Chapter 1
Introduction

Atomic nucleus is a highly quantal-mechanical, finite many-body system comprised of protons and neutrons, where the strong, the weak and the electromagnetic fundamental interactions play an important role at the most profound level. The study of the atomic nucleus has been therefore crucial for elucidating the origin of matter (or nucleosynthesis processes), the tests of fundamental symmetries, and even the purpose of practical applications. Furthermore the way to understand the structure of nucleus is interdisciplinary since it applies to other fields of mesoscopic quantum systems such as condensed matter, atomic and polyatomic molecular physics. Thanks to the rigorous experimental efforts worldwide that make use of a new generation of rare-isotope beams e.g., at RIKEN in Japan, FRIB and TRIUMF in North America, CERN, GANIL and GSI in Europe etc, it has nowadays become possible to produce and to accelerate extremely unstable, i.e., short-lived, nuclei with considerable proton or neutron excess. The nuclei under such extreme conditions present many unexpected facets, and are therefore called *exotic nuclei*.

Since the pioneering work by Mayer and Jensen [1, 2], formation of shell structure has been one of the remarkable features of atomic nucleus in understanding the nuclear structure. In what is called independent-particle (or shell) model, a nucleon in the nucleus is taken as being moving with an average potential created by all other nucleons. This is much alike the dynamics of electrons in an atom, and similarly to these exhibits discrete single-particle energies. When protons and/or neutrons are filled from the lowest- up to the higher-lying orbitals to reach specific values like 2, 8, 20, 28, 50, 82, 126, …, then a nucleus is notably stable and hence large amount of energy is needed to excite the nucleus from the closed shell to the next. These numbers are called magic numbers, which become evident as a sudden drop of the observed nucleon separation energies. In exotic nuclei, conventional magic numbers may become no longer valid, even giving rise to novel shell structures not heretofore recognized.

Besides these intriguing features that reflect single-nucleon degrees of freedom, the nucleus as a whole exhibits collective properties associated with a distinct shape, where all the constituent nucleons are coherently involved. The collective motion,

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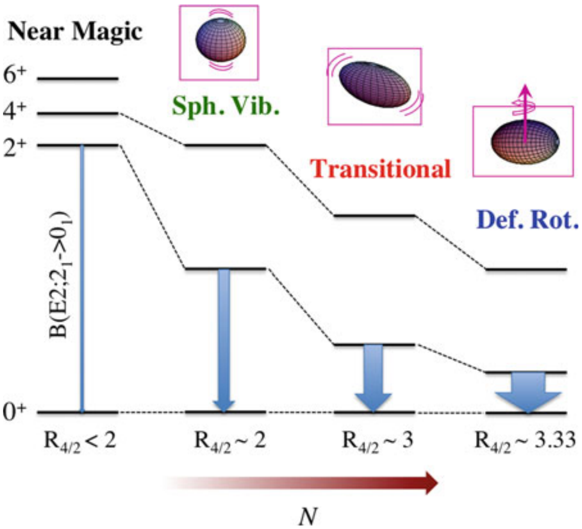

Fig. 1.1 Pictorial description of the quadrupole collective states of atomic nucleus. When departing from the closed shell (Near Magic) with the increase of the valence nucleon number N, the shape changes from spherical vibrator (Sph. Vib.) to deformed rotor (Def. Rot.), passing through the transitional nuclei in between. Each shape results in the characteristic level structure: phonon-like level scheme for a vibrator, and a clear rotational band for a rotor, which are well indicated by the ratio of 4_1^+ to 2_1^+ excitation energies, denoted by $R_{4/2}$. As the collectivity evolves with the number of valance nucleons, the electric quadrupole (E2) transition intensity from the 2_1^+ excited state to the 0_1^+ ground state becomes stronger

observed normally in low-energy[1] regime, stems from the deformation of nuclear surface, that is induced by the multi-fermion dynamics [3–7]. The microscopic interpretation on such a nuclear collective motion was already come up with by Rainwater in 1950 [3], on top of which Bohr and Mottelson established an well-known geometrical model in the middle of 1950s [4–7]. The collective model incorporates the single-particle (shell-model) feature into the purely classical description of the intrinsic nuclear shape as a macroscopic droplet. Particularly the most basic, yet significant nuclear collective motion can be of quadrupole type: the shape of a nucleus can be a spherical vibrator, an ellipsoidal deformed rotor and an object in between, depending on the number of active nucleons. Consequently, a class of remarkable regularities emerge in the corresponding spectroscopic properties (cf. Fig. 1.1). Deformation occurs as a consequence of the intrinsic spontaneous symmetry breaking of the nuclear mean field (in analogy with Jahn-Teller effect [8]), and the rotational motion manifests itself as a realization of symmetry-restoration mechanism [9, 10], which is highly relevant to understanding the microscopy of the nuclear quadrupole deformation.

[1] The energy scale for the collective mode of excitation is typically of the order of 1–10 MeV.

The nucleus is a strongly correlating system governed by the complex nuclear force acting among individual nucleons, while it is, as a whole, a self-bound object characterized by a rather distinct shape seen through the regular patterns of the collective excitations. Therefore, to understand the regularities of the collective mode of excitation from a more microscopic degree of freedom has been a theme of major interest in nuclear physics [3–7, 11–20]. The purpose of this thesis is to address this issue from the viewpoint of the interacting boson model [16, 17] that is formulated by microscopic nuclear energy density functionals. Note that *microscopic* in this context refers to the single-nucleon degrees of freedom, and that we basically assume nucleons (both protons and neutrons) as elementary degrees of freedom throughout this thesis.

Microscopic studies based on nuclear energy density functionals (EDFs) have been quite successful in reproducing with remarkable accuracy various intrinsic (bulk) properties of almost all medium-mass and heavy nuclei on the periodic table such as binding energies, density distributions, surface deformations, charge radii, giant resonances, etc [14, 15]. The current and well-established generation of EDFs includes non-relativistic Skyrme- [21–24], which is of zero-range nature, and Gogny- [25, 26], which is of finite-range type, functionals as well as other density functionals associated with the relativistic mean-field Lagrangian of the effective theory of two-flavor quantum chromodynamics [27–29]. The framework of EDFs has also been extended beyond the mean-field level to describe excitation spectra and electromagnetic transition rates. Models have been developed that perform restoration of symmetries broken by the static nuclear mean field, and take into account quadrupole fluctuations: configuration mixing calculations in the spirit of the generator coordinate method [14, 15, 30–38], and solutions of the Bohr-type collective model Hamiltonian with quadrupole degrees of freedom [39–43].

A static self-consistent mean-field solution in the intrinsic frame, for instance a map of the energy surface as a function of quadrupole deformation, is characterized by symmetry breaking: translational, rotational, particle number, and can only provide an approximate description of bulk ground-state properties. To calculate excitation spectra and electromagnetic transition rates in individual nuclei, it is necessary to include correlations that arise from symmetry restoration and fluctuations around the mean-field minimum. Both types of correlations can be included simultaneously by mixing angular-momentum projected states corresponding to different quadrupole moments. The most effective approach for configuration mixing calculations is the generator coordinate method (GCM), with multipole moments used as coordinates that generate the intrinsic wave functions. It must be noted that, while GCM configuration mixing of axially symmetric states has been implemented by several groups and routinely used in nuclear structure studies [44–47], the application of this method to triaxial shapes presents a much more involved and technically difficult problem [33, 38]. In addition, the use of general EDFs, that is, with an arbitrary dependence on nucleon densities, in GCM type calculations, often leads to discontinuities or even divergences of the energy kernels as a function of deformation [48, 49]. Only for certain types of density dependence a regularization method can be implemented, which corrects energy kernels and removes the discontinuities and divergences [50–52].

As a sound approximation to the full GCM approach to five-dimensional quadrupole dynamics that restores rotational symmetry and that allows for fluctuations around the triaxial mean-field minima, a collective Hamiltonian can be formulated, with deformation-dependent parameters determined by constrained microscopic self-consistent mean-field calculations. The dynamics of the five-dimensional Hamiltonian for quadrupole vibrational and rotational degrees of freedom is governed by the seven functions of the intrinsic quadrupole deformations: the collective potential, three vibrational mass parameters, and three moments of inertia for rotations around the principal axes [39–43].

Another successful approach to the low-lying structure of medium-heavy and heavy nuclei consists in mapping[2] of the multi-nucleon dynamics onto the appropriate system of interacting bosons [16, 17]. The interacting boson model (IBM) of atomic nucleus, originally invented by Arima and Iachello [16, 17], has witnessed great deal of success for the phenomenological description of the low-lying quadrupole collective states of medium-heavy and heavy nuclei. The main ansatz of IBM is to employ the $J^\pi = 0^+$ (s) and 2^+ (d) bosons, which are supposed to simulate the motion of the collective nucleon pairs coupled to angular momentum $J^\pi = 0^+$ and 2^+, respectively, and to introduce the relevant interactions between the bosons [53, 54]. The IBM embodies an entire class of symmetries and regularities of the low-lying quadrupole collective states: three dynamical symmetries arising from the spontaneous breaking of U(6) symmetry, U(5) [55], SU(3) [56] and O(6) [57] limits, where the boson Hamiltonian can be written in some specific forms based on simple algebraic relations, and the intermediate situations of these limits, to which most realistic nuclei belong. The IBM, as well as its algebraic feature, is so general that it has been applied not only in but outside of nuclear physics [16, 17, 58, 59], and thus is itself of wide interest. The IBM in its earliest version (referred to as IBM-1) is purely phenomenological so that the interaction strengths of the model Hamiltonian have been determined from experiment or taken from earlier fitting calculations. Therefore, the IBM itself should have a certain microscopic foundation starting from the nucleonic degrees of freedom.

From a microscopic viewpoint [53, 54, 60], the IBM is essentially a vast truncation of the nuclear shell model, where the so-called proton monopole s_π and quadrupole d_π bosons and neutron monopole s_ν and quadrupole d_ν bosons reflect collective pairs of valence protons, S_π and D_π, and neutrons, S_ν and D_ν, respectively. As the numbers of valence protons and neutrons are constant for a given nucleus, the numbers of proton and neutron bosons, denoted respectively by N_π and N_ν, are set equal to half of the valence proton and neutron numbers. The interaction strengths of the boson Hamiltonian have been determined by the mapping from the *SD* subspace of the full shell-model space onto the *sd* boson space. The mapping scheme for deriving the IBM Hamiltonian of this type is usually referred to as the Otsuka-Arima-Iachello (OAI) mapping and can be extended as the proton-neutron interacting boson model (IBM-2) as a natural consequence [53, 54]. The OAI mapping has been practiced for limited realistic cases of nearly spherical or γ-unstable

[2] Further explanation of the terminology "mapping" will be given in Sect. 2.4.1.

shapes [61–64] by using zero- and low-seniority states of the shell model [53, 54, 60], and has been also tested for deformed Sm isotopes by renormalizing the contribution from the G-pairs as a perturbation [65]. A fermion-boson mapping for deformed nuclei has been studied partly by the "independent-pair" property of condensed coherent fermion pairs [66] and by the rotation of the intrinsic state (a state in the body-fixed frame) [67]. In addition, there are many systematic calculations within the IBM-2 phenomenology for, e.g., Xe-Ba-Ce [68], Ru-Pd [69], Kr [70] and W-Os [71, 72] regions. The microscopic basis of the IBM has been studied for many years, but is still an open problem for the cases involving the strongly deformed nuclei.

More recently a general way of deriving the Hamiltonian of IBM-2 was proposed by Nomura et al. [73]. Under the assumption that the multi-fermion dynamics of the surface deformation is simulated by effective bosonic degrees of freedom, the energy expectation value with varying quadrupole deformation (so-called potential energy surface; PES) within the self-consistent mean-field calculation with a fixed microscopic EDF is mapped onto the corresponding classical limit of the appropriate boson Hamiltonian. Energies and wave functions of excited states are yielded with good angular momentum and particle number [73, 75]. As a given EDF allows universal description of the nuclear intrinsic properties including deformation of ground-state shape, this mapping process in principle provides the interaction strengths of the IBM Hamiltonian for any situations of the quadrupole collective states. While any popular EDF has a direct correspondence to the quadrupole deformation and is certainly suitable to start with, the IBM is a model for nuclear spectroscopy, that provides almost complete description of low-lying structure in medium-heavy and heavy nuclei and that embodies relevant physics in a straightforward way. Therefore we try to incorporate a successful EDF approach in the IBM framework. The validity of the initial work of Ref. [73] was further examined in Ref. [75]: the uniqueness of the derived parameters have been examined carefully using the method of the Wavelet transform [76].

When it is formulated microscopically, however, the IBM is shown to have a crucial problem of not capable of reproducing the moment of inertia of rotational band of strongly deformed nuclei. The problem occurs also in the new scheme of Ref. [73]: the moment of inertia calculated by the IBM turns out be by several tens per cent smaller than the experimentally observed one. Originally, the issue arose as a consequence of the critical comment made by Bohr and Mottelson in 1980, based on a microscopic theory using Nilsson plus BCS model [77]. They concluded that the *SD* truncation might not be sufficient to account for the intrinsic state of rotational deformed nuclei. This question should lead to the problem concerning whether or not the *sd*-IBM can be justified for deformed nuclei. In spite of considerable amounts of theoretical works for the past decades concerning the critique by Bohr and Mottelson, any conclusive work that justifies the validity of IBM for rotational motion has been missing. An important piece of information as to the critique was provided recently by Nomura et al. [78]. They suggested that the deformed nucleon system is substantially different in its response to infinitesimal rotation (cranking) from the corresponding deformed boson system.[3] It was shown [78] that, when the difference in the rotational response becomes sizable, then it can be a possible microscopic origin of the problem concerning the rotational moment of inertia. To correct the difference in the rotational response between fermion and boson systems, the rotational kinetic-like term (so-called LL term) was introduced in the boson system. As a consequence, the rotational bands of strongly-deformed rare-earth and actinoid nuclei were reproduced almost perfectly without any phenomenological adjustment. This study revisited the criticism made in the past by Bohr and Mottelson, and showed, for the first time, how the IBM can be justified for rotational motion of strongly deformed nuclei.

In most isotopic or isotonic sequences the transition between different shapes is gradual, but in a number of cases, with the addition or subtraction of only few nucleons, one finds signatures of abrupt changes in observables that characterize equilibrium shapes. These structure phenomena have been investigated using concepts of quantum shape/phase transitions in finite nuclear system [18, 19, 79–82], and advanced self-consistent (beyond) mean-field approaches [15, 37, 42, 43, 83–94]. In particular, the complex interplay between several deformation degrees of freedom, taking place in different regions of the nuclear chart, offers the possibility of testing microscopic descriptions of atomic nuclei under a wide variety of conditions. In this context, mean-field approximations based on effective EDFs, which as shown already are a cornerstone to almost all microscopic approximations to the nuclear many-body problem, appear to be a first tool to rely on when looking for fingerprints of nuclear shape/phase transitions. On the other hand, it has also become possible to recast mean-field equations in terms of efficient minimization procedures such as the so-called gradient method [95, 96]. One of the advantages of the gradient method is the way it handles constraints, which is well adapted to the case where a large number of constraints are required (like the case which requires, in addition to the proton and neutron number constraints, constrains on both β and γ degrees of freedom characterizing the nuclear shape). Another advantage is its robustness in reaching a solution, a convenient property when large scale calculations requiring the solution of many HFB equations are performed. Experimentally, low-lying spectroscopy provides one with a very powerful source of information that allows establishing signatures correlating nuclear shape transitions with excitation spectra [97–107]. Along these works, the method of [73] has been already tested in a number of spectroscopic calculations in order to clarify the collective structural evolution in various mass regions: Neutron-rich Kr isotopes with mass $A \approx 90$–100 [108], Ru-Pd isotopes with $A \approx 100$–120 [75], Ba-Xe isotopes with $A \approx 110$–130 [75], Sm-Gd isotopes with $A \approx 150$ [73, 75, 78], Pt [109] and Os-W [110] isotopes with $A \approx 180$–200, as well as more systematic analysis on Yb-Hf isotopes in addition to the last three in the same mass region [111].

What is also of interest concerns whether the IBM Hamiltonian, derived from an EDF, can have equal predictive power as other EDF-based schemes, such as

[3] The rotational response in this context means the change of the ground-state energy due to the infinitesimal rotation.

the collective Hamiltonian approach. In Ref. [112], the spectroscopic observables resulting from the IBM-2 Hamiltonian were compared with the solutions of the five-dimensional collective Hamiltonian, with both models starting from the density-dependent point-coupling interaction (DD-PC1) [113] of the relativistic Hartree-Bogoliubov model. The comparison of the two schemes has been done in heavy Pt isotopes, and it was shown in Ref. [112] that both methods do work similarly quite well in the ground-state band spectra but that a certain difference between the two prescriptions comes out e.g., in the structure of the quasi-γ band and in the E2 transition pattern within the ground-state band.

Meanwhile, the structure of non-axial nuclei has been described by the two major geometrical models: the rigid-triaxial rotor model of Davydov and Filippov [114] and the γ-unstable rotor model of Wilets and Jean [115]. However, presumably all observed non-axial medium-heavy and heavy nuclei fall exactly in between the rigid-triaxial and the γ-unstable rotor pictures. This puzzle was addressed in Ref. [116], which showed that, based on a microscopic energy density functional calculation, neither of the rigid-triaxial nor γ-unstable rotor descriptions is realized in actual nuclei. This empirically known fact can be explained naturally only with the inclusion of the three-body boson term into the IBM-2 system, and is shown to be independent of the choice and the details of the EDFs. The result also points to the most appropriate IBM description of γ-soft systems.

This thesis is organized as follows: Chap. 2 explains the *proof of principle*, i.e., the way to determine the IBM Hamiltonian by the EDF approach, as well as its physical interpretations. Crucial limitation inherent to the microscopic IBM, which one encounters in reproducing the moment of inertia of rotational band, is pointed out. This naturally casts a question as to the validity of IBM for deformed nuclei, and a possible answer to this question is proposed in Chap. 3. In Chap. 4, spectroscopic calculations are presented for sets of medium-heavy and heavy nuclei over the wide range of the nuclear chart. We will mainly consider weakly deformed nuclei where the triaxial dynamics plays an important role. The results will be compared with the available experimental data and with the recent studies of quantum phase transitions as well. In Chap. 5, the predictive power of the method presented in Chap. 2 is examined by comparing the spectroscopic properties resulting from the IBM Hamiltonian derived from a relativistic EDF with those obtained from the five-dimensional collective Hamiltonian based on the same EDF. Chapter 6 addresses the question of whether a non-axial nucleus is γ-rigid or unstable, presents a robust regularity of the γ-soft nuclei and how it is realized from a microscopic calculation. The result points to the most suitable IBM description of the γ-soft systems. Chapter 7 discusses the impact of the quantal-mechanical correlation energy on the measurable ground-state properties as an implication of the structural evolution. Chapter 8 is devoted to summary and outlook for possible future research directions. Figure 1.2 indicates how this thesis is organized, and the goal and the motivation of each chapter. For readers' convenience, each chapter and/or section contains an introduction as well as a brief summary. Special attention has been paid so as to clarify the interrelationship among chapters and sections in order to describe a variety of topics in a unified way.

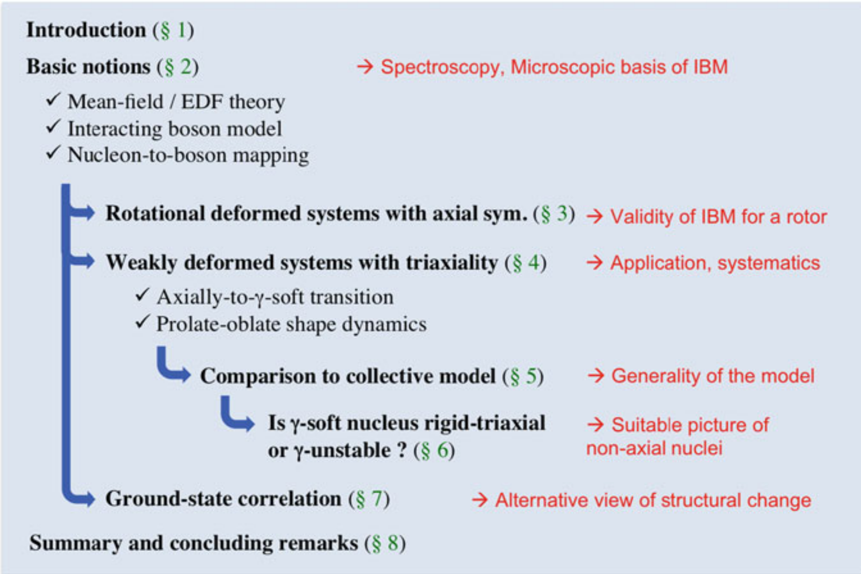

Fig. 1.2 Organization of this thesis. Interrelationship among chapters and sections are indicated. The motivation of each chapter and the outcome drawn from there are indicated on the *right-hand side*

Chapters 2–6, Sect. 7.1, and the Appendices A–B in this thesis are based on the author's original works published already [73, 75, 78, 108–112, 116, 117], coauthoring with (in alphabetical order) M. Albers (Argonne National Laboratory), L. Guo (Graduate University of Chinese Academy of Sciences), T. Nikšić (University of Zagreb), T. Otsuka (University of Tokyo), Zs. Podolyák (University of Surrey), P. H. Regan (University of Surrey), L. M. Robledo (Universidad Autónoma de Madrid), R. Rodríguez-Guzmán (Rice University), P. Sarriguren (Consejo Superior de Investigaciones Científicas, Madrid), N. Shimizu (University of Tokyo), P. D. Stevenson (University of Surrey), and D. Vretenar (University of Zagreb).

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