given from a viewpoint of constrained dynamical systems in a recent paper [181].

8.5. Solution with the LQRPA method

The LQRPA method used in section 5 for the microscopic derivation of the Bohr-Mottelson collective Hamiltonian may be regarded as a non-iterative solution of (97)–(100) in the ASCC method, without the consistency in the generator $\hat{Q}^i(q)$ between the moving-frame HFB equation and the moving-frame QRPA equations. It may also be regarded as a first step of the iterative procedure for solving the self-consistent equations. Equation (40) corresponds to the moving-frame HFB equation (97) with $\hat{Q}^i(q)$ replaced by global one-body operators $\hat{D}_{2m}^{(+)}$. It is worth noting that the moving-frame HFB Hamiltonian $\hat{H}_M$ contains terms, $-\lambda^{(\tau)}\hat{N}^{(\tau)} - \mu_m\hat{D}_{2m}^{(+)}$, which naturally appear from the ASCC equations with the approximation to replace $\hat{Q}^i(q)$ in $\hat{H}_M(q)$ by $\hat{D}_{2m}^{(+)}$. In fact, the origin of these terms are not constraints, but the time-derivative terms in equation (105). The LQRPA equations, (44) and (45), are obtained by ignoring the curvature term in the moving-frame QRPA equations, (99) and (100).

The validity of the LQRPA method was examined for the cases where a well-defined valley (collective path) exists in the collective potential $V(\beta, \gamma)$ [105]. The rotational and vibrational inertial masses calculated by using the LQRPA method were compared with those obtained by the fully self-consistent ASCC calculations. It was confirmed that they

agree very well, indicating that the LQRPA is a good approximation to the ASCC calculation along the collective path on the (β, γ) plane. The accuracy of the LQRPA method on the full (β, γ) plane may be checked by making an iterative calculation; that is, by solving equation (40) replacing $\hat{D}_{2m}^{(+)}$ with the solutions $\hat{Q}^i(q)$ of the LQRPA equations (44) and (45), and evaluate the deviations from the result of the lowest-order LQRPA calculation. This task remains for future, however.

9. Open problems in quadrupole collective dynamics

Nowadays, the domain of quadrupole collective phenomena awaiting applications of the Bohr–Mottelson collective model is increasing enormously covering wide regions from low to highly excited states, from small to large angular momenta, and from proton-drip line to neutron-drip line. Among many interesting subjects, we remark here on only a few.

9.1. Shape coexistence, pairing fluctuation and mysterious 0^+ states

As mentioned in section 2, when two different HFB equilibrium shapes coexist in the same energy region, large-amplitude shape mixings through the potential barriers take place. These phenomena may be regarded as a kind of macroscopic quantum tunneling where the potential barrier itself is generated as a consequence of the dynamics of the self-bound quantum system. For instance, two strongly distorted rotational bands built on the oblate and prolate shapes, which seem to coexist and interact with each other, have been found in ^{68}Se [41, 105]. Such phenomena are widely seen in low-energy spectra from light to heavy nuclei [41]. We have applied the Bohr–Mottelson collective Hamiltonian to some of these shape coexistence/mixing phenomena with the use of the collective inertial masses microscopically calculated by means of the LQRPA method. An illustrative example is presented for ^{74}Kr in section 6.

One of the issues related to the shape coexistence/fluctuation is to clarify the nature of deformation in neutron-rich nuclei around ^{32}Mg having the magic number $N = 20$ of the spherical shell model [41]. In the P + Q model, the major properties of low-lying states in open-shell nuclei are determined by the competition between the pairing (particle-particle, hole-hole) and quadrupole (particle-hole) correlations acting among nucleons in partially filled major shells. On the other hand, in situations where the pairing and quadrupole correlations *across* the spherical major shells play the major role, such as in neutron-rich Mg isotopes around ^{32}Mg, the two different correlations seem to act coherently and generate interesting collective phenomena where large-amplitude fluctuations in the monopole and quadrupole pairing gaps as well as the quadrupole shape take place simultaneously [107].

In some nuclei, the first excited 0^+ state appears below the first excited 2^+ state. An example is the first excited 0^+ state of ^{72}Ge which is known from old days but still poorly understood. This anomaly occurs in the vicinity of $N = 40$

where the $g_{9/2}$ shell starts to be partially filled (due to the pairing). It has been pointed out [182–185] that the mode-mode coupling between the 0^+ member of the two quadrupole-phonon triplet and the neutron pairing vibration becomes especially strong near $N = 40$ and generates such anomalous 0^+ states with extremely low-excitation energy.

As reviewed by Hyde and Wood [41] and by Garrett [186], the nature of the low-lying excited 0^+ states systematically found in recent experiments, in addition to those known from old days, is not well understood. It is thus quite challenging to apply, in a systematic ways, the Bohr–Mottelson collective Hamiltonian approach to all of these data, from light to heavy and from stable to unstable nuclei, and explore the limit of the applicability. Considering the suggestion [182–185] about the coupling effects with pairing vibrations, one of the basic questions is *'under what situations we need to extend the 5D collective Hamiltonian to 7D by explicitly treating the proton and neutron pairing gaps as dynamical variables.'*

We should mention about a few fundamental subjects that are closely related to the shape coexistence phenomena in low-lying states: in the decays of superdeformed rotational bands [187], macroscopic quantum tunnelings through self-consistently generated barriers are very clearly seen. Needless to say, microscopic description of spontaneous fissions is a longstanding yet modern fundamental subject of nuclear structure physics [20, 75]. Recent experimental progress in deep sub-barrier fusion reactions [188] provides another modern problem of macroscopic tunnelings in finite quantum systems.

9.2. Vibrational and rotational modes at high angular momentum

As a nucleus rotates rapidly, excitations of aligned quasi-particles take place [189, 190]. Rapid rotation changes the deformation and shell structure of the mean field. The pair field also disappears eventually at high-spin [191]. These structural changes in the high-spin yrast states significantly affect the properties of vibrational motions built on them (the yrast state is the 'ground' states for given angular momenta). Unfortunately experimental data for low-frequency shape vibrations in the vicinity of the high-spin yrast states have not been accumulated enough. Considering the role of the BCS pairing in forming the collective low-frequency quadrupole vibrations built on the ground state, existence of low-frequency collective vibrations built on the high-spin yrast states is actually not evident, since we expect that the role of the pairing is much less in high-spin states. On the other hand, we expect that the vibrations could compete with rotations in high-spin states because the rotational frequency increases with the angular momentum, and becomes comparable to the vibrational frequencies [192].

Discovery of superdeformed bands [32, 33] shed a new light on the above situation. In superdeformed states, a new shell structure called *superdeformed shell structure* emerges and it creates new low-frequency octupole vibrations on superdeformed states at high angular momentum [193, 194].

These vibrational modes simultaneously break the axial symmetry and the reflection symmetry. Moreover, some experimental data for γ vibrations (quadrupole shape vibration that breaks the axial symmetry) at high spin have been reported [195, 196]. It has been discussed for a long time that the triaxial deformation may be realized at high spin states due to the weakening of the pairing correlations. When the mean field breaks the axial symmetry, a new rotational mode called *wobbling motion* is expected to emerge. Observation of the wobbling rotational band is therefore a clear signature of the occurrence of the triaxial deformation in the mean field. About 15 years ago, the first experimental data on the wobbling band were obtained [197] (see also [198, 199]). Their properties have been theoretically analyzed from various points of view [200–203]. These investigations show that the aligned quasiparticle plays a crucial role in the emergence of the wobbling motion. There is another new phenomenon expected to emerge in the axial-symmetry-broken nuclei under certain conditions: *chiral rotation* and its experimental signature, chiral doublet bands [189]. Experimental search for chiral doublet bands and its precursor phenomena called *chiral vibrations* [204] is currently in progress.

The Bohr–Mottelson collective Hamiltonian as reviewed in this paper is not applicable to quadrupole collective phenomena at high angular momenta. This is because the collective inertial masses and the collective potential $V(\beta, \gamma)$ are calculated at low angular momenta. It seems, however, possible to extend it to describe such high-spin phenomena. We have learned through the success of the cranked shell model [189, 190] that the concept of single-particle motion in a rotating mean field holds very well. This means that major effects of rapid rotation (Coriolis- and centrifugal-force effects) can be captured in the self-consistent mean-field by defining the single-particle motion in a rotating frame of reference attached to the rapidly rotating nucleus. In the extension of the self-consistent mean field to a rotating frame, the time-reversal symmetry is broken, but it opens a new dimension in nuclear structure physics. *In the history of nuclear structure physics, we have been successfully extending the concept of the single-particle motion to a more general mean field. Such extensions have been achieved by breaking some symmetries of the self-consistent mean field.* Let us recall that extension of the concept of single-particle excitation (with spontaneous breaking of the symmetry) and appearance of new collective excitation (restoring the broken symmetry) are *dual concepts* that underline the quantum many-body theory of nuclear structure.

9.3. Low-frequency collective excitations in nuclei near the neutron drip line

The mean field in unstable nuclei near the neutron drip line possesses new features associated with the large neutron to proton ratio, the formation of neutron skin, the weak binding of single-particles states near the Fermi surface, the excitation of neutron pairs into the continuum, etc. The collectivity of surface vibrations may change reflecting the modification of shell structure [205] and the variation of pairing properties

[206]. Thus, the QRPA method has been extended to properly treat the excitations into the continuum [207]. The extended version is called *continuum QRPA*, and it has been applied to weakly bound unstable nuclei [208–210]. The particle-vibration coupling theory has also been extended to include the continuum effects by means of the continuum QRPA method [211].

In stable nuclei, overlaps of different single-particle wave functions become maximum at the surface and generate a strong coherence among many quasiparticle excitations [2]. In the weak binding situation, single-particle wave functions significantly extend from the surface (half-density radius) to the low-density region and acquire strong individualities. It is an open problem how the pairing correlation in such a situation acts to generate the collectivity of vibrational modes. Nowadays, it is one of the central subject in nuclear structure-reaction theory to carry out fully self-consistent HFB+QRPA calculations using the same energy density functional and simultaneously taking into account the deformation, pairing and excitations into the continuum [210]. From such microscopic calculations, for instance, it is suggested [82] that a strong coherence among the quadrupole shape fluctuation and the fluctuations of the monopole and quadrupole pairing gaps may generate a collective vibration unique to the weakly bound neutron-rich nuclei.

At the present time, the major efforts are devoted to clarifying the properties of the ground states and a few excited states of nuclei near the drip line. In the coming future, more experimental data on excitation spectra will be obtained with the progress of ambitious experimental projects now ongoing in the world. We shall then encounter a variety of phenomena that cannot be understood within the small-amplitude approximation for collective motions. It will become necessary to explore the nature of collective motions in nuclei near the drip line by an extension of the collective Hamiltonian approach reviewed in this paper.

10. Concluding remarks

We have reviewed recent approaches to microscopically derive the Bohr–Mottelson collective Hamiltonian on the basis of the time-dependent self-consistent mean field. The *moving* self-consistent mean field is the key concept to the unified understanding of the single-particle and collective motions in nuclei. We hope that this paper fits the aim of this special edition for the 40 year anniversary of Nobel Prize 1975.

Although the progress achieved during these 40 years with the Bohr–Mottelson collective Hamiltonian is spectacular, many interesting subjects of fundamental significance are awaiting our challenge in our road towards understanding quantum collective dynamics in nuclei. As we briefly remarked in the preceding section, it will be very interesting to explore the limits of applicability of the Bohr–Mottelson collective Hamiltonian by systematically applying it to shape coexistence/fluctuation/mixing phenomena. At the present time, the quadrupole collective Hamiltonian is used mainly

for low-spin states. It seems possible, however, to extend the microscopic approach reviewed in this paper to collective phenomena at high-spin states by taking into account the effects of rapid rotation from the beginning in the self-consistent mean fields. In a similar manner, it will be interesting to extend the collective Hamiltonian approach to describe low-lying excited states in neutron-rich unstable nuclei, by taking into account the effects of weak binding and continuum coupling in constructing the self-consistent mean fields. These extensions will open new dimensions in quantum collective dynamics of nuclear structure. Finally, it should be emphasized that one of the great challenges is to calculate the collective inertial masses using the LQRPA method on the basis of the density functional theory.

Appendix A. Quantization in curvilinear coordinates

For Cartesian coordinates $q = (q^1, q^2, ..., q^f)$ in a f-dimensional space, the kinetic energy in classical mechanics is given by $T = \frac{1}{2}\sum_{i=1}^{f}(\dot{q}^i)^2$ in a unit with mass $m = 1$, where $\dot{q}^i$ are time derivatives (velocities) of q^i. After the canonical quantization, we obtain the kinetic energy operator

$$\hat{T} = -\frac{1}{2}\sum_{i=1}^{f}\frac{\partial^2}{\partial q^{i2}} = -\frac{1}{2}\Delta \qquad (107)$$

in the unit with $\hbar = 1$, where Δ is the Laplacian in the Cartesian coordinates.

For the curvilinear coordinates $x = (x^1, x^2, ..., x^f)$ in a f-dimensional curved space, the line element squared may be written as

$$\mathrm{d}s^2 = \sum_{i,j} g_{ij}(x)\mathrm{d}x^i \mathrm{d}x^j \qquad (108)$$

with $g_{ij}(x) = g_{ji}(x)$, using the metric tensor $\{g_{ij}(x)\}$ characterizing the curved space. The kinetic energy in classical

mechanics is then given by

$$
\begin{aligned}
T &= \frac{1}{2}\left(\frac{ds}{dt}\right)^2 \\
&= \frac{1}{2}\sum_{i,j}g_{ij}(x)\frac{dx^i}{dt}\frac{dx^j}{dt}.
\end{aligned}
\tag{109}
$$

Note that the metric tensor $\{g_{ij}(x)\}$ depends on the coordinate x.

According to the Pauli prescription for quantization in curvilinear coordinates, the corresponding kinetic energy operator in quantum mechanics is given by

$$
\begin{aligned}
\hat{T} &= -\frac{1}{2}\Delta \\
&= -\frac{1}{2\sqrt{g(x)}}\sum_{i,j}\frac{\partial}{\partial x^i}\sqrt{g(x)}\,g^{ij}(x)\frac{\partial}{\partial x^j},
\end{aligned}
\tag{110}
$$

where $g(x)$ denotes the determinant of the metric tensor, $g(x) = \det\{g_{ij}(x)\}$, and $g^{ij}(x)$ are the components of the inverse matrix $\{g_{ij}(x)\}^{-1}$. This expression is obtained in a straightforward way by rewriting the Laplacian Δ in the curvilinear coordinates. The Schrödinger equation is written as

$$
\begin{aligned}
&\left(-\frac{1}{2\sqrt{g(x)}}\sum_{i,j}\frac{\partial}{\partial x^i}\sqrt{g(x)}\,g^{ij}(x)\frac{\partial}{\partial x^j} + V(x)\right) \\
&\times \psi(x) = E\psi(x).
\end{aligned}
\tag{111}
$$

The normarization of the wave function is

$$
\int |\psi(x)|^2 d\tau = 1
\tag{112}
$$

with the volume element $d\tau = \sqrt{g(x)}\,dx \equiv \sqrt{g(x^1, x^2, \ldots, x^f)}\,dx^1 dx^2 \cdots dx^f$.

For the Bohr–Mottelson collective model, $f = 5$ and the five collective variables consist of the (β, γ) deformation variables and the three Euler angles ϑ_k; that is, $(x^1 = \beta, x^2 = \gamma, x^3 = \vartheta_1, x^4 = \vartheta_2, x^5 = \vartheta_3)$. The three components of the angular velocity (time-derivatives of the rotational angle) on the intrinsic axes, $\dot{\varphi}_k$ appearing in the classical expression of the rotational energy $T_{\text{rot}} = \frac{1}{2}\sum_{k=1}^3 \mathcal{J}_k(\beta, \gamma)\dot{\varphi}_k^2$, are related with the time derivatives of the Euler angles $\dot{\vartheta}_k$ by

$$
\dot{\varphi}_k = \sum_{k'=1}^3 V_{kk'}\dot{\vartheta}_{k'}
\tag{113}
$$

with

$$
V_{kk'} = \begin{pmatrix} -\sin\vartheta_2\cos\vartheta_3 & \sin\vartheta_3 & 0 \\ \sin\vartheta_2\sin\vartheta_3 & \sin\vartheta_3 & 0 \\ \cos\vartheta_2 & 0 & 1 \end{pmatrix}.
\tag{114}
$$

After the quantization, the classical expression T_{rot} for the rotational energy becomes to $\hat{T}_{\text{rot}} = \sum_k \frac{\hat{I}_k^2}{2\mathcal{J}_k(\beta, \gamma)}$, where the components of the angular-momentum operator on the intrinsic axes, $(\hat{I}_1, \hat{I}_2, \hat{I}_3)$, are represented in terms of the Euler angles $(\vartheta_1, \vartheta_2, \vartheta_3)$ and the derivatives with respect to them. In the same way, we obtain, after carrying out somewhat lengthy but straightforward calculations, the quantum operator $\hat{T}_{\text{vib}}$ for

the kinetic energy of the vibrational motion, given in equation (6), and the determinant of the metric tensor,

$$
g(\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3) = G(\beta, \gamma)\sin^2\vartheta_2,
\tag{115}
$$

with $G(\beta, \gamma)$ given by equation (17). Note that the determinant does not depend on ϑ_1 and ϑ_3. For the definitions of the Euler angles and more details of the calculation, see, e.g., chapter 6 in the textbook of Eisenberg and Greiner [43].

Appendix B. Calculation of E2 transitions and moments

The electric quadrupole ($E2$) operators in the body-fixed frame are given as a sum of neutron and proton contributions with effective charges $e_{\text{eff}}^{(\tau)}$,

$$
\hat{D}_m^{(E2)} = \sum_{\tau=n,p} e_{\text{eff}}^{(\tau)}\hat{D}_{2m}^{(\tau)},
\tag{116}
$$

where $\hat{D}_{2m}^{(\tau)}$ are the quadrupole operator of neutrons and protons, and $\sum_\tau \hat{D}_{2m}^{(\tau)} = \hat{D}_{2m}$. The $E2$ operator in the laboratory frame is related with that in the intrinsic frame as

$$
\hat{D}_m^{\prime(E2)} = \sum_{m'}\mathcal{D}_{mm'}^2(\Omega)\hat{D}_{m'}^{(E2)},
\tag{117}
$$

where $\mathcal{D}$ are Wigner's rotational matrices. The experimental observables such as the $B(E2)$ and the spectroscopic quadrupole moment Q are defined as

$$
B(E2; \alpha I \to \alpha'I') = (2I+1)^{-1}|\langle\alpha I\|\hat{D}^{\prime(E2)}\|\alpha'I'\rangle|^2,
\tag{118}
$$

$$
Q(\alpha I) = \sqrt{\frac{16\pi}{5}}\langle\alpha, I, M=I|\hat{D}_0^{\prime(E2)}|\alpha, I, M=I\rangle.
\tag{119}
$$

Here, the reduced matrix element in equation (118) is defined with the Wigner-Eckart theorem,

$$
\begin{aligned}
&\langle\alpha, I, M=I|\hat{D}_0^{\prime(E2)}|\alpha', I', M'=I\rangle \\
&= \begin{pmatrix} I & 2 & I' \\ -I & 0 & I \end{pmatrix}\langle\alpha I\|\hat{D}^{\prime(E2)}\|\alpha'I'\rangle.
\end{aligned}
\tag{120}
$$

Substituting equation (13) into $|\alpha, I, M\rangle$, we obtain [46]

$$
\begin{aligned}
\langle\alpha I\|\hat{D}^{\prime(E2)}\|\alpha'I'\rangle =\ & \sqrt{(2I+1)(2I'+1)}\,(-)^I \\
\times \sum_K \Bigg\{& \begin{pmatrix} I & 2 & I' \\ -K & 0 & K \end{pmatrix}\langle\Phi_{\alpha,I,K}|\hat{D}_{0+}^{(E2)}|\Phi_{\alpha',I',K}\rangle \\
& + \sqrt{(1+\delta_{K0})}\Bigg[\begin{pmatrix} I & 2 & I' \\ -K-2 & 2 & K \end{pmatrix} \\
& \times \langle\Phi_{\alpha,I,K+2}|\hat{D}_{2+}^{(E2)}|\Phi_{\alpha',I',K}\rangle \\
& + (-)^{I+I'}\begin{pmatrix} I & 2 & I' \\ K & 2 & -K-2 \end{pmatrix} \\
& \times \langle\Phi_{\alpha,I,K}|\hat{D}_{2+}^{(E2)}|\Phi_{\alpha',I',K+2}\rangle\Bigg]\Bigg\}
\end{aligned}
\tag{121}
$$

with $\hat{D}_{m+}^{(E2)} = (\hat{D}_m^{(E2)} + \hat{D}_{-m}^{(E2)})/2$.

The quadrupole matrix elements between the intrinsic states are evaluated using the collective wave functions as

$$
\begin{aligned}
&\langle \Phi_{\alpha,I,K}| \ \hat{D}_{m+}^{(E2)} \ |\Phi_{\alpha',I',K'}\rangle \\
&= \int \mathrm{d}\beta \mathrm{d}\gamma \sqrt{G(\beta,\gamma)} \Phi_{\alpha IK}^*(\beta,\gamma) D_{m+}^{(E2)}(\beta,\gamma) \Phi_{\alpha' I' K'}(\beta,\gamma),
\end{aligned}
\tag{122}
$$

where

$$
D_{m+}^{(E2)}(\beta,\gamma) = \langle \phi(\beta,\gamma)| \ \hat{D}_{m+}^{(E2)} \ |\phi(\beta,\gamma)\rangle.
\tag{123}
$$

Appendix C. Illustration of triaxial deformation dynamics

We consider a simple model that may be useful to understand several interesting limits of triaxial deformation dynamics in a unified perspective. The model discussed below includes several situations, such as the axially symmetric rotor model, the γ-unstable model [51], the triaxial rigid rotor model [52], and oblate-prolate shape coexistence in an ideal situation. This model enables us to describe the smooth change between these extreme situations by changing a few parameters. Here we show only the simplest example, referring [212] for more general cases. To focus our attention on the γ degree of freedom, we fix the β degree of freedom at a constant value β_0 in the Bohr–Mottelson collective Hamiltonian (5) and parametrize the collective potential $V(\beta,\gamma)$ as $V(\beta_0,\gamma) = V_\beta(\beta_0) + V_\gamma(\beta_0,\gamma)$ with

$$
V_\gamma(\beta_0,\gamma) = V_0(\beta_0)\sin^2 3\gamma + V_1(\beta_0)\cos 3\gamma.
\tag{124}
$$

This form is readily obtained by expanding $V(\beta,\gamma)$ in powers of the basic second- and third-order invariants, β^2 and $\beta^3 \cos 3\gamma$, and keeping up to the second order in $\beta^3 \cos 3\gamma$.

When $V_1 = 0$, the collective potential is symmetric with respect to the reflection about $\gamma = 30°$. For positive V_0, two minima appear at the oblate ($\gamma = 60°$) and prolate ($\gamma = 0°$) shapes. They are degenerated and separated by a barrier located at $\gamma = 30°$. For negative V_0, on the other hand, the barrier top at $\gamma = 30°$ turns out to be the single minimum, and it becomes deeper as $|V_0|$ increases. The term V_1 breaks the oblate-prolate symmetry, and controls the magnitude of the symmetry breaking. For positive (negative) V_1, the oblate (prolate) shape becomes the minimum (when V_0 is positive).

Let us discuss the simplest case where $V_1 = 0$, and the collective inertial masses $(D_{\beta\beta}, D_{\gamma\gamma}\beta_0^{-2}, D_1, D_2, D_3)$ are replaced by a common constant D, and $D_{\beta\gamma}$ is ignored. In this case, both the collective potential and the moments of inertia $\mathcal{J}(\beta,\gamma)$ are symmetric with respect to the reflection about $\gamma = 30°$, so that the collective Hamiltonian possesses the oblate-prolate symmetry. Furthermore, D and β_0 appear only in the form $(2D\beta_0^2)^{-1}$ in the kinetic energy. Therefore the ratio $2D\beta_0^2 V_0$ is a single quantity that enters in the collective Schrödinger equation (12) and determines the dynamics. A particular case of $V_0 = 0$ is known to be the Wilets-Jean

γ-unstable model [51]. In this case the excitation spectra just scale with the factor $(2D\beta_0^2)^{-1}$.

Figure 6 shows excitation spectra as functions of V_0. The excitation energies are normalized with the excitation energy of the second 0^+ state (first excited 0^+ state) $E(0_2^+)$ at $V_0 = 0$ (which is 1.8 MeV for $\beta_0^2 = 0.1$ and $D = 50$ MeV^{-1}). Because of the scaling property of the collective Schrödinger equation, this figure is valid for any value of $(2D\beta_0^2)^{-1}$. In the lower panels, the collective potentials $V(\beta_0,\gamma)$ are shown for three extreme situations, namely 1) a triaxially deformed case with a deep minimum at $\gamma = 30°$, 2) a γ-unstable case, and 3) an ideal case of oblate-prolate shape coexistence with two degenerated minima. Note that the collective potential $V(\beta,\gamma)$ is a periodic function of 60° in γ. The solid line in figure 6(d) shows the region $0° \leqslant \gamma \leqslant 60°$.

When V_0 is positive, a doublet structure appears with increasing the barrier-height parameter V_0. In other words, an approximately degenerated pair of eigenstates emerges for every angular momentum when $V_0/E(0_2^+) \gg 1$. This is a well-known doublet pattern in the double-well potential problem. We can associate this doublet structure with the oblate-prolate symmetry as seen in figure 6(d). Furthermore, we notice a very unique behavior of the 0_2^+ state; when V_0 decreases in the positive-V_0 side, its energy rises more rapidly than those of the yrare 2_2^+, 4_2^+, and 6_2^+ states. It crosses with $E(2_2^+)$ at $V_0/E(0_2^+) \simeq 3$, and finally at $V_0 = 0$, the 0_2^+ state is degenerated with 4_2^+ and 6_1^+ states, as expected in the Wilets-Jean model [51].

In the negative-V_0 side, the excitation energies of 3_1^+ and 5_1^+ states rapidly decrease with decreasing V_0, and when the potential minimum at $\gamma = 30°$ becomes very deep, the spectrum becomes similar with that of the Davydov-Filippov rigid triaxial rotor model [52].

## Appendix D. Time-dependent unitary transformation of the HFB state vectors

Let us first consider the TDHF case. It is convenient to define the particle-hole concept with respect to the HF ground state $|\phi_{\mathrm{HF}}\rangle$ for doubly even nuclei by

$$
\begin{aligned}
c_i^\dagger &= (1 - n_i)c_i^\dagger + n_i c_i^\dagger = a_i^\dagger + b_{\bar{i}}, \\
c_{\bar{i}} &= (1 - n_i)c_{\bar{i}} + n_i c_{\bar{i}} = a_{\bar{i}} - b_i^\dagger.
\end{aligned}
\tag{125}
$$

Here $c_i^\dagger$ and $c_{\bar{i}}$ are the nucleon creation and annihilation operators in the HF states i and its time-conjugate states $\bar{i}$, respectively, and n_i is 1 or 0 according to whether a pair of the HF states $(i, \bar{i})$ is occupied or unoccupied. The nucleon operators $(c_i^\dagger, c_{\bar{i}})$ correspond to the particle operators $(a_i^\dagger, a_{\bar{i}})$ for unoccupied space and the hole operators $(b_{\bar{i}}, b_i^\dagger)$ for the occupied space. Obviously, the HF ground state is a vacuum for the particles and holes:

$$
a_i|\phi_{\mathrm{HF}}\rangle = b_j|\phi_{\mathrm{HF}}\rangle = 0.
\tag{126}
$$
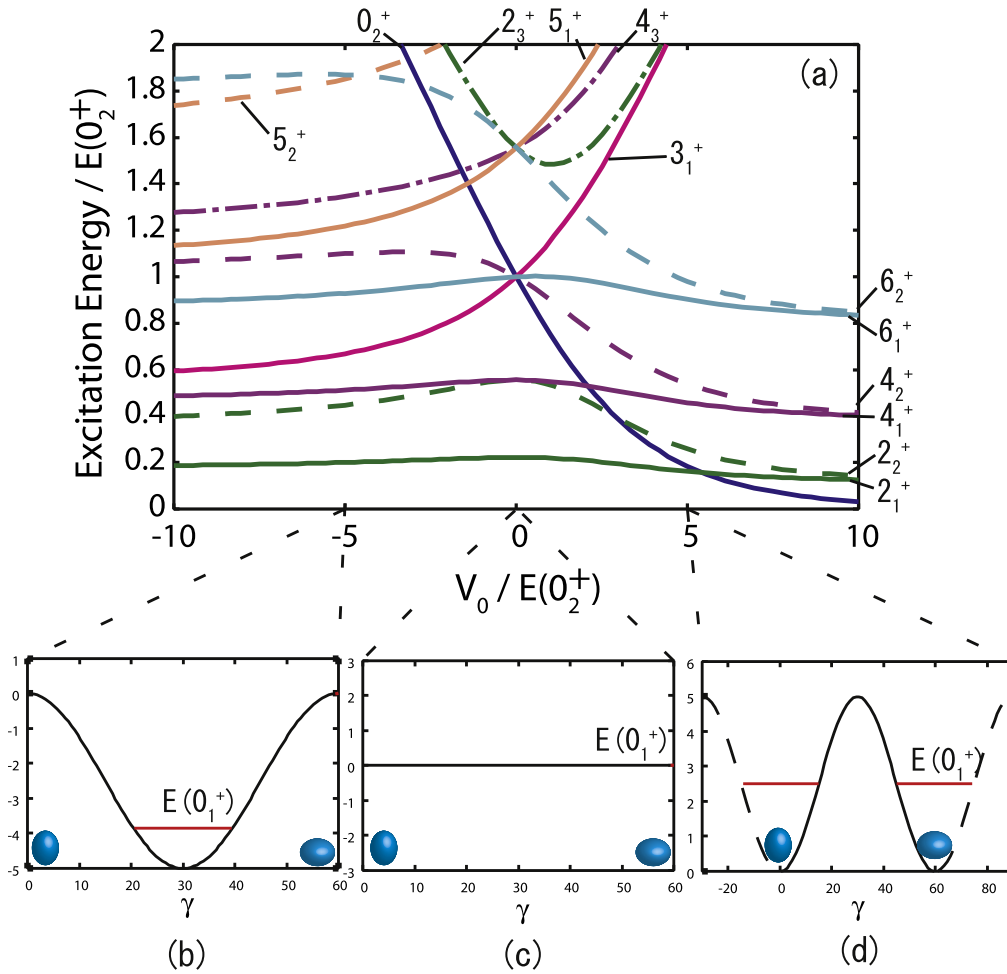
Figure 6. (a): excitation energies as functions of the parameter V_0. Both the excitation energies and the V_0 are normalized by the excitation energy of the second 0^+ state for $V_0 = 0$. (b), (c), (d): the collective potentials $V(\gamma)$ and the ground state energies $E(0_1^+)$ at $V_0/E(0_2^+) = -5.0$ (b), 0.0 (c), and 5.0 (d). Note that $E(0_1^+) = 0$ for $V_0 = 0$. The collective potential is a periodic function of $60°$ in γ, and only the region $0° \leqslant \gamma \leqslant 60°$ is drawn with a solid line in (d). This figure is taken from [212].

According to the Thouless theorem [213], another HF state $|\phi_{\mathrm{HF}}(t)\rangle$ non-orthogonal to $|\phi_{\mathrm{HF}}\rangle$ can be written as

$$|\phi_{\mathrm{HF}}(t)\rangle = N(t) \exp\left(\sum_{ij} z_{ij}(t) a_i^\dagger b_j^\dagger\right)|\phi_{\mathrm{HF}}\rangle \qquad (127)$$

with the normalization constant $N(t)$. It may be more convenient to describe the same HF state as a unitary transformation of $|\phi_{\mathrm{HF}}\rangle$ [59, 214]:

$$|\phi_{\mathrm{HF}}(t)\rangle = e^{i\hat{G}_{\mathrm{HF}}(t)}|\phi_{\mathrm{HF}}(t=0)\rangle \qquad (128)$$

with

$$i\hat{G}_{\mathrm{HF}}(t) = \sum_{ij}(f_{ij}(t) a_i^\dagger b_j^\dagger - f_{ij}^*(t) b_j a_i). \qquad (129)$$

Here, $|\phi_{\mathrm{HF}}\rangle$ is denoted $|\phi_{\mathrm{HF}}(t=0)\rangle$ to emphasize that equation (128) can be regarded as a time-dependent unitary transformation describing the time evolution of the TDHF state vectors. In this generalized form, in contrast to the original Thouless theorem, even the HF states orthogonal to $|\phi_{\mathrm{HF}}(t=0)\rangle$ can be described.

It is straightforward to generalize the above formulation to the TDHFB case including the pairing correlations. The particle-hole concept in the HF theory is replaced by the quasiparticle concept, which is introduced through the generalized Bogoliubov transformations [54],

$$c_i^\dagger = \sum_j (u_{ij}^* a_j^\dagger + v_{ij} a_j),$$

$$c_i = \sum_j (u_{ij} a_j + v_{ij}^* a_j^\dagger), \qquad (130)$$

(separately for protons and neutrons) in the HFB theory. (The use of the same notation ($a_i^\dagger$, $a_{\bar{i}}$) for the quasiparticles in the HFB theory and the particles in the HF theory may not cause any confusion.) The particle-hole pair creation and annihilation operators ($a_i^\dagger b_j^\dagger$, $b_j a_i$) are then replaced by the two-quasiparticle creation and annihilation operators ($a_i^\dagger a_j^\dagger$, $a_j a_i$). Similarly to equation (128) in the TDHF case, the time evolution of the TDHFB state $|\phi(t)\rangle$ can be described as a time-dependent unitary transformation [62, 215]:

$$|\phi(t)\rangle = e^{i\hat{G}(t)}|\phi(t=0)\rangle, \qquad (131)$$

where $i\hat{G}(t)$ is a one-body anti-Hermitian operator given by

$$i\hat{G}(t) = \sum_{(ij)}(g_{ij}(t)a_i^\dagger a_j^\dagger - g_{ij}^*(t)a_j a_i). \qquad (132)$$

Here, the sum is taken over independent two-quasiparticle configurations (ij). For the HFB state at $t = 0$, one may choose the HFB ground state $|\phi_0\rangle$ which satisfies the vacuum condition for the quasiparticles:

$$a_i\,|\phi_0\rangle = 0. \qquad (133)$$

It is important to note that equation (131) is valid for any choice of the initial HFB state $|\phi(t=0)\rangle$, if the quasiparticle operators in $i\hat{G}(t)$ are defined with respect to $|\phi(t=0)\rangle$.

Because $\hat{G}(t)$ is a one-body operator, it is possible to define quasiparticle creation and annihilation operators $\{a_i^\dagger(t), a_j(t)\}$ with respect to $|\phi(t)\rangle$ as follows:

$$
\begin{aligned}
a_i(t) &= \mathrm{e}^{i\hat{G}(t)}a_i\mathrm{e}^{-i\hat{G}(t)} \\
&= a_i + [i\hat{G}, a_i] + \frac{1}{2}[i\hat{G}, [i\hat{G}, a_i]] \\
&\quad + \frac{1}{6}[i\hat{G}, [i\hat{G}, [i\hat{G}, a_i]]] + \cdots \\
&= \sum_j (U_{ji}a_j + V_{ji}a_j^\dagger).
\end{aligned}
\qquad (134)
$$

The matrices, $U(t)$ and $V(t)$, composed of the amplitudes $U_{ij}(t)$ and $V_{ij}(t)$, are given by [60, 215]

$$U^T(t) = \cos\sqrt{G^\dagger G}, \qquad (135)$$

$$V^T(t) = G^\dagger \frac{\sin\sqrt{GG^\dagger}}{\sqrt{GG^\dagger}}, \qquad (136)$$

where G is a matrix composed of the components g_{ij}. Obviously, the quasiparticle operators $\{a_i^\dagger(t), a_j(t)\}$ satisfy the vacuum condition for $|\phi(t)\rangle$:

$$
\begin{aligned}
a_i(t)|\phi(t)\rangle &= \mathrm{e}^{i\hat{G}(t)}a_i\mathrm{e}^{-i\hat{G}(t)}\mathrm{e}^{i\hat{G}(t)}|\phi(t=0)\rangle \\
&= \mathrm{e}^{i\hat{G}(t)}a_i|\phi(t=0)\rangle \\
&= 0.
\end{aligned}
\qquad (137)
$$

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