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Open problems in the microscopic theory of large-amplitude collective motion

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Abstract
Construction of the microscopic theory of large-amplitude collective motion, capable of describing a wide variety of quantum collective phenomena in nuclei, is a long-standing and fundamental subject in the study of nuclear many-body systems. The present status of the challenge toward this goal is discussed taking the shape coexistence/mixing phenomena as typical manifestations of the large-amplitude collective motion at zero temperature. Some open problems in rapidly rotating cold nuclei are also briefly discussed in this connection.

1. Introduction

Low-frequency collective modes of excitation in cold nuclei near the yrast line exhibit a number of unique features of the nucleus as a finite quantum many-body system. To understand the nature of these collective excitations, we need to develop a microscopic theory of large-amplitude collective motion (LACM), which has sound theoretical basis and, at the same time, is practical enough for applications to a wide variety of nuclear collective phenomena. This is a very broad and long-term pursuit in nuclear structure physics. Through the attempts up to now to construct the microscopic theories of LACM, promising new concepts and methods have been proposed and developed (see [1] for a review), but it may be fair to say that the challenge is still in its infancy. In this paper, we discuss the present status of the challenge taking mainly the shape coexistence/mixing phenomena as typical manifestations of LACM at zero temperature. Open problems in the theoretical formulation of microscopic LACM theory and collective phenomena awaiting its application are listed including those in rapidly rotating cold nuclei. This paper is not intended to be a comprehensive review of this broad field of nuclear structure physics, and we apologize that the selection of topics and references is leaning to our personal interest. Certainly, microscopic description of spontaneous fission from the viewpoint of nonlinear/non-equilibrium physics is one of the major goals, but this

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subject will be discussed by other contributors to this special issue on *open problems in nuclear structure*.

2. Shape coexistence/mixings as large-amplitude collective phenomena

2.1. Shape coexistence phenomena

In recent years, new experimental data exhibiting coexistence of different shapes (like spherical, prolate, oblate and triaxial shapes) in the same energy region (of the same nucleus) have been obtained in low-energy spectra of nuclei in various regions of a nuclear chart (see [2, 3] for reviews and [4–6] for examples of recent data). These data indicate that the shape coexistence is a universal phenomenon representing essential features of the nucleus.

2.2. Necessity of going beyond the small-amplitude approximation

Let us define 'shape of the nucleus' as a semi-classical, macroscopic concept introduced by a self-consistent mean-field approximation, such as the Hartree–Fock–Bogoliubov (HFB) approximation, to the quantum-mechanical many-nucleon system. Needless to say, any HFB equilibrium shape inevitably accompanies quantum zero-point oscillations. If only one HFB equilibrium state exists, we can describe various kinds of vibrational mode about this point using the standard many-body methods like the random-phase approximation (RPA) or the boson-expansion methods [7, 8]. In the situations where two different HFB equilibrium shapes coexist in the same energy region, however, the large-amplitude shape vibrations tunneling through the potential barrier between the two HFB local minima may take place. To describe such LACM, we need to go beyond the perturbative approaches based on an expansion about one of the local minima.

2.3. Quantum field theory point of view

Different from the well-known tunneling of a single particle through the barrier created by an external field, the shape mixing of interest between different HFB local minima is a macroscopic tunneling phenomenon where the potential barrier itself is generated as a consequence of the dynamics of the self-bound quantum system. A HFB local minimum corresponds to a vacuum for quasiparticles in the quantum field-theoretical formulation. In contrast to infinite systems, different vacua in a finite quantum system are not exactly orthogonal to each other. Thus, the shape coexistence phenomena provide us precious opportunities to make a detailed study of the many-body dynamics of LACM connecting different vacua in terms of quantum spectra and electromagnetic transition properties associated with them.

2.4. Unique feature of the oblate–prolate coexistence

When the self-consistent mean field breaks the reflection symmetry (like the pear shape), parity doublets appear as the symmetric and anti-symmetric superpositions of two degenerate states associated with the two local minima. In contrast, there is no exact symmetry like parity when two local minima having the oblate and prolate shapes coexist. In this case, we do not know the relevant collective degree(s) of freedom through which the two shapes mix. It is obviously needed to develop a microscopic theory capable of describing the shape mixing dynamics of this kind.

2.5. Mysterious 0^+ *states*

There are only a few nuclei in which the first excited 0^+ state appears below the first excited 2^+ state. A well-known example is the 0^+ state at 0.69 MeV in ^{72}Ge which appears below the 2^+ state at 0.83 MeV. The nature of this state is poorly understood. Experimental systematics including neighboring nuclei indicates that the excitation energy of the 0^+ state takes the minimum around $N = 40$ where the neutron pairs start to occupy the $g_{9/2}$ shell. Microscopic calculations [9, 10] using the boson expansion method indicate that the mode–mode coupling between the quadrupole anharmonic vibration and the neutron pairing vibration plays an indispensable role in bringing about the peculiar behavior of the excited 0^+ states. On the other hand, these states are often interpreted in terms of the phenomenological shape coexistence picture [11]. Relations between the two interpretations are not well understood. Closely examining the properties of the excited 0^+ states in a wide region of nuclear chart, one finds that they exhibit features that cannot be understood in terms of the traditional concepts alone (see [12] for an example of recent data).

3. Characteristics of low-frequency collective excitations in nuclei

As is well known, shell structure and pairing correlations play essential roles for the emergence of low-frequency collective modes of excitation in medium–heavy and heavy nuclei. They exhibit unique features of the nucleus as a finite quantum many-body system and their amplitudes of vibration tend to become large. In this section, we discuss their characteristics in a wider perspective including the shape mixing phenomena and argue for the need of a microscopic theory capable of describing them.

3.1. Deformed shell structure

Nuclei exhibit quite rich shell structures comprising a variety of single-particle motions in the mean field localized in space. Let us define the shell structure as a regular oscillating pattern in the single-particle level density coarse-grained in energy. The nucleus gains an extra binding energy, called the shell energy, when the level density at the Fermi surface is low. The shell structure changes as a function of deformation. If the level density at the Fermi surface is high at the spherical shape, the nucleus prefers a deformed shape with lower level density. When different deformed shell structures give almost the same energy gain, we may obtain approximately degenerate HFB equilibrium shapes.

3.2. Pairing correlations and quasiparticles

It should be emphasized that both the mean field and the single-particle modes are collective phenomena. Needless to say, the nuclear mean field is self-consistently generated as a result of cooperative motion of strongly interacting nucleons. We learned from the BCS theory of superconductivity that the single-particle picture emerges as a consequence of collective phenomena: the Bogoliubov quasiparticles are nothing but the elementary modes of excitation in the presence of the Cooper pair condensate, and they have a gap in their excitation spectra (become ‘massive’). As is well known, this idea has been greatly extended to understand dynamical mechanisms for generating the masses of ‘elementary’ particles [13]. The HFB theory is a generalized mean field theory taking into account both the pair condensation and the HF mean field in a unified manner [7, 8, 14].

3.3. Spontaneous breaking of symmetry

The self-consistent mean field of a finite quantum system inevitably breaks some symmetries. Even the spherical mean field breaks the translational symmetry. When the mean field breaks another symmetry of a higher order, the concept of single-particle motion is generalized accordingly. For instance, the Bogoliubov quasiparticle is introduced by breaking the number conservation. Struggles for finding a better concept of single-particle motion comprise the heart of nuclear structure study. When the mean field breaks some continuous symmetries, collective modes (Nambu–Goldstone modes) restoring the broken symmetries emerge. Nuclear rotations are typical examples: they restore the rotational symmetries broken by the mean field [15]. In this way, the (generalized) single-particle picture and the symmetry-restoring collective motions are inextricably linked like 'two sides of the same coin'. This fact has been beautifully demonstrated by the success of the 'rotating (cranked) shell model' [16], which describes the interplay of the rotational motions and 'the single-particle motions in the rotating mean field' in a simple manner. One of the fascinations of nuclear structure physics is that we can study the microscopic dynamics of symmetry breaking and restoration by means of a detailed study of quantum spectra. Finite quantum systems localized in space, such as the nucleus, provide us with such unique and invaluable opportunities.

3.4. Origin of oblate–prolate asymmetry

It should be noted that breaking of the spherical symmetry does not necessarily lead to the regular rotational band structure. For instance, even when the HFB mean field has an equilibrium point at a prolate shape which is deep with respect to the axial deformation parameter β, it should be deep also with respect to the axially asymmetric deformation parameter γ. In HFB calculations restricted to the axially symmetric shapes, we often obtain two solutions having the prolate and oblate shapes, but the oblate solution might be unstable with respect to γ. Even if both minima are stable, a strong mixing of the two shapes might occur through quantum mechanical large-amplitude collective vibrations in the γ degree of freedom. To suppress such a mixing, we need a sufficient amount of the potential barrier and the energy difference between the oblate and prolate solutions. Otherwise, identities of the rotational bands built on the oblate and prolate shapes will be easily lost due to the large-amplitude γ vibrations. These problems point to the critical need for the microscopic theory of LACM capable of describing such γ-soft situations, the oblate–prolate shape coexistence (where two rotational bands built on them can be identified) and various intermediate situations in a unified manner. In spite of the obvious importance for understanding low-energy collective spectra, the microscopic origin of the oblate–prolate asymmetry in nuclear structure (the reason why the prolate shapes are energetically more favored in many cases than the oblate shapes) still remains as one of the long-standing and fundamental problems. On this issue, quite recently, Hamamoto and Mottelson suggested that the surface diffuseness plays a key role in bringing about the asymmetry [17]. A useful approach to investigate the dynamical origin of appearance of the deformed shell structure is the semi-classical theory of the shell structure [18–20]. It may be interesting to apply this approach to the problem in question for a deeper understanding of the oblate–prolate asymmetry.

3.5. Collective motion as moving mean field

Nuclear rotational and vibrational motions can be described as moving self-consistent fields. This is one of the basic ideas of the unified model of Bohr and Mottelson [21, 22]. The time-dependent HFB (TDHFB) mean field is a generalized coherent state and its time development can be described as a trajectory in the large-dimensional TDHFB phase space. Such a formulation of the TDHFB theory as a Hamilton dynamical system provides a microscopic foundation for using a classical picture of rotating and vibrating mean fields [23–25]. Thus, nuclear collective motions are beautiful examples of emergence of classical properties in genuine quantum many-body systems. For small-amplitude vibrations around a HFB equilibrium point, one can make the linear approximation to the TDHFB equations and obtain the quasiparticle RPA (QRPA). One of the merits of the QRPA is that it determines the microscopic structures of the normal modes (collective coordinates) without postulating them from the outset. The small-amplitude approximation is valid for giant resonances (high-frequency collective vibrations), and the (Q)RPA is used as the standard method for their microscopic descriptions.

3.6. Need for a microscopic theory of LACM

In contrast to giant resonances, the small-amplitude approximation is often insufficient for low-frequency collective modes. This is especially the case for the quadrupole collective modes in open-shell nuclei. The oblate–prolate shape coexistences/mixings are typical examples. It is also well known that the amplitude of the quadrupole vibration becomes very large in transient situations of the quantum phase transition from spherical to deformed, where the spherical mean field is barely stable or the spherical symmetry is broken only weakly. Many nuclei are situated in such a transitional region. It seems that this is one of the characteristic features of the quantum phase transition in the nucleus as a finite quantum many-body system. We need to go beyond the QRPA for describing such low-frequency quadrupole collective excitations. In view of the crucial role that the deformed shell structure and the pairing correlation play in generating the collectivity and determining the characters of these modes, it is desirable to construct a microscopic theory of LACM as an extension of the QRPA keeping its merit of deriving the collective coordinates from a huge number of microscopic degrees of freedom. Another important merit of the QRPA is that it is a quantum theory derived also with a new Tamm–Dancoff approximation in quantum field theory. Because we aim at constructing, on the basis of the TDHFB picture, a quantum theory of LACM capable of describing quantum spectra, it may be imperative, for justification of quantization of the collective coordinate, to formulate the quantum theory in such a way that it reduces to the QRPA in the small amplitude limit. In the next section, we briefly review various attempts toward this goal.

4. Problems in microscopic theories of collective motions

4.1. Boson expansion method

One of the microscopic approaches to treat nonlinear vibrations is the boson expansion method [26]. For describing the quadrupole vibrations in transitional nuclei, the collective QRPA normal modes at the spherical shape are represented as boson operators and anharmonic effects ignored in the QRPA are evaluated in terms of a power series of the boson creation and annihilation operators. The boson expansion methods have been widely used for the investigation of low-frequency quadrupole collective phenomena. This approach is perturbative in the sense that the microscopic structures of the collective coordinates and momenta are fixed at the spherical shape and nonlinear effects are evaluated by a power-series expansion in terms of these collective variables. To treat situations where the collective vibrations become increasingly larger amplitude and the nonlinear effects grow to such a degree that the microscopic structures of the collective variables themselves may change during the vibrational motion, it is desirable to develop a microscopic theory which can treat the nonlinear effects in a non-perturbative way.

4.2. Generator coordinate method (GCM)

In the application of the GCM to quadrupole collective phenomena, quantum eigenstates are described as superpositions of mean-field (generalized Slater determinant) states parametrized by the generator coordinates. This microscopic approach is widely used in conjunction with the angular momentum and number projections [14]. A long-standing open problem in the GCM is the reliability of the collective masses (inertial functions) evaluated with the real generator coordinates. For the center of mass motion, complex generator coordinates are needed to reproduce the correct mass, indicating that we have to explicitly treat the collective momenta in addition to the coordinates [7]. Another important problem in the GCM is the choice of the generator coordinates. Holzwarth and Yukawa [27] once tried to find an optimal collective path by variationally determining the generator coordinate. This work stimulated the attempts to construct the microscopic theory of LACM.

4.3. Time-dependent HF (TDHF) method

Needless to say, the TDHF is a powerful tool to microscopically describe the LACM taking place in heavy-ion collisions [23]. The TDHF is insufficient for the description of quantum spectra of low-lying states, however, because of its semi-classical feature. On the other hand, as emphasized in section 3.6, its small-amplitude approximation, the RPA, can be formulated as a quantum theory and gives us a physical insight how the collective modes are generated as coherent superpositions of a large number of particle-hole excitations. It is thus desirable to extend the idea of deriving the RPA from the TDHF to large amplitude motions.

4.4. Adiabatic TDHF (ATDHF) method

Challenges for constructing microscopic theory of LACM can be traced back to the pioneering works by Belyaev [28], Baranger and Kumar [29] in which the collective potential and collective masses (inertial functions) appearing in the quadrupole collective Hamiltonian of Bohr and Mottelson are microscopically calculated on the basis of the time-dependent mean-field picture and with the use of the pairing-plus-quadrupole force [30]. In the ATDHF theories, developed by Baranger and Vénéroni [31], Brink *et al* [32], Goeke and Reinhard [33], more general schemes applicable to general effective interactions are given. There, under the assumption that the LACM is slow, the time-dependent density matrix is expanded in terms of the collective momentum, and the collective coordinate is introduced as a parameter describing the time dependence of the density matrix. Another ATDHF theory by Villars [34] resembles the above approaches, but it is more ambitious in that it provides a set of equations to self-consistently determine the collective coordinates. It turned out, however, that these equations are insufficient to uniquely determine the collective coordinates. This problem was solved by properly treating the second-order equation (with respect to the collective momentum) in the time-dependent variational principle (see Mukherjee and Pal [35] and the series of papers by Klein, Do Dang, Bulgac and Walet, reviewed in [36]). It was also clarified through these works that the optimal collective path maximally decoupled from non-collective degrees of freedom coincides in a very good approximation with the valley in the large-dimensional configuration space associated with the TDHF states.

4.5. Self-consistent collective coordinate (SCC) method

Attempts to construct the LACM theory without assuming the adiabaticity and treating the collective coordinates and momenta on the same footing were initiated by Rowe [37] and Marumori [38]. The problems remaining in these early works were solved in the SCC method formulated by Marumori *et al* [39]. The major aim of this approach is to extract the optimal collective path (collective submanifold), maximally decoupled from non-collective degrees of freedom, in the TDHF phase space of large dimension. The collective submanifold is a geometrical object independent of the choice of the canonical coordinate system. This idea was developed also by Rowe [40], Yamamura and Kuriyama [41]. These works yield a new insight into the fundamental concepts of collective motion. The SCC method was extended [42] to include the pairing correlations and applied to anharmonic quadrupole vibrations [43–45]. In these works, a perturbative method of solving its basic equations was adopted and it remained as an open task to develop a non-perturbative method of solution for genuine LACM. This task was attained by the adiabatic SCC (ASCC) method [46], in which the basic equations of the SCC method is solved using an expansion with respect to the collective momentum. Therefore, the method is applicable to the change of the system in a wide range of the collective coordinate. This new method may also be regarded as a modern version of the ATDHF method initiated by Villars [34]. Another approach similar to the ASCC method has been developed also by Almehed and Walet [47] although the method of restoring the gauge invariance (number conservation) broken in the TDHFB states is not given there. In the next section, we briefly summarize the basic ideas of the microscopic theory of LACM along the lines of the ASCC method which is formulated respecting the gauge invariance.

5. Basic concepts of the microscopic theory of LACM

5.1. Extraction of the collective submanifold

As mentioned in the previous sections, the TDHFB theory can be formulated as a Hamilton dynamical system: the dimension of the phase space is quite large (twice the number of all possible two quasiparticle states). The major aim of the microscopic theory of LACM is to extract the collective submanifold from the TDHFB space, which is describable in terms of a few numbers of collective coordinates and momenta. The collective Hamiltonian is then derived and requantized yielding the collective Schrödinger equation.

5.2. Basic equations of the microscopic theory of LACM

Let us assume that the time development of the TDHFB state is describable in terms of the single collective coordinate $q(t)$ and momentum $p(t)$. To describe the superfluidity, we need to introduce also the number variable $n(t)$ and the gauge angle $\varphi(t)$ conjugate to it (for both protons and neutrons in applications to nuclei). We assume that the TDHFB state can be written in the following form:

$$|\phi(q, p, \varphi, n)\rangle = e^{-i\varphi\tilde{N}}|\phi(q, p, n)\rangle, \tag{1}$$

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

Here $|\phi(q, p, n)\rangle$ is an intrinsic state for the pairing rotational degree of freedom parametrized by φ, $|\phi(q)\rangle$ represents a non-equilibrium HFB state called *moving-frame HFB state*, $\hat{Q}(q)$ and $\hat{\Theta}(q)$ are one-body operators called *infinitesimal generators* and $\tilde{N}$ and n are defined by

$\tilde{N} \equiv \hat{N} - \langle\phi(q)|\hat{N}|\phi(q)\rangle \equiv \hat{N} - N_0$ and $n \equiv \langle\phi(q,p,n)|\hat{N}|\phi(q,p,n)\rangle - N_0 \equiv N - N_0$, $\hat{N}$ being the number operator.

We determine the microscopic structure of the infinitesimal generators $\hat{Q}(q)$, $\hat{\Theta}(q)$ and the moving-frame HFB state $|\phi(q)\rangle$ on the basis of the time-dependent variational principle:

$$\delta\langle\phi(q,p,\varphi,n)|\mathrm{i}\frac{\partial}{\partial t} - \hat{H}|\phi(q,p,\varphi,n)\rangle = 0, \tag{3}$$

where $\hat{H}$ is a microscopic many-body Hamiltonian. Expanding in powers of p and n and keeping terms up to the second order in p, we obtain *the moving-frame HFB equation*

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

where $\hat{H}_M(q)$ is the moving-frame Hamiltonian defined by

$$\hat{H}_M(q) = \hat{H} - \lambda(q)\tilde{N} - \frac{\partial V}{\partial q}\hat{Q}(q), \tag{5}$$

and *the moving-frame QRPA equations* also called *local harmonic equations*

$$\delta\langle\phi(q)|[\hat{H}_M(q),\hat{Q}(q)] - \frac{1}{\mathrm{i}}B(q)\hat{P}(q)|\phi(q)\rangle = 0, \tag{6}$$

$$\delta\langle\phi(q)|\left[\hat{H}_M(q),\frac{1}{\mathrm{i}}\hat{P}(q)\right] - C(q)\hat{Q}(q) - \frac{1}{2B(q)}\left[\left[\hat{H}_M(q),\frac{\partial V}{\partial q}\hat{Q}(q)\right],\hat{Q}(q)\right] - \frac{\partial\lambda}{\partial q}\tilde{N}|\phi(q)\rangle = 0, \tag{7}$$

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

$$|\phi(q+\delta q)\rangle = \mathrm{e}^{-\mathrm{i}\delta q\hat{P}(q)}|\phi(q)\rangle, \tag{8}$$

and

$$C(q) = \frac{\partial^2 V}{\partial q^2} + \frac{1}{2B(q)}\frac{\partial B}{\partial q}\frac{\partial V}{\partial q}. \tag{9}$$

The quantities $C(q)$ and $B(q)$ are related to the eigenfrequency $\omega(q)$ of the local normal mode obtained by solving the moving-frame QRPA equations through $\omega^2(q) = B(q)C(q)$. Note that these equations are valid also for regions with a negative curvature ($C(q) < 0$) where $\omega(q)$ takes an imaginary value. The double commutator term in (7) stems from the q derivative of $\hat{Q}(q)$ and represents the curvature of the collective path.

Solving the above set of equations, the microscopic structure of the infinitesimal generators, $\hat{Q}(q)$ and $\hat{P}(q)$, are determined: they are explicitly expressed as bilinear superpositions of the quasiparticle creation and annihilation operators locally defined with respect to the moving-frame HFB state $|\phi(q)\rangle$. The collective Hamiltonian is given by

$$\mathcal{H}(q,p,n) = \langle\phi(q,p,n)|\hat{H}|\phi(q,p,n)\rangle = V(q) + \tfrac{1}{2}B(q)p^2 + \lambda(q)n, \tag{10}$$

where $V(q)$, $B(q)$ and $\lambda(q)$ represent the collective potential, inverse of the collective mass and the chemical potential, respectively. Note that they are functions of the collective coordinate q. The basic equations, (4), (6) and (7), reduce to the well-known HFB and QRPA equations at the equilibrium points where $\partial V/\partial q = 0$. Thus, the LACM theory outlined above is a natural extension of the HFB-QRPA theory to non-equilibrium states.

5.3. Relation to the constrained HFB approach

The moving-frame HFB equation (4) looks like the constrained HFB (CHFB) equation, but it is essentially different from the CHFB in that the infinitesimal generator $\hat{Q}(q)$ (corresponding to the constraint operator) is self-consistently determined together with $\hat{P}(q)$ as a solution of the moving-frame QRPA equations, (6) and (7), locally at every point of the collective coordinate q. Therefore, unlike the constraint operator in the CHFB method, its microscopic structure changes as a function of q. In other words, the LACM takes place choosing the locally optimal 'constraint operator' at every point of q along the collective path. When the LACM of interest is described by more than one collective coordinates, we try to extract the collective hypersurface embedded in the large-dimensional TDHFB space by extending the above equations to the multi-dimensional cases and derive the collective Schrödinger equation by requantization. This attempt has some features in common with the problem of *quantization of a constrained dynamical system* [40]. It is interesting to discuss the microscopic foundation of the so-called Pauli prescription (frequently used in quantizing phenomenological collective Hamiltonians) from this point of view. In discussing this issue, it is important to note that the LACM is constrained on the collective hypersurface not by external constraining forces but by the dynamics of itself. Namely, the collective hypersurface is generated as a consequence of the dynamics of the quantum many-body system under consideration. It seems that this is a unique and quite attractive feature of the subject under discussion.

5.4. Gauge invariance with respect to the pairing rotational angle

An important problem in formulating the microscopic LACM theory based on the TDHFB approximation is how to respect the number conservation. As is well known, one of the merits of the QRPA is that the zero-frequency Nambu–Goldstone mode restoring the number conservation is decoupled from other normal modes of vibration [48]. Our problem is how to generalize this concept to non-equilibrium HFB states. A clue for solving this problem is obtained by noting that the basic equations, (4), (6) and (7), are invariant against rotations of the gauge angle φ at every point of q. Actually, we can determine the infinitesimal generator $\hat{\Theta}(q)$ associated with the pairing-rotational degree of freedom in the same way as $\hat{Q}(q)$ and $\hat{P}(q)$, and obtain the pairing rotational energy proportional to n^2 as an additional term to the collective Hamiltonian (10). Although this term vanishes by setting $N = N_0$ to respect the number conservation, the consideration of the gauge invariance is essential for correctly treating the LACM in systems with superfluidity. Specifically, we need to set up a gauge fixing condition in practical calculations (see [49] for details).

6. Open problems in the microscopic theory of LACM

6.1. Contributions of the time-odd mean field to the collective mass

In the microscopic calculation of the collective mass (inertial function), the cranking mass is widely used. It is obtained through the adiabatic perturbation treatment of the time development of the mean field. As stressed by Belyaev [28], Baranger and Vénéroni [31], the effects of the time-odd components (breaking the time-reversal invariance) induced by the time evolution of the mean field are ignored in the cranking mass. These effects are self-consistently taken into account in the ASCC collective mass obtained by solving equations (6) and (7). On the other hand, one can derive the collective Schrödinger equation from the GCM equation by making the Gaussian overlap approximation (GOA). It is not clear, however, to what extent the time-odd mean-field effects are taken into account in the GCM-GOA mass evaluated in this way with real generator coordinates. In view of the importance of the collective mass in the dynamics of LACM, the time-odd mean-field effects have been studied extensively (see e.g. [50]). In spite of these efforts, it may be fair to say that we are still far from a full understanding of the time-odd effects. Thus, it remains as a great subject for future to evaluate the time-odd mean-field effects on the collective mass using energy density functionals currently under active development.

6.2. Different meaning of 'adiabatic'

There is another important difference between the ASCC collective mass and the cranking mass. Let us first note that the meaning of the adjective 'adiabatic' in the ASCC method is different from that of the adiabatic perturbation theory. In the ASCC method, it just means that the collective kinetic energy term higher than the second order in the power-series expansion with respect to the collective momentum is omitted and, in contrast to the adiabatic perturbation, the smallness of the collective kinetic energy in comparison with the intrinsic two-quasiparticle excitation energies is not indispensable. Recalling that the ASCC collective mass coincides with the QRPA collective mass at the HFB equilibrium point, one can easily confirm this difference by considering the spherical QRPA limit in the pairing-plus-quadrupole force model, where the time-odd mean-field effect is absent. At the spherical HFB equilibrium point, in fact, the QRPA collective mass reduces to the cranking mass in the limit that the frequency of the QRPA normal mode vanishes [30]. In this connection, it may be pertinent to emphasize the difference between the ASCC collective mass and the ATDHFB collective mass of Baranger and Vénéroni. Specifically, the former is determined by the local QRPA mode and reduces to the QRPA collective mass at the HFB equilibrium point, while the latter is related to the cubic inverse energy-weighted sum rule [51] and does not reduce to the QRPA collective mass in this limit. Therefore, it is also interesting to make a systematic comparison between different collective masses including the ASCC, cranking, GCM-GOA and ATDHFB collective masses.

6.3. Deeper understanding of the pair-hopping mechanism

The collective mass represents the inertia of the many-body system against an infinitesimal change of the collective coordinate q during the time evolution of the mean field. It is a local quantity and varies as a function of q. What is the microscopic mechanism that determines the collective mass? This is one of the central questions in our study of many-body dynamics of the LACM. Concerning this question, it is well known that the pairing correlation plays a crucial role. Because the single-particle-energy spectrum in the mean field changes as a function of q, the level crossing at the Fermi energy successively occurs during the LACM. In the presence of the pairing correlation, the many-body system can easily rearrange to take the lowest energy configurations at every value of q, i.e. the system can easily change q. The easiness/hardness of the configuration rearrangements at the level crossings determines the adiabaticity/diabaticity of the system. Since the inertia represents a property of the system trying to keep a definite configuration, we expect that the stronger the pairing correlation, the smaller the collective mass. The nucleon-pair hopping mechanism at the successive level crossings at the Fermi surface is modeled by Barranco *et al* [52]. It yields the collective mass, called hopping mass, which has been applied to the exotic decays and the tunneling phenomena between the superdeformed (SD) and normal deformed states [52, 53]. Of course, smooth changes of single-particle wavefunctions as functions of q also contribute to the collective mass in addition to the configuration changes. To deepen our understanding of the collective mass of LACM, it is desirable to make a comprehensive analysis of the microscopic mechanism determining it. A systematic comparison between the hopping mass and other collective masses discussed above will certainly serve for this purpose.

6.4. Application to the shape coexistence/mixing phenomena

As discussed in section 2, one of the most interesting LACM phenomena is the oblate–prolate shape coexistence/mixing in the proton-rich ^{68}Se and ^{72}Kr region. Quite recently, we have applied the ASCC method to them and successfully determined the collective path which runs through the triaxially deformed valley and connects the oblate and prolate HFB minima. Evaluating the rotational moments of inertia on the collective path and requantizing the collective Hamiltonian, we have derived the collective Schrödinger equation describing the coupled motion of the large-amplitude shape vibrations and the three-dimensional (3D) rotational motions [54, 55]. We have thus found a number of interesting features which change when going from nucleus to nucleus. For instance, the ^{68}Se nucleus exhibits intermediate features between the oblate–prolate shape coexistence and the γ-soft rotors, while in the neighboring $N = Z$ nucleus ^{72}Kr, we have found that the localization of the collective wavefunction in the (β, γ) plane significantly develops with increasing rotational angular momentum. It is certainly desirable to carry out this kind of microscopic analysis for a wide variety of shape coexistence/mixing phenomena. We believe that theoretical and experimental investigations of these phenomena will be very fruitful and bring about plenty of new ideas on nuclear structure and dynamics.

6.5. Microscopic derivation of the Bohr–Mottelson collective Hamiltonian

Extending the one-dimensional (1D) collective path to the two-dimensional (2D) hypersurface and mapping it on the (β, γ) plane, we shall be able to microscopically derive the five-dimensional (5D) quadrupole collective Hamiltonian of Bohr and Mottelson [15]. In this derivation, the moments of inertia of the 3D rotation may be evaluated at every point of the 2D hypersurface generalizing the Thouless–Valatin equations to those at non-equilibrium points. The microscopic derivation of the Bohr–Mottelson collective Hamiltonian is a well-known long-standing subject in nuclear structure physics, but we are still on the way to the goal (see [56, 57] for examples of recent works and [58] for a review). We illustrate in figure 1 the basic concepts of the microscopic LACM theory and the result of a recent calculation.

6.6. Extension to high-spin states

In the above approach, variations of intrinsic structure due to rotation are not taken into account. Therefore, the range of its applicability is limited to low-spin states. A promising way of constructing LACM theory applicable to high-spin states is to adopt the rotating mean-field picture. Specifically, it is interesting to develop LACM theory on the basis of the HFB approximation in a rotating frame (it is possible to formulate the SCC method in a form suitable for treating the rotational motions [59, 60]). Such an approach was once tried in [47]. It remains as a future challenge to construct the microscopic theory of LACM at high spin, which is capable of self-consistently taking into account variation of intrinsic structure due to rapid rotation.

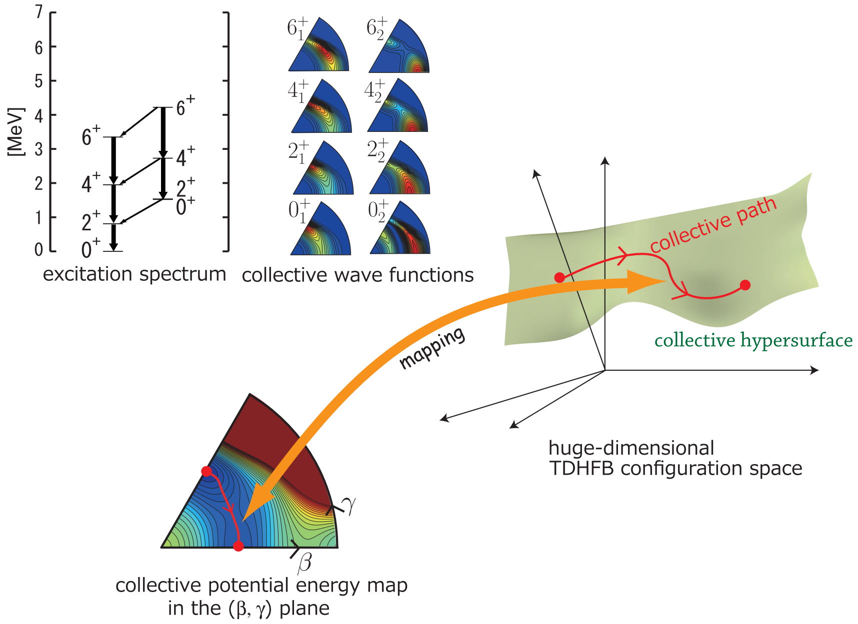

Figure 1. Illustration of basic concepts of LACM. The collective path and the collective hypersurface embedded in the huge-dimensional TDHFB configuration space (*right-hand side*). Mapping of the collective path and the hypersurface into the (β, γ) plane and the collective potential energy on it (*lower part on the left-hand side*). The excitation spectrum and collective wavefunctions obtained by solving the collective Schrödinger equation (*upper part on the left-hand side*). In this illustration, the result of a microscopic calculation for the oblate–prolate shape coexistence/mixing phenomenon in ^{68}Se is used, where the collective path is self-consistently determined by solving the ASCC equations while the collective potential and the collective masses are evaluated by solving the CHFB and the moving-frame QRPA equations, respectively, with the pairing-plus-quadrupole force (the quadrupole pairing is also taken into account). This calculation may be regarded as a first step toward a fully self-consistent microscopic derivation of the 5D quadrupole collective Hamiltonian starting from modern density functionals.

(This figure is in colour only in the electronic version)

6.7. Combining with better density functionals

As seen in a number of contributions to this special issue on open problems in nuclear structure, very active works are going on to build a universal nuclear energy density functional. It is certainly a great challenge to make a systematic microscopic calculation for LACM phenomena using better energy density functionals. For carrying out such ambitious calculations, it is certainly necessary to develop efficient numerical algorithms to solve the basic equations of the LACM theory. In practical applications, for instance, we need to iteratively solve the moving-frame HFB equation and the moving-frame QRPA equations at every point on the collective path. When we extend these equations to 2D hypersurfaces, the numerical calculation grows to a large scale. Especially, an efficient method of solving the moving-frame QRPA equations is needed. An extension of the finite amplitude method [61] into a form suitable for this purpose may be promising. It may also be worthwhile to examine the applicability of the separable approximation [62] to the effective interaction derived from the energy density functionals.

6.8. LACM in odd-A nuclei

So far we have limited our discussions to LACM in doubly even nuclei only. In fact, microscopic description of LACM in odd-A nuclei remains as a vast unexplored field. Needless to say, unified treatment of the seemingly contradictory concepts of single-particle and collective modes of motion is the central theme of the phenomenological Bohr–Mottelson model of nuclear structure. Low-lying states in odd-A nuclei provide a wealth of data exhibiting their interplay. In view of the great success of the Bohr–Mottelson approach, it is extremely important to develop a microscopic theory capable of treating the single-particle and collective modes in a unified manner. In fact, various microscopic theories of particle–vibration coupling have been developed: e.g. the nuclear field theory [63] and the boson-expansion method for odd-A nuclei [26]. These available theories treat the particle–vibration couplings in a perturbative manner starting from the small-amplitude approximation (RPA/QRPA) for collective excitations at an equilibrium point of the mean field. Non-perturbative method capable of treating LACM in odd-A nuclei (generally speaking, LACM in the presence of several quasiparticles) is lacking, however. This is an extremely difficult but challenging subject for future.

7. Large-amplitude collective phenomena at high spin

The nucleus exhibits a rich variety of nonlinear collective phenomena awaiting applications of the microscopic LACM theory. Certainly, microscopic description of spontaneous fission from the viewpoint of nonlinear/non-equilibrium physics is one of the major goals. Another vast unexplored field is the microscopic study of LACM at finite temperature. Microscopic mechanism of damping and dissipation of various kinds of LACM is a long-term subject. It seems particularly interesting to explore both theoretically and experimentally how the character of LACM changes when going from the yrast to the compound-nucleus regions. These subjects are outside the scope of the present paper, however. Restricting our scope to the LACM at zero temperature, in this section, we discuss a few open problems in rapidly rotating nuclei (see [64] for a review on high-spin states).

7.1. Tunneling decay of superdeformed (SD) states and high-K isomers

It is quite interesting to apply the microscopic LACM theory to the quantum tunneling phenomena from the SD states (with an axis ratio of about 2:1) to the compound-nucleus states [53], because the tunneling probability depends quite sensitively on the collective mass and the collective path connecting the initial and final states. The tunneling decay from high-K to low-K isomers is also interesting [65], because it poses a unique question as to which of the two competing decay paths dominates; one through LACM in the triaxial shape degree of freedom and the other in the orientation degree of freedom of the angular momentum vector (with respect to the principal axes of the body-fixed frame).

7.2. Large-amplitude wobbling motions and chiral vibrations

A new mode of 3D rotation associated with the spontaneous breaking of the axial symmetry is called wobbling motion; it is describable as a boson (small-amplitude vibration-like) excitation from the yrast line [15, 66]. The observed rotational band associated with the double excitations of the wobbling mode indicates, however, the presence of significant anharmonicity [67]. It is an interesting open problem to explore what will happen when the amplitude of the wobbling mode increases and the uniformly rotating nucleus becomes unstable against this collective rotational degree of freedom [68, 69]. Another interesting issue concerning new modes of 3D rotation is the possibility of doublet rotational bands called chiral band [16, 70, 71]. In triaxially deformed nucleus, one can define *chirality* in terms of the directions of the collective rotational angular momentum and those of the quasiparticle angular momenta of both protons and neutrons. When the rotating HFB mean field involves such an intrinsic structure, the two solutions corresponding to the right-handed and left-handed configurations are degenerate. Then, a chiral doublet pattern is expected to appear in the rotational band structure. In a transient situation, where the barrier separating the two HFB solutions is still in an early stage of development, the large-amplitude vibrations connecting the two configurations, called chiral vibrations, may occur [16, 70, 71]. It remains for the future to apply the microscopic LACM theory to these phenomena unique to rapidly rotating nuclei with triaxial shape.

7.3. Large-amplitude vibrations associated with the reflection symmetry breaking

Rich experimental data exhibiting the parity-doublet pattern are available, indicating that the reflection symmetry is broken in their mean fields [72]. The energy splitting of the doublet changes as a function of rotational angular momentum [73]. Thus, it is quite interesting to investigate, on the basis of the microscopic LACM theory, how the quantum tunneling motion between the left- and right-configurations is affected by rapid rotation. Also interesting in this connection is the recent observation of alternating parity bands [74, 75] that exhibit a transitional feature toward the static octupole deformation. A considerable number of SD states are expected to be very soft with respect to the shape vibrational degrees of freedom simultaneously breaking the reflection and axial symmetries. In fact, the soft octupole vibrations built on the SD yrast states have been observed [76, 77]. When the SD mean field becomes unstable against this kind of vibrations, a new class of SD states having exotic shapes (like a banana) may appear [78, 79]. In transitional situations, the large-amplitude vibrations associated with the instability toward such exotic shapes may take place. Possible appearance of exotic shapes is not restricted to SD high-spin states. For example, the symmetry-unrestricted HFB calculation [80] yields a local minimum with the tetrahedral shape near the ground state of ^{80}Zr. The potential energy surface is shallow, however, indicating that we need to take into account the large-amplitude tetrahedral shape fluctuation [81]. Generally speaking, microscopic LACM theories are required for describing collective motions in transitional regions of quantum phase transition, where some symmetry is weakly broken or tends to be broken.

8. Concluding remarks

One of the fundamental questions of nuclear structure physics is why and how a variety of LACM emerges in consequence of quantum many-body dynamics. The nucleus provides us valuable opportunities to make a detailed study of the microscopic dynamics generating the collectivities. The microscopic derivation of the quadrupole collective Hamiltonian started more than half a century ago, but the challenge to construct a fully self-consistent microscopic theory of LACM has encountered a number of serious difficulties. Finally, however, these long-term efforts have yielded the new concept of *collective submanifold* and a deeper understanding of what is *collectivity*. At the same time, new efficient methods of numerical calculation are now under active development. Thus, in the coming years, fruitful applications to low-frequency collective phenomena are envisaged. This means that a new era in the microscopic study of nuclear collective dynamics is opening.

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