Chapter 1

Introduction

1.1 Background of this thesis

The nuclear self-consistent mean field (SCMF) models have been one of the central theoretical tools in the nuclear structure and low-energy dynamics [1]. The SCMF method occupies an intermediate position between microscopic approach such as *ab initio* method and macroscopic approach such as liquid drop model. The nuclear mean field of SCMF method is determined self-consistently using an effective interaction. The SCMF approach with local effective density-dependent interaction is considered as an analogy of energy-density-functional theory of electronic systems. The SCMF approach plays a key role to understanding global properties of nuclear ground as well as excited states for wide mass region in a unified way.

At present, there are mainly three approaches of SCMF theory. One is based on a relativistic mean field (RMF) theory (cf. [2]). The others are based on a non-relativistic mean field theory with a zero-range effective (Skyrme) interaction [3, 4, 5] and a finite-range effective (Gogny) interaction [6, 7]. The non-relativistic mean field theory with Skyrme interaction has been most widely studied among the SCMF theories.

The Skyrme interaction was introduced by Skyrme more than forty years ago [3, 4]. Vautherin and Brink proposed Skyrme SII interaction and showed that the Hartree-Fock calculation with the Skyrme interaction is successful in describing nuclear global properties more than thirty years ago [5]. Beiner *et al.* showed that the Skyrme-Hartree-Fock (SHF) method with SIII interaction succeeds in reproducing the binding energy and charge radii of several spherical nuclei [8]. The SHF method has been developed up to the present (cf. [9, 10, 11, 12, 13, 14]). Recently, the Skyrme Hartree-Fock-BCS method with MSk7 interaction by S. Goriely *et al.* [15] and the Skyrme

Hartree-Fock-Bogoliubov method with BSk1 interaction by M. Samyn et al. [16] fairly succeed in reproducing the binding energies for nuclei in a wide range of mass region, where the root-mean square error is less than 0.8 MeV.

For excited states, the random phase approximation (RPA) based on the Skyrme-Hartree-Fock theory has been developed. The RPA response function method with Skyrme force was proposed by Bertsch and Tsai [17]. Van Giai and Sagawa proposed Skyrme SGII force in order to reproduce the giant resonances of spherical nuclei by means of the RPA response function method [18]. Blaizot and Gogny applied the diagonalization method of the RPA equation in particle-hole configuration space, where the RPA equation is diagonalized in the spherical harmonic oscillator basis, to the low-lying state of spherical nuclei in terms of the Skyrme and Gogny interaction [19]. Krewald *et al.* [20] and Waroquier *et al.* [21, 22] proposed the extended Skyrme forces in order to reproduce the ground state properties, the giant resonances and the low-lying excited levels of spherical nuclei by means of the diagonalization method and so on. Recently, Bender *et al.* studied the possibility to improve the Skyrme interaction with respect to the Gamow-Teller resonance and superdeformed band [23]. At present, it is uncertain whether the Skyrme interactions are able to reproduce the low-lying excited states of deformed nuclei. In the future, we foresee that the Skyrme interaction with the ability to reproduce the excited states of deformed nuclei is realized. In this thesis, we formulate a method to be beneficial for such a situation.

1.2 Self-consistent RPA calculation of low-lying states in mesh representation

The three-dimensional (3D) Cartesian mesh calculation is suitable to describe the deformation of nuclei. In nuclear physics, the 3D Cartesian mesh calculation was first performed in solving the time dependent Hartree-Fock equation [24, 25]. In calculating the SHF, Bonche *et al.* showed that the 3D Cartesian mesh calculation is suitable to describe nuclear deformation [26]. Baye and Heenen proposed Lagrange mesh method which provides an explanation for the unexpected accuracy of the Hartree-Fock calculations performed on the 3D Cartesian mesh [27]. Tajima *et al.* performed the SHF plus BCS calculation on the 3D Cartesian mesh in throughout the periodic table of even-even nuclei [28].

Recently, Muta *et. al.* reported a computational method for solving the self-consistent RPA equations in the coordinate representation on 3D Cartesian mesh [29]. They succeeded in calculating a few low-lying states of deformed nuclei with a simplified local effective interaction. In their method, the RPA equations are given in the mixed configuration space of coordinate, instead of unoccupied orbitals, and occupied orbitals, which was first derived by Lemmer and Vénéroni [30]. In solving the RPA equation in a mixed configuration space, the construction of the unoccupied state is not necessary in the procedure, i.e., no truncation of the unoccupied orbitals is required. So, the RPA method in the mixed configuration space corresponds to the RPA response function method [31, 32], which consider the continuum effect. The method by Muta *et al.* has three difficulties. The first point is that fine mesh size is required in their calculation in order to separate physical modes from the spurious zero modes. The second point is that imaginary eigenvalues of the RPA equations cannot be treated with their method. The third point is that it is probably difficult to calculate the low-lying states of heavy nuclei because the memory and the time that are necessary for numerical computation are enormous.

In this thesis, we propose the formulation of self-consistent SHF plus RPA calculation in the mesh representation for the even-even nuclei with reflection symmetry with respect to $x = 0$, $y = 0$ and $z = 0$ planes (cf. [33]). Our formulation is based on the method of Ref. [29] but improved to get over the difficulties in their method. First, in order to reduce a cost to be necessary for numerical computation, we take advantage of the time-reversal properties and spatial symmetry in solving the RPA equation. The introduced spatial symmetries can be also utilized so as to specify the quantum number of the excited state. Second, we develop the numerical method for treating solutions with pure imaginary eigenvalues of the RPA equation. The method is essential for calculation with imposed spatial symmetries because there is a possibility that the RPA equation has the solutions with pure imaginary eigenvalues when the spatial symmetries are imposed on the RPA calculation. Third, we develop the numerical method for obtaining accurate numerical results even though coarse mesh is employed in the calculation. It enables us to calculate the spurious state and physical state accurately.

1.3 Superdeformed state for ^{40}Ca

Very recently, the superdeformed band built on 0_3^+ state for the doubly magic nucleus ^{40}Ca was observed by Ideguchi *et al.* [34]. From the theoretical side, it was suggested more than thirty years ago that the 0_3^+ state of ^{40}Ca is considered as 8-particle 8-hole (8p-8h) excitation with the shell model [35] and has large deformations with the Strutinsy type calculation [36]. It was also studied with Skyrme Hartree-Fock calculation more than ten years ago [37, 38], in which the 0_3^+ state is predicted as the 8p-8h state with the quadrupole deformation $\beta_2 = 0.599$. After the observation of superdeformed band of ^{40}Ca, the several calculations were performed with cranked-Skyrme-Hartree-Fock method [39], AMD [40, 41] and shell model [42].

Fig. 1.1 shows experimental levels of ^{40}Ca [34]. The Band 1 built on a 0_3^+ state at 5.213 MeV is a superdeformed band. From the analysis with fractional Doppler shifts, the transition quadrupole moment $Q_t = 1.80^{+0.39}_{-0.29}$eb was determined. The quadrupole deformation is determined as $\beta_2 = 0.59^{+0.11}_{-0.07}$ from the above transition quadrupole moment by means of the rigid axially symmetric rotor model [34].

This superdeformed band has special features which other superdeformed bands do not have: One is that the ^{40}Ca is a well known doubly magic nucleus and has same number of protons and neutrons. The other is that the superdeformed band is built on the excited 0^+ state.

The octupole softness of the superdeformed band is an interesting topic (cf. [43]). Nakatsukasa *et al.* studied octupole correlations of the SD band by means of the cranked RPA method [44, 45]. Inakura *et al.* studied octupole softness of the SD band of ^{40}Ca by means of the constrained SHF method [39].

We apply our formulation to the superdeformed state of ^{40}Ca.

This thesis is organized as follows. In chapter 2, we derive the RPA equation in the mixed configuration space of spatial coordinate and hole orbitals. We also study the time reversal property of the RPA equation under time-reversal. In chapter 3, we derive the HF equation in the coordinate representation and the RPA equation in the mixed configuration space with Skyrme interaction, which are used in our numerical calculation. In chapter 4, we explain our numerical method in detail. We present the solution method that is useful to solve the SHF equation on the 3D Cartesian mesh. We also present the solution method of the RPA equation in the mixed configuration space on the 3D Cartesian mesh. We introduce the spatial symmetries in the SHF and RPA calculations in order to solve the equations on one eighth of the mesh space. These spatial symmetries are made use of in order to specify the quantum numbers of excited states. We explain the simple method for obtaining the accurate results of the excitation energies and reduced transition probabilities in terms of the 3D cartesian mesh calculation with Lagrange mesh method. This method allows us to obtain accurate results even when we employ course mesh size. We propose a computational method for calcu-

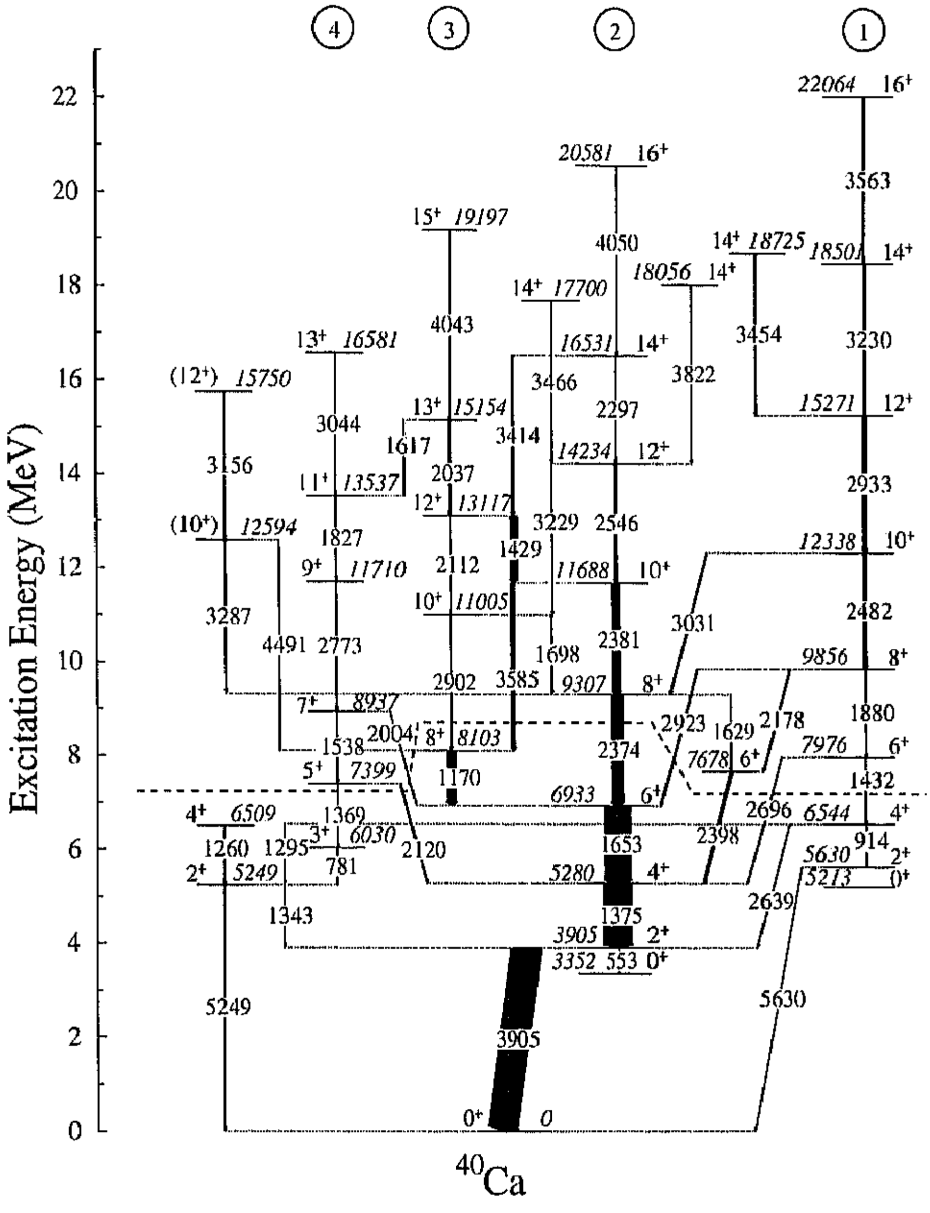

Figure 1.1: Partial level scheme of ^{40}Ca. The Band 1 built on a 0_3^+ state at 5.213 MeV is a superdeformed band. (From Ref. [34]).

lating RPA correlation energies associated with the spatial symmetries. and for obtaining collective mass for translation as well as moment of inertia for rotation of the nucleus. We compare our results of the RPA calculation with the ones by other's RPA calculations. We make comment on the instability due to the $\boldsymbol{s} \cdot \triangle \boldsymbol{s}$ terms in Skyrme energy functional. In chapter 5, we apply our method to spherical nuclei. In chapter 6, we apply our formulation to the superdeformed state of ^{40}Ca. We show that our formulation with SkI4 force reproduce the SD rotational band. We also study the octupole softness of SD band.