Covariant Density Functional Theory: Global Performance and Rotating Nuclei

Debisree Ray

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Covariant density functional theory: Global performance and rotating nuclei

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Covariant density functional theory (CDFT) is a modern theoretical tool for the description of nuclear structure physics. Here different physical properties of the ground and excited states in atomic nuclei have been investigated within the CDFT framework employing three major classes of the state-of-the-art covariant energy density functionals.

The global performance of CEDFs for even-even nuclei are investigated and the systematic theoretical uncertainties are estimated within the set of four CEDFs in known regions of the nuclear chart and their propagation towards the neutron drip line. Large-scale axial relativistic Hartree-Bogoliubov (RHB) calculations are performed for even-even nuclei to calculate different ground state observables. The predictions for the two-neutron drip line are also compared in a systematic way with the non-relativistic results.

CDFT has been applied for systematic study of extremely deformed, rotating $N \sim Z$ nuclei of the $A \sim 40$ mass region. At spin zero such structures are located at high energies which prevents their experimental observation. The rotation acts as a tool to bring these
exotic shapes down to the yrast line so that their observation could become possible with a future generation detectors such as GRETA or AGATA. The major physical observables of such structures, the underlying single-particle structure and the spins at which they become yrast or near yrast are defined. The search for the fingerprints of clusterization and molecular structures is performed and the configurations with such features are discussed.

CDFT has been applied to study fission barriers of superheavy nuclei and related systematic theoretical uncertainties in the predictions of inner fission barrier heights in superheavy elements. Systematic uncertainties are substantial in superheavy elements and their behavior as a function of proton and neutron numbers contains a large random component. The benchmarking of the functionals to the experimental data on fission barriers in the actinides allows reduction of the systematic theoretical uncertainties for the inner fission barriers of unknown superheavy elements. However, even then they on average increase when moving away from the region where benchmarking has been performed.

Key words: covariant density functional theory, driplines, theoretical uncertainties, superdeformation, hyperdeformation, megadeformation, yrast, fission barriers, superheavy elements
DEDICATION

To my parents
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LIST OF SYMBOLS

Following are the technical abbreviations and special nomenclature used in this dissertation.

**DFT**  Density Functional Theory

**CDFT**  Covariant density Functional Theory

**CEDF**  Covariant energy density functional

**SDFT**  Skyrme Density Functional Theory

**rms**  root-mean-square

**CRMF**  Cranked Relativistic Mean Field

**Superdeformed**  Deformed nucleus, far from spherical shape forming an ellipsoid where the semiaxis ratio is around 2:1:1

**Hyperdeformed**  Deformed nucleus, far from spherical shape forming an ellipsoid where the semiaxis ratio is around 3:1:1

**Yrast**  Lowest in energy state at a given spin.

**PES**  Potential Energy Surface

**SHE**  Super Heavy Element
CHAPTER 1
INTRODUCTION

For the last few decades, the Kohn-Sham density functional theory (DFT) \[1, 2\] has been successfully applied to the description of quantum mechanical many body systems in atomic, molecular and condensed matter physics. In Coulombic systems, the functional can be derived directly from the coulombic interaction, without any phenomenological adjustments. However, in nuclear physics the situation is much more complicated.

Atomic nuclei are considered as self-bound, quantum mechanical many-body systems with translational invariance. There are spin and isospin degrees of freedom which cannot be neglected. Many open shell nuclei are superfluid systems. There are strong indications that an optimal description of nuclei should be relativistic \[3, 4\]. As a consequence the single-particle wave functions at each point in r-space form a spinor of dimension 16 (in relativistic case) \[3\], which substantially complicates a theoretical description.

In spite of all these complications, for the last 40 years, both non-relativistic and relativistic (covariant) DFTs have been developed and extensively applied to various nuclear physics problems \[5, 6, 7, 8\] with great success. These are extremely useful for medium and heavy mass nuclei where the \textit{ab-initio} type few body calculations are at least currently not possible. The DFT calculations are achieved in terms of effective parametrizations of
the energy density functionals (EDF). Most of them are determined by symmetry arguments and the rest by fitting to experimental data in finite nuclei; such as binding energy, charge radii etc. Amongst these nuclear DFTs, the covariant density functional theory (CDFT) is one of the most sophisticated theories because ([3]):

- Covariant energy density functionals (CEDFs) exploit basic properties of QCD at low energies, such as symmetries and the separation of scales [6].
- They provide a consistent treatment of spin degrees of freedom.
- They include the complicated interplay between the large Lorentz scalar and vector self-energies induced at the QCD level by the in-medium changes of the scalar and vector quark condensates [9].
- These functionals include nuclear magnetism [10], i.e. a consistent description of currents and time-odd mean fields important for odd-mass nuclei [11], the excitations with unsaturated spins, magnetic moments [12] and nuclear rotations [13, 14].

This class of relativistic theories, based on the concepts of non-renormalizable effective relativistic field theories and DFT, provides the most useful tool to study atomic nuclei at and far away from stability. At present, all attempts to derive these functionals directly from the bare forces [15, 16, 17, 18] do not reach the required accuracy. However, in recent years modern covariant energy density functionals have been derived [19, 20, 21] which provide an excellent description of ground and excited states all over the nuclear chart [7, 22] with a high predictive power. Modern versions of these forces derive the density
dependence from state-of-the-art ab-initio calculations and use only the remaining few parameters for a fine tuning of experimental masses in finite spherical [21] or deformed [20] nuclei.

In this dissertation we have investigated different physical properties of ground and excited state atomic nuclei in the CDFT framework. In the first project we have applied CDFT for axially symmetric systems to the investigation of the global performance of CEDFs for even-even nuclei and related systematic theoretical uncertainties. In the second project CDFT has been applied to the study of extreme deformations and clusterization in the rotating $N \sim Z$ nuclei of the $A \sim 40$ mass region. And finally, in the third project, CDFT has been applied to triaxial systems to study fission barriers of superheavy nuclei and related theoretical uncertainties. The outlines of these projects are:

- The theoretical description of ground state properties and its extrapolation to nuclei with large isospin are important to understand nuclear structure physics and nuclear astrophysics. Many such nuclei will not be studied experimentally even with the next generation experimental facilities. Hence, it is very important to understand how well the nuclear EDFs describe globally the available experimental data and how well they extrapolate to the region of unknown nuclei with large isospin. Unfortunately, even the answer to the first question was not known for the state-of-the-art covariant energy density functionals before our study.

Thus, the goal of the first project was the global assessment of the accuracy of the description of the ground state properties of even-even nuclei and the estimate of the theoretical uncertainties in known regions of the nuclear chart and their propa-
gation towards the neutron-rich side. To achieve this, we have undertaken the first ever systematic study of all \( Z \leq 104 \) even-even nuclei between the two-proton and two-neutron driplines in a relativistic Hartree-Bogoliubov (RHB) framework with four state-of-the-art covariant energy density functionals such as NL3*, DD-ME2, DD-ME\( \delta \) and DD-PC1. The physical observables of interest include binding energies, two-particle separation energies, charge quadrupole deformations, charge radii, neutron skin thickness and the positions of the two-proton and two-neutron driplines.

Theoretical results are always associated with some uncertainties. In the present study of ground-state observables, these are theoretical uncertainties which come from the selection of the form of EDF as well as from the fitting protocol details of EDFs, such as the selection of the nuclei under investigation, the physical observables or the corresponding weights. The theoretical uncertainties can be separated into systematic and statistical ones. The systematic uncertainties emerge from the underlying theoretical approximations. In the DFT framework, there are two major sources of these approximations, namely, the range of interaction and the form of the density dependence of the effective interaction \([5, 23]\). In the CDFT, the point coupling and the meson exchange models have an interaction of zero and of finite range, respectively \([7, 19, 20, 24]\). The density dependence is introduced either through an explicit dependence of the coupling constants \([19, 20, 25]\) or via non-linear meson couplings \([23, 24]\). This ambiguity in the definition of the range of the interaction and its density dependence leads to several major classes of the covariant energy density functionals (CEDF) which have been discussed in Ref. \([3]\). Therefore we
define *systematic theoretical uncertainties* for a given physical observable via the spread of theoretical predictions within the selected set of CDEFs.

The *statistical errors* arise from the details of the fitting protocol such as the choice of experimental data and the selection of adopted errors. It applies only to a given functional and can be calculated from a statistical analysis during the fit. However, it is difficult to perform the analysis of statistical errors on a global scale since the properties of transitional and deformed nuclei have to be calculated repeatedly for different variations of the original CEDF. Thus, such statistical analysis has been performed mostly for spherical nuclei [26, 27] or selected isotopic chains of deformed nuclei [28].

- There is a considerable interest in the study of cluster structures and extremely deformed shapes in light nuclei. In recent years, these investigations of exotic cluster configurations have been undertaken also in the density functional theory. The clustering phenomenon in light stable and exotic nuclei was studied within the relativistic mean field (RMF) approach in Ref. [29] and within the Hartree-Fock (HF) approach based on the Skyrme energy density functionals (EDF) in Ref. [30]. Linear chain configurations of four α-clusters in $^{16}$O and the relationship between the stability of such states and angular momentum were investigated using Skyrme cranked HF method in Ref. [31] and Cranked RMF (CRMF) in Ref. [32]. This is an example of a “rod shaped” nucleus. Another case of such structures is a linear chain of three α clusters, suggested about 60 years ago [33] which was recently studied in the CRMF...
theory in Ref. [34]. This exotic structure (the “Hoyle” state) plays a crucial role in the synthesis of $^{12}\text{C}$ from three $^4\text{He}$ nuclei in stars [35]. The stability of rod-shaped structures in highly-excited states of $^{24}\text{Mg}$ was studied in Ref. [36] using cranked Skyrme HF calculations.

However, the difficulty in investigating these extremely deformed states is that they are either unbound and/or lie at high excitation energies at low spins. The high density of nucleonic configurations at these energies and possible mixing among them is another factor hindering their observation with current and future generations of experimental facilities. Moreover, obtaining unambiguous evidences for clustering (such as a transition strengths between different states and the structure of the wavefunction) is equally challenging and frequently ambiguous from an experimental point of view. In addition, the mechanisms of the reactions used in experimental studies frequently favor the population of yrast or near-yrast states [37].

The rotation of the nucleus could help to overcome these problems in experimental observation of extremely deformed structures. Two factors contribute to lowering these states. First, very large deformation configurations (such as super-, hyper- and mega-deformed configurations) are favored by rotation at high spins (see, for example, the discussion in Refs. [38, 39]). Second, normal- and highly-deformed configurations, which are forming yrast or near-yrast structures at low and medium spins, have limited angular momentum content. As a consequence, only extremely deformed structures could be populated above some specific spin values in the nuclei of the interest.
Thus, the second project of this dissertation deals with a systematic search for extremely deformed and clustered configurations in the rotating $N = Z$ and $N = Z + 2$ even-even $S$ ($Z = 16$), Ar ($Z = 18$), Ca ($Z = 40$), Ti ($Z = 42$), Cr ($Z = 44$) (and also on $N = Z + 4$ $^{44}$Ca) and odd-odd $N = Z = 21$ $^{42}$Sc nuclei in the CDFT framework. At spin zero such structures are located at high excitation energies which prevents their experimental observation. The rotation acts as a tool to bring these exotic shapes to the yrast line or its vicinity so that their observation could become possible with a future generation of $\gamma$-tracking (or similar) detectors such as GRETA or AGATA.

- The third project deals with fission barriers in superheavy nuclei. The region of superheavy elements (SHE), characterized by the extreme values of proton number $Z$, is one of the extremes of the nuclear landscape and an arena of active experimental and theoretical studies (see Refs. [40, 41, 42] and references therein). The stability of SHEs is defined by the fission barriers. In addition, the experimental studies of SHEs are based on the observation of $\alpha$-decays. As a consequence, only SHEs with spontaneous fission half-lives $\tau_{SF}$ longer than the half-lives $\tau_{\alpha}$ of the $\alpha$-decays could be observed in experiment. An additional limit is set up by the fact that only $\alpha$-decays longer than 10 $\mu$s can be observed in experiment. Therefore it is of great importance to study the fission barriers in SHEs. The height of the fission barrier, $B_f$, which is the difference of the energies of the respective saddle in the potential energy surface (PES) and the ground state, is one of most important quantities. It defines the survival probability of SHEs synthesized in heavy-ion reactions and impacts the
spontaneous fission half-lives. The later is important for an understanding of the competition between the fission process and $\alpha$ particle emission.

Theoretical investigations require also an estimate of theoretical uncertainties. This becomes especially important when one deals with the extrapolations beyond the known regions, as for example in particle number or deformation and related systematic theoretical uncertainties. Thus, the impact of triaxial deformation on inner fission barriers and related systematic uncertainties have been investigated within the triaxial RHB framework.

The dissertation is organized as follows: Ch. 2 contains the basic formalism of covariant density functional theory. Ch. 3 is devoted to global assessment of the accuracy of the description of the ground state properties of even-even nuclei. Ch. 4 is dedicated to the study of extreme deformations and clusterization at high spin in the $N \sim Z$ nuclei of the $A \sim 40$ mass region. In Ch. 5 theoretical uncertainties in fission barriers of superheavy nuclei are evaluated. Finally, the summary of the major results is presented in Ch. 6.
CHAPTER 2
FORMALISM : COVARIANT DENSITY FUNCTIONAL THEORY

2.1 Basic features of covariant density functional theory

Covariant density functional theory (CDFT) is a microscopic description of atomic nuclei, which can be regarded as a quantum mechanical many particle system. In CDFT a nucleus is described as a system of Dirac nucleons interacting via the exchange of effective mesons with finite masses leading to a finite range interaction. Three classes of covariant density functional models have been used in this dissertation. These are the nonlinear meson-nucleon coupling model (NL), the density-dependent meson-exchange model (DD-ME) and the density-dependent point-coupling model (DD-PC). The main differences between them are in the treatment of the range of the interaction, the mesons and the density dependence of the interaction. The interaction in the first two classes has a finite range that is determined by the mass of the mesons. For fixed density it is of Yukawa type and the range is given by the inverse of the meson masses. For large meson masses, i.e. for small ranges, the meson propagator can be expanded in terms of this range. In zeroth order we obtain δ-forces and higher order derivative terms. This leads to the third class of density functionals, the point coupling models. There is no meson in this type of model, therefore the interaction is of zero-range. The density dependence is explicit in the last two models. They are taken into account by density dependent meson-nucleon vertices in the DD-ME
and DD-PC models. In nonlinear meson nucleon coupling model the density dependence is introduced through the powers of the $\sigma$-meson. Each of these classes is represented by the energy density functionals considered to be state-of-the-art. They are NL3* [24] for the NL-models, DD-ME2 [19] and DD-ME$\delta$ [21] for the DD-ME models, and by DD-PC1 [20] for the point coupling models.

2.2 Covariant Energy Density Functionals

2.2.1 Meson-exchange model

In the meson-exchange models [19, 21, 24], the nucleus is described as a system of Dirac nucleons interacting via the exchange of mesons with finite masses leading to finite-range interactions. The starting point of covariant density functional theory for these two models is a standard Lagrangian density [43]

\[
\mathcal{L} = \bar{\psi} \gamma \cdot \left( i \partial - g_\omega \omega - g_\rho \vec{\rho} \vec{\gamma} - eA \right) \psi - m - g_\sigma \sigma - g_\delta \vec{\sigma} \vec{\delta} \psi \\
+ \frac{1}{2} (\partial \sigma)^2 - \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{2} (\partial \bar{\delta})^2 - \frac{1}{2} m_\delta^2 \bar{\delta}^2
\]

\[
- \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega^2 - \frac{1}{4} \bar{F}_{\mu\nu} \bar{F}^{\mu\nu} + \frac{1}{2} m_\rho^2 \rho^2
\]

\[
- \frac{1}{4} F_{\mu\nu} F^{\mu\nu}
\] (2.1)

The nucleons are described by the Dirac spinors $\psi$ of mass $m$ and several effective mesons characterized by the quantum numbers of spin, parity, and isospin. These mesons are, the $\sigma$ meson with respective quantum numbers of angular momentum $J$, isospin $T$ and parity $P(J = 0, T = 0, P = +1)$, the $\rho$ meson($J = 1, T = 1, P = -1$) and the $\omega$ meson ($J = 1, T = 0, P = -1$). Fig. 2.1 shows the Feynman diagrams for the
respective interactions. These mesons create the effective fields in a Dirac equation, which corresponds to the Kohn-Sham equation [1] in the non-relativistic DFT. The Lagrangian (2.1) contains as parameters the meson masses $m_\sigma$, $m_\omega$, $m_\delta$, and $m_\rho$ and the coupling constants $g_\sigma$, $g_\omega$, $g_\delta$, and $g_\rho$. While $e$ is the charge of the proton which vanishes for the neutrons.

![Feynman diagrams for respective meson-nucleon effective interactions](image)

**Figure 2.1**

Feynman diagrams for respective meson-nucleon effective interactions

This linear model was first introduced by Walecka [44, 45]. However, it has failed to describe the surface properties of realistic nuclei. In particular, the resulting incompressibility of infinite nuclear matter is much too large [23] and nuclear deformations are too small [43]. This problem has been resolved by Boguta and Bodmer in Ref. [23]. They in-
introduced a density dependence via a non-linear meson coupling replacing the term $\frac{1}{2}m^2_\sigma \sigma^2$ in Eq. (2.1) by

$$U(\sigma) = \frac{1}{2}m^2_\sigma \sigma^2 + \frac{1}{3}g_2 \sigma^3 + \frac{1}{4}g_3 \sigma^4. \quad (2.2)$$

The nonlinear meson-coupling models are represented by the parameter set NL3* [24]. This is a modern version of the widely used parameter set NL3 [46]. Both contain no $\delta$ meson. Apart from the fixed values for the masses $m$, $m_\omega$, and $m_\rho$, there are six phenomenological parameters $m_\sigma$, $g_\sigma$, $g_\omega$, $g_\rho$, $g_2$, and $g_3$ which have been fitted in Ref. [24] to a set of experimental data in spherical nuclei: 12 binding energies, 9 charge radii, and 4 neutron skin thicknesses [3].

The density-dependent meson-nucleon coupling model has an explicit density dependence for the meson-nucleon vertices. There are no non-linear terms for the $\sigma$ meson, i.e. $g_2 = g_3 = 0$. For the form of the density dependence the Typel-Wolter ansatz [25] has been used:

$$g_i(\rho) = g_i(\rho_{\text{sat}}) f_i(x) \quad \text{for } i = \sigma, \omega, \delta, \rho \quad (2.3)$$

where the density dependence is given by [19, 21, 25]

$$f_i(x) = a_i \frac{1 + b_i (x + d_i)^2}{1 + c_i (x + e_i)^2}. \quad (2.4)$$

Here $x$ is defined as the ratio between the baryonic density $\rho$ at a specific location and the baryonic density at saturation $\rho_{\text{sat}}$ in symmetric nuclear matter. The parameters in Eq. (2.4) are not independent, but constrained as follows: $f_i(x = 1) = 1$, $f''_\sigma(x = 1) = f''_\omega(x = 1)$, and $f''_i(x = 0) = 0$. In addition, the constraints $d_\sigma = e_\sigma$ and $d_\omega = e_\omega$ are used. Thus the number of independent parameters for the density dependence has been reduced.
The density-dependent meson-nucleon coupling model is represented here by the CEDF’s DD-ME2 [19] and DD-MEδ [21]. The parameters of the NL3*, DD-ME2 and DD-MEδ CEDF’s are tabulated in the Table 2.1. The masses are given in MeV and the dimension of $g_2$ in NL3* is fm$^{-1}$. All other parameters are dimensionless. Note that $g_\sigma = g_\sigma(\rho_{\text{sat}})$, $g_\omega = g_\omega(\rho_{\text{sat}})$, $g_\delta = g_\delta(\rho_{\text{sat}})$ and $g_\rho = g_\rho(\rho_{\text{sat}})$ in the case of the DD-ME2 and DD-MEδ CEDF’s.

The difference between DD-MEδ and DD-ME2 in this class of the models is related to the role of the extra ($\delta$) meson. In DD-ME2 there is no $\delta$-meson and the density dependence of Eq. (2.4) is used only for the $\sigma$ and $\omega$ mesons and for the $\rho$ meson we have an exponential density dependence

$$f_\rho(x) = \exp(-a_\rho(x - 1)).$$

The difference between the functional NL3* and other three functionals is related to the fact that NL3* has no non-linearities in the isovector channel. Therefore, in infinite nuclear matter, the isovector fields are proportional to the isovector density, which are given by $N - Z$. This leads to a very stiff symmetry energy as a function of the density and to relatively large values for the symmetry energy $J$ and its slope $L$ at saturation (see Table IV in the Ref. [3]). The fits of other above-mentioned non-linear meson coupling functionals have tried to reduce this value. However, because of the stiffness of the linear ansatz this is possible only to a certain extent. Although these functionals are very successful for static CDFT close to the valley of stability [24], their common feature is that the neutron skin thicknesses are larger than those of successful Skyrme EDF’s and DD-ME* CEDF’s.
Table 2.1

The parameters of NL3*, DD-ME2 and DD-MEδ CEDF’s.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>NL3*</th>
<th>DD-ME2</th>
<th>DD-MEδ</th>
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<tbody>
<tr>
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<td>939</td>
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<td>783.000</td>
<td>783.00</td>
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<tr>
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<td>983.0</td>
<td>983.0</td>
</tr>
<tr>
<td>$m_{\rho}$</td>
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<td>763.000</td>
<td>763.00</td>
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<tr>
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<td>7.152</td>
<td>7.152</td>
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<tr>
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</tr>
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<td>$g_3$</td>
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</tr>
<tr>
<td>$e_{\sigma}$</td>
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</tr>
<tr>
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<tr>
<td>$a_{\delta}$</td>
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<td>$b_{\delta}$</td>
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<td>$c_{\delta}$</td>
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</tr>
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<td>$d_{\delta}$</td>
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<td></td>
</tr>
<tr>
<td>$e_{\delta}$</td>
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<td></td>
<td></td>
</tr>
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<td>$a_{\rho}$</td>
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</tr>
<tr>
<td>$b_{\rho}$</td>
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</tr>
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<td>$c_{\rho}$</td>
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</tr>
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<td>$d_{\rho}$</td>
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</tr>
<tr>
<td>$e_{\rho}$</td>
<td></td>
<td>0.9737</td>
<td></td>
</tr>
</tbody>
</table>
For the functional DD-ME2 [19] the masses $m$, $m_\omega$ and $m_\rho$ are kept at fixed values. As discussed above the density dependence of the coupling constants $f_i(x) \ i = \sigma, \omega, \rho$ is given by four independent parameters. Therefore, together with the four parameters $m_\sigma$, $g_\sigma(\rho_{\text{sat}})$, $g_\omega(\rho_{\text{sat}})$, and $g_\rho(\rho_{\text{sat}})$ DD-ME2 contains eight independent parameters which have been fitted in Ref. [19] to a set experimental data in spherical nuclei: 12 binding energies, 9 charge radii, and 3 neutron skin thicknesses.

The functional DD-ME$\delta$ [21] differs from the earlier DD-ME functionals also in the fitting strategy. It tries to use only a minimal number of free parameters adjusted to the data in finite nuclei and to use ab-initio calculations to determine the density dependence of the meson-nucleon vertices. Relativistic ab-initio calculations [16, 17] show clearly that the isovector scalar self-energy, i.e. the field of the $\delta$-meson, is not negligible. Therefore, the functional DD-ME$\delta$ differs also from the other functionals by including the $\delta$-meson, which leads to a different effective Dirac mass for protons and neutrons:

$$m_{n,p}^* = m + g_\sigma \sigma \pm g_\delta \delta.$$  \hspace{1cm} (2.6)

As a consequence, the splittings of the spin-orbit doublets with large orbital angular momentum $l$ are slightly different in the models with and without a $\delta$-meson. However, this effect is too small to be seen in present experiments [21]. All the other effects of the $\delta$-meson on experimental isovector properties of nuclear structure at densities below and slightly above saturation can be completely absorbed by a renormalization of the $\rho$-meson-nucleon vertex [21]. Therefore, successful phenomenological CEDF’s do not need to include the $\delta$-meson. However, the effects of the $\delta$-meson are important for a proper description of
the nuclear equation of state (EoS) at higher densities (see Ref. [21] and references given there) which play a role in heavy-ion reactions and in astrophysics.

In the earlier parameters sets DD-ME1 [47] and DD-ME2 [19], all eight independent parameters were adjusted to experimental data in finite nuclei, whereas for DD-MEδ only the four independent parameters $m_\sigma$, $g_\sigma(\rho_{\text{sat}})$, $g_\omega(\rho_{\text{sat}})$, and $g_\rho(\rho_{\text{sat}})$ have been adjusted to experimental data in finite nuclei. This data set includes 161 binding energies and 86 charge radii of spherical nuclei. The parameter $g_\delta(\rho_{\text{sat}})$ and the density dependence $f_i(x)$ have been fitted to parameter-free ab-initio calculations of infinite nuclear matter of various densities, as for instance the equations of state (EoS) for symmetric nuclear matter and pure neutron matter, and the difference in the effective Dirac masses $m_p^* - m_n^*$. Thus, the functional DD-MEδ is the most microscopically justified CEDF among these four.

2.2.2 Point coupling model

Table 2.2

The parameters of the DD-PC1 CEDF

<table>
<thead>
<tr>
<th>Parameter</th>
<th>DD-PC1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
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</tr>
<tr>
<td>$a_S$</td>
<td>-10.04616</td>
</tr>
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<td>$b_S$</td>
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<td>$c_S$</td>
<td>-6.42729</td>
</tr>
<tr>
<td>$d_S$</td>
<td>1.37235</td>
</tr>
<tr>
<td>$a_V$</td>
<td>5.91946</td>
</tr>
<tr>
<td>$b_V$</td>
<td>8.86370</td>
</tr>
<tr>
<td>$d_V$</td>
<td>0.65835</td>
</tr>
<tr>
<td>$b_{TV}$</td>
<td>1.83595</td>
</tr>
<tr>
<td>$d_{TV}$</td>
<td>0.64025</td>
</tr>
</tbody>
</table>
For the density-dependent point coupling model [20, 48], the Lagrangian is given by

\[ \mathcal{L} = \bar{\psi} (i\gamma \cdot \partial - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - e \bar{\psi} \gamma \cdot A \psi - \frac{1}{2} \alpha_S(\rho) \bar{\psi} \gamma \cdot \bar{\psi} + \frac{1}{2} \alpha_V(\rho) \bar{\psi} \gamma^\mu \gamma \cdot \bar{\psi} + \delta_S \bar{\psi} \gamma \cdot \bar{\psi} \tag{2.7} \]

This model is represented by the parametrization DD-PC1 [20] given in Table 2.2. The ansatz used for the functional form of the couplings is

\[ \alpha_i(\rho) = a_i + (b_i + c_i x) e^{-d_i x}, \quad \text{for } i = S, V, TV \tag{2.8} \]

where \( x = \rho/\rho_{\text{sat}} \) denotes the nucleon density in units of the saturation density of symmetric nuclear matter. In the isovector channel a pure exponential dependence is used, i.e. \( a_{TV} = 0 \) and \( c_{TV} = 0 \). The remaining set of 10 constants \( a_S, b_S, c_S, d_S, a_V, b_V, c_V, d_V, b_{TV}, a_{TV} \) that control the strength and density dependence of the interaction Lagrangian, was adjusted in a multistep parameter fit exclusively to the experimental masses of 64 axially deformed nuclei.

The Lagrangian (2.7) contains the free-nucleon part, the coupling of the proton to the electromagnetic field, and the point coupling interaction terms. The derivative term with the D’Alembert operator \( \Box \) accounts for the leading effects of finite-range interaction which are important in nuclei. In analogy with meson-exchange models, this model contains isoscalar-scalar (S), isoscalar-vector (V) and isovector-vector (TV) interactions. The coupling constants \( \alpha_i(\rho) \) are density dependent.
The nuclei shown in the \((N, Z)\) plane, which were used in the fit of indicated CDFT parametrization.

The nuclei shown in the \((N, Z)\) plane, which were used in the fit of indicated CDFT parametrizations
Figure 2.4

The nuclei shown in the \((N, Z)\) plane, which were used in the fit of indicated CDFT parametrization.

Figure 2.5

The nuclei shown in the \((N, Z)\) plane, which were used in the fit of indicated CDFT parametrization.
2.2.3 The fitting protocols

Fig. 2.2, Fig. 2.3, Fig. 2.4, Fig. 2.5 show the nuclei which were used in the fits of the different covariant energy density functionals. One can see that the fitting protocols used for the derivation of the various CEDF’s differ in the amount and the type of experimental data. NL3*, DD-ME2 and DD-MEδ CEDF were fitted to spherical nuclei, while DD-PC1 was fitted to deformed nuclei in the rare-earth and actinide regions. Only 12 spherical nuclei were used in the fitting protocols of NL3* and DD-ME2. On the contrary, the fits of other two CEDF’s rely on more extensive sets of experimental data (161 spherical nuclei in the DD-MEδ CEDF and 64 deformed nuclei in the DD-PC1 CEDF). In all these fitting protocols, the binding energies, charge radii and neutron skin thicknesses were used. In contrast to non-relativistic models, no single-particle information has been used in the fits. The number of independent parameters in the NL3*, DD-ME2, DD-MEδ and DD-PC1 CEDF is 6, 8, 14, and 10, respectively. Note, however, that in the case of DD-MEδ, only 4 parameters are fitted to the properties of finite nuclei while the additional 10 parameters are fitted to pseudo-data obtained from ab initio calculations of nuclear matter.

2.3 The cranked relativistic mean field (CRMF) framework

As already described, in the CDFT the nucleus is described as a system of pointlike nucleons, Dirac spinors, coupled to mesons and to the photons [7, 45, 49]. The nucleons interact by the exchange of several mesons, namely a scalar meson $\sigma$ and three vector particles, $\omega$, $\rho$ and the photon. The CRMF theory [10, 50, 51] represents the realization of covariant density functional theory for rotating nuclei with no pairing correlations [7].
It is formulated in the rotating frame in one-dimensional cranking approximation. It has successfully been tested in a systematic way on the properties of different types of rotational bands in the regime of weak pairing such as normal-deformed [52], superdeformed [51, 53], as well as smooth terminating bands [7] and the bands at the extremes of angular momentum [54].

The formalism and the applications of the CRMF theory to the description of rotating nuclei have recently been reviewed in Ref. [55] (see also Refs. [7, 56]). A clear advantage of the CRMF framework for the description of rotating nuclei is the treatment of time-odd mean fields which are uniquely defined via the Lorentz covariance [11]; note that these fields substantially affect the properties of rotating nuclei [13, 14].

In the one-dimension cranking approximation, with rotation around the $x$-axis, the stationary Dirac equation for the nucleons is given as (See Ref. [11, 14] for more details)

$$\hat{h}_D \psi_i = \hat{J}_x \psi_i = \epsilon_i \psi_i$$  \hspace{1cm} (2.9)

here $\hat{h}_D$ represents the Dirac Hamiltonian and is given by

$$\hat{h}_D = \alpha (-i \nabla - V(r)) + V_0(r) + \beta (m + S(r))$$  \hspace{1cm} (2.10)

and the Coriolis term is

$$-\Omega_x \hat{J}_x = -\Omega_x (\hat{L}_x + \frac{1}{2} \hat{\Sigma}_x)$$  \hspace{1cm} (2.11)

The rotational frequency $\Omega_x$ along the $x$-axis is defined from the condition that the expectation value of the total angular momentum at spin $I$ has a definite value [11, 14]

$$J(\Omega_x) = \langle \Phi_\Omega | \hat{J}_x | \Phi_\Omega \rangle = \frac{I(I+1)}{2}.$$  \hspace{1cm} (2.12)
The Dirac Hamiltonian contains the attractive scalar field

\[ S(r) = g_\sigma \sigma(r), \]  

(2.13)
determined by the mesons, and the repulsive time-like vector field \( V_0(r) \) given by

\[ V_0(r) = g_\omega \omega_0(r) + g_\rho \tau_3 \rho_0(r) + e \frac{1 - \tau_3}{2} A_0(r). \]  

(2.14)
The magnetic potential

\[ V(r) = g_\omega \omega(r) + g_\rho \tau_3 \rho(r) + e \frac{1 - \tau_3}{2} A(r), \]  

(2.15)
originates from the space-like components of the vector mesons.

Note that here we have assumed \( \hbar = 1 \). The last term in the last equation breaks time-reversal symmetry and induces currents in odd-mass nuclei [11]. In the Dirac equation, the space-like components of the vector mesons \( \omega(r) \) and \( \rho(r) \) have the same structure as the space-like component \( A(r) \) generated by the photons. Since \( A(r) \) is the vector potential of the magnetic field, by analogy the effect due to presence of the vector field \( V(r) \) is called nuclear magnetism [10]. It affects the properties of odd-mass nuclei [11]. Thus, the spatial components of the vector mesons are properly taken into account for such nuclei. This is done only for the study of odd-even mass staggerings as it has been successfully done earlier for the studies of single-particle [57, 58] and pairing [56] properties of deformed nuclei. Nuclear magnetism, i.e. currents and time-odd mean fields, plays no role in the studies of even-even nuclei.

In these equations, the four-vector components of the vector fields \( \omega^\mu, \rho^\mu, \) and \( A^\mu \) are separated into the time-like (\( \omega_0, \rho_0 \) and \( A_0 \)) and space-like (\( \omega = (\omega^x, \omega^y, \omega^z), \rho = \)) components.
\((\rho^x, \rho^y, \rho^z)\), and \(\mathbf{A} = (A^x, A^y, A^z)\) components. In the Dirac equation the magnetic potential has the structure of a magnetic field. The meson fields and the electromagnetic potential are given by the Klein-Gordon equations with source terms involving the various nucleonic densities and currents [14].

\[-\Delta - (\Omega_x L_x)^2 + m^2_{\sigma} \{ \sigma(\mathbf{r}) = -g_{\sigma}[\rho^\sigma_n(\mathbf{r}) + \rho^\sigma_p(\mathbf{r})] - g_2\sigma^2(\mathbf{r}) - g_3\sigma^3(\mathbf{r}), \quad (2.16)\]

\[-\Delta - (\Omega_x L_x)^2 + m^2_{\omega} \{ \omega_0(\mathbf{r}) = g_{\omega}[\rho^\omega_n(\mathbf{r}) + \rho^\omega_p(\mathbf{r})], \quad (2.17)\]

\[-\Delta - (\Omega_x J_x)^2 + m^2_{\omega} \{ \omega(\mathbf{r}) = g_{\omega}[j^\omega_n(\mathbf{r}) + j^\omega_p(\mathbf{r})], \quad (2.18)\]

\[-\Delta - (\Omega_x J_x)^2 + m^2_{\rho} \{ \rho_0(\mathbf{r}) = g_{\rho}[\rho^\rho_n(\mathbf{r}) - \rho^\rho_p(\mathbf{r})], \quad (2.19)\]

\[-\Delta - (\Omega_x J_x)^2 + m^2_{\rho} \{ \rho(\mathbf{r}) = g_{\rho}[j^\rho_n(\mathbf{r}) - j^\rho_p(\mathbf{r})], \quad (2.20)\]

\[-\Delta A_0(\mathbf{r}) = e\rho^\rho_p(\mathbf{r}), \quad -\Delta A(\mathbf{r}) = ej^\rho_p(\mathbf{r}) \quad (2.21)\]

The spatial components of the vector potential \(\mathbf{A}(\mathbf{r})\) are neglected because the coupling constant of the electromagnetic interaction is small compared to that of mesonic fields. One needs to replace \(\Omega_x\) by zero in case of no rotation.

In the description of rotating nuclei the Coriolis operator is always present in the cranking model framework. The description of experimental moments of inertia is improved by the inclusion of the currents \(j^{n,p}(r)\) into the Klein-Gordon equations. The spatial components of the vector \(\omega\) and \(\rho\) mesons lead to the interactions between possible currents. For \(\omega\)-meson this interaction is attractive for \(pp\), \(nn\) and \(pn\) combinations of currents, where as for \(\rho\)-meson it is attractive only for \(pp\) and \(nn\) currents and repulsive for \(pn\) currents. In the Klein-Gordon equations, the currents are isoscalar and isovector in nature for \(\omega\) and
$\rho$ mesons respectively. As a consequence of that, in most of the cases, even at the neutron driplines the contribution of the $\rho$-meson to magnetic potential and the total energy is marginal. Therefore, the time-odd mean fields in the CDFT framework depend on the spatial components of the $\omega$ meson. Neglecting the $\rho$-meson effects, clearly, the properties of the time-odd mean fields are governed by the mass $m_\omega$ and the coupling constant $g_\omega$.

The stationary solution of the CDFT equations correspond to the ground state of the nucleus. For any point in deformation space, in order to get a solution, we need to impose constraints on the mass moments. The method of quadratic constraints uses a variation of the function

$$E_{RHB} + \frac{C_{20}}{2} (\hat{Q}_{20} - q_{20})^2$$

where $E_{RHB}$ is the total energy and $\hat{Q}_{20}$ denotes the expectation value of the mass quadrupole operator,

$$\hat{Q}_{20} = 2z^2 - x^2 - y^2$$

$q_{20}$ is the constrained value of the multipole moment, and $C_{20}$ the corresponding stiffness constant [59]. In order to provide the convergence to the exact value of the desired multipole moment we use the method suggested in Ref. [60]. Here the quantity $q_{20}$ is replaced by the parameter $q_{20}^{eff}$, which is automatically modified during the iteration in such a way that we obtain $\hat{Q}_{20} = q_{20}$ for the converged solution. This method works well in our constrained calculations.

In this dissertation, the CRMF equations are solved to study the rotating $N = Z$ nuclei of the $A \sim 40$ mass region. The pairing correlations are neglected in these calculations. There are several reasons behind that. First, the pairing correlations are quenched by ro-
tation (the Coriolis antipairing effect). Second, the calculations for blocked-configurations within a cranked relativistic Hartree-Bogoliubov (CRHB) framework are frequently numerically unstable. The details of these have been discussed in the Chapter 4 of this dissertation.

2.4 Solution of the RHB Equations

For all open shell nuclei the pairing correlations play an important role. On the mean field level they are taken into account by Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogoliubov (HFB) theory, and in the relativistic case by Relativistic Hartree-Bogoliubov (RHB) theory \[61, 62, 63\]. The nuclear energy density functionals depend on two densities; the normal density

\[ \rho_{n_1n_2} = \Phi | c_{n_2}^\dagger c_{n_1} | \Phi, \] \hspace{1cm} (2.24)

and the anomalous density

\[ \kappa_{n_1n_2} = \Phi | c_{n_2} c_{n_1} | \Phi. \] \hspace{1cm} (2.25)

usually called the pairing tensor. \( | \Phi \) is the RHB wave function, a generalized Slater determinant \[59\] and, therefore, the density \( \rho \) as well as \( \kappa \) depend on the pairing correlations. In particular, the density matrix \( \rho \) is no longer a projector on the subspace of occupied states:

\[ \rho^2 - \rho = \kappa \kappa^*. \] \hspace{1cm} (2.26)

In the relativistic form the nuclear energy functional is usually given by

\[ E_{RHB}[\rho, \kappa] = E_{RMF}[\rho] + E_{pair}[\kappa], \] \hspace{1cm} (2.27)
where $E_{RMF}[\rho]$ has the same functional form as the CEDF’s discussed in the last section, but it is now a functional of the density $\rho$ in Eq. (2.24) depending on the RHB wave function $|\Phi\rangle$. The pairing energy\(^1\) is given by

$$E_{pair}[\kappa] = \frac{1}{4} \sum_{n_1n_2n_1'n_2'} \kappa_{n_1n_2}^* \kappa_{n_1'n_2'} \langle \Phi \rangle \overline{\langle \rho \rangle} |V_{pp}^n|_{n_1n_2} \kappa_{n_1'n_2'}$$

(2.28)

The Dirac equation for fermion fields $\psi(r)$ is now replaced by the RHB equation. It has the proper coupling to the continuum at the neutron drip line and, therefore, it allows a correct description of weakly bound nuclei close to the neutron drip line. Even nuclear halo phenomena can be described by this method, if a proper basis is used, such as the coordinate space \cite{64, 65} or a Woods-Saxon basis \cite{66}.

The RHB equations for the fermions are given by \cite{63}

$$\begin{pmatrix}
\hat{h}_D - \lambda & \hat{\Delta} \\
-\hat{\Delta}^* & -\hat{h}_D^* + \lambda
\end{pmatrix}
\begin{pmatrix}
U(r) \\
V(r)
\end{pmatrix}
= E_k
\begin{pmatrix}
U(r) \\
V(r)
\end{pmatrix}
,$$

(2.29)

Here, $\hat{h}_D$ is the Dirac Hamiltonian for the nucleons with mass $m$, $\lambda$ is the chemical potential defined by the constraints on the average particle number for protons and neutrons, $U_k(r)$ and $V_k(r)$ are quasiparticle Dirac spinors \cite{61, 62, 63}, and $E_k$ denotes the quasiparticle energies.

### 2.5 Pairing correlations

The pair field $\hat{\Delta}$ in RHB theory is given by

$$\hat{\Delta} \equiv \Delta_{n_1n_2} = \frac{1}{2} \sum_{n_1'n_2'} \langle \Phi \rangle \overline{\langle \rho \rangle} |V_{pp}^n|_{n_1n_2} \kappa_{n_1'n_2'}$$

(2.30)

\(^1\)The details for the treatment of pairing are presented in the next section.
It contains the pairing tensor $\kappa$ of Eq.(2.25)

$$\kappa = V^* U^T$$

(2.31)

and the effective interaction $V_{pp}$ in the particle-particle channel. In the literature on nuclear density functional theory several types of effective pairing forces $V_{pp}$ have been used. The most simple force is the seniority force of Kerman [67] with constant pairing matrix elements $G$. For problems with time-reversal symmetry the corresponding pairing matrix $\Delta$ in Eq. (2.30) is proportional to unity for this force and RHB theory is equivalent to RMF + BCS. This force is widely used, but has many limitations, e.g. correlations in pairs with higher angular momentum are neglected, the scattering between pairs with different shells is not constant in realistic forces, the coupling to the continuum is not properly taken into account and the predictive power is limited. Nonetheless this method is used in the constant gap approximation in most of the large scale adjustments of CEDF’s, in particular, also for DD-ME2 [19] and DD-PC1 [20].

In the present dissertation the separable pairing interaction, introduced by Tian et al. [68] has been used. This is finite range and, therefore, provides an automatic cutoff of the high-momentum component. Its matrix elements in $r$-space have the form

$$V(r_1, r_2, r_1', r_2') = -f G \delta(R - R') P(r) P(r') \frac{1}{2} (1 - P^*)$$

(2.32)

with $R = (r_1 + r_2)/2$ and $r = r_1 - r_2$ being the center of mass and relative coordinates. The form factor $P(r)$ is of Gaussian shape

$$P(r) = \frac{1}{(4\pi a^2)^{3/2}} e^{-r^2/4a^2}$$

(2.33)
The parameters of this interaction have been derived by a mapping of the $^1S_0$ pairing gap of infinite nuclear matter to that of the Gogny force D1S. The resulting parameters are: \( G = 738 \text{ fm}^3 \) and \( a = 0.636 \text{ fm} \) [68].

As discussed in Ref. [56], in many applications of RHB theory with the pairing force D1S the same scaling factor \( f \) has been used across the nuclear chart. However, it was found a decade ago that a proper description of rotational properties in actinides [57] requires weaker pairing as compared with the rare-earth region [63, 69]. Subsequent systematic studies of pairing (via the three-point indicator \( \Delta^{(3)} \)) and rotational properties of actinides confirmed this observation in Refs. [56, 70]. The investigation of odd-even mass staggering in spherical nuclei in Ref. [71] also confirms the need for a scaling factor \( f \) which depends on the region in the nuclear chart. The studies of Refs. [56, 57, 71] show also a weak dependence of the scaling factor \( f \) on the CEDF. We therefore introduce in Eq. (2.32) a scaling factor \( f \) for a fine tuning of the effective pairing force.

The scaling factor \( f \) used in the present dissertation has been selected based on the results of a comparison between experimental moments of inertia and those obtained in cranked RHB calculations with the CEDF NL3*. As verified in the actinides in Ref. [56], the strengths of pairing defined by means of the moments of inertia and by the three-point indicators \( \Delta^{(3)} \) strongly correlate in deformed nuclei. Following the results obtained in Ref. [56], the scaling factor has been fixed at \( f = 1.0 \) in the \( Z \geq 88 \) actinides and superheavy nuclei. The analysis of the moments of inertia in the rare-earth region [?] leads to a scaling factor of \( f = 1.075 \) for the \( 56 \leq Z \leq 76 \) rare-earth nuclei. For \( Z \leq 44 \) nuclei, the scaling factor was fixed at \( f = 1.12 \) [?]. The scaling factor gradually changes with \( Z \) in between of
these regions. Since the strength parameter $G$ of the separable force has been determined in Ref. [68] by a direct mapping to the Gogny force D1S, the same scaling factors are also used in the following RHB calculations with separable pairing.
CHAPTER 3

GLOBAL PERFORMANCE OF COVARIANT ENERGY DENSITY FUNCTIONALS:
GROUND STATE OBSERVABLES OF EVEN-EVEN NUCLEI AND THE ESTIMATE
OF THEORETICAL UNCERTAINTIES.

3.1 Introduction

One might wonder how many atomic nuclei can be found in the universe. This has
always been a very basic and an open question related to the eternal quest of mankind to
understand the birth and origin of the universe. Each of the atomic nuclei in the universe
must occupy a point in the graphical representation called the nuclear landscape shown in
Fig.1 in Ref. [72]. This is a triangular enclosure bounded by the two boundaries called the
neutron and proton drip lines, respectively. The drip lines represent the limits of particle
stability. So the location of both drip lines measures the exact area of the nuclear landscape
and eventually answers the question perfectly.

The proton drip line has been delineated experimentally up to $Z = 91$. However, the
position of neutron drip line beyond $Z = 8$ is given by model calculations. Because of ex-
perimental limitations, the predictions of the neutron drip line are dependent on theoretical
calculations. However, different models involve different assumptions and parametriza-
tions. They show a large variation in the predictions of the location of neutron drip line.
The comparison of the uncertainties in the definition of two-proton and two-neutron drip lines obtained in CDFT and SDFT.

In such a situation it is important to estimate the theoretical uncertainties introduced by different models.

We have undertaken a systematic study of the location of two-proton and two-neutron drip lines (because our calculation is restricted to even-even nuclei) in the relativistic Hartree-Bogoliubov (RHB) framework with 4 different state-of-the-art covariant energy density functionals (CEDF)s. We also estimated theoretical uncertainties in the predictions of drip lines. We compared our results with those obtained in the framework of Skyrme density functional theory (SDFT) [28] and with existing experimental data [73].

In the context of low-energy nuclear structure physics it is very important to understand how well the state-of-the-art CEDF’s describe available experimental data and also how well they extrapolate to the region of unknown nuclei. This is also very important for nuclear astrophysics. To understand the astrophysical r-process etc., we have to un-
nderstand nuclei with large isospin. Most of these neutron-rich nuclei cannot be studied experimentally even with the next generation facilities.

New generation covariant energy density functionals such as NL3* [24], DD-ME2 [19], DD-MEδ [21] and DD-PC1 [20] have not been tested with respect to experimental data in a global scale before this study. So it was not known how well they describe the ground state observables on a global scale, and what are their strong and weak points in that context.

It was suggested in Refs. [26, 28, 74] to define the uncertainties in the EDF parameters. These uncertainties come from the selection of the form of EDF as well as from the fitting protocol details, such as the selection of the nuclei under investigation, the physical observables, or the corresponding weights. Some of them are called statistical errors and can be calculated from a statistical analysis during the fit, others are systematic errors, such as the form of the EDF under investigation. It is very difficult to perform the analysis of statistical errors on a global scale since the properties of transitional and deformed nuclei have to be calculated repeatedly for different variations of original CEDF. Thus, such statistical analysis has been performed mostly for spherical nuclei [26, 27] or selected isotopic chains of deformed nuclei [28].

Although such an analysis has its own merits, at present, it does not allow to fully estimate theoretical uncertainties in the description of physical observables. This is because they originate not only from the uncertainties in model parameters, but also from the definition and the limitations of the model itself, in particular, from an insufficient form of the nuclear energy density functional. The later uncertainties are very difficult to estimate. As a consequence, any analysis of theoretical uncertainties (especially, for extrapolations
to neutron-rich nuclei) contains a degree of arbitrariness related to the choice of the model and fitting protocol.

Thus, in the given situation in our study we concentrate mostly on the uncertainties related to the present choice of energy density functionals which can be relatively easily deduced globally. We therefore define theoretical uncertainties for a given physical observable via the spread of theoretical predictions within the four sets of CEDF’s:

\[
\Delta O(Z, N) = |O_{\text{max}}(Z, N) - O_{\text{min}}(Z, N)|
\]  

(3.1)

where \(O_{\text{max}}(Z, N)\) and \(O_{\text{min}}(Z, N)\) are the largest and smallest values of the physical observable \(O(Z, N)\) obtained with the four employed CEDF’s for the \((Z, N)\) nucleus. Three different classes of the CEDF’s are used for this purpose (see Sec. II in the Ref. [3]). Note that these theoretical uncertainties are only spreads of physical observables due to a very small number of functionals and, thus, they are only a crude approximation to the systematic theoretical errors discussed in Ref. [74]. As in the case of present Skyrme functionals, the different covariant functionals do not form an independent statistical ensemble. Their number is very small and they are all based on a very similar form. For example, no tensor terms are present in the relativistic case and simple power laws are used for the density dependence in the Skyrme DFT. The parameters of these functionals are fitted according to similar protocols including similar types of physical observables such as binding energies, radii etc.
3.2 The details of numerical calculation

The calculations have been carried out in the RHB framework. The details of the calculational scheme are as follows:

- Three classes of covariant density functional models are used throughout this study. These are the nonlinear meson-nucleon coupling model (NL), the density-dependent meson-exchange model (DD-ME) and the density-dependent point-coupling model (DD-PC). The main differences between them lay in the treatment of the range of the interaction and in the density dependence and in their fitting protocol. They are represented by four CEDFs NL3* [24], DD-ME2 [19], DD-MEδ [21] and DD-PC1 [20]. The details have already been discussed in the preceding chapter.

- The RHB equations are solved in a parity conserving cartesian oscillator basis [63, 75]. For each nucleus the potential energy curve is calculated in a large deformation range from $\beta_2 = -0.4$ up to $\beta_2 = 1.0$ by means of a constraint on the quadrupole moment $q_{20}$. The lowest energy minimum is defined from the potential energy curve. Then, unconstrained calculations are performed in this minimum and the correct ground state configuration and its energy are determined. This procedure is especially important for the cases of shape coexistence.

- The truncation of the basis is performed in such a way that all states belonging to the major shells up to $N_F = 20$ fermionic shells for the Dirac spinors and up to $N_B = 20$ bosonic shells for the meson fields are taken into account. In constrained calculations, the deformation of the basis is selected in such a way that it corresponds to the
desired deformation of the converged solution. The Coulomb field is determined by integrating over the Greens function [76]. The comparison with the results obtained with $N_F = 26$ and $N_B = 26$ clearly shows that this truncation scheme provides sufficient numerical accuracy for the description of weakly bound nuclei in the vicinity of the neutron drip line and of superheavy nuclei. This is even more true for the nuclei in the vicinity of the $\beta$-stability line and for the nuclei with masses $A \leq 260$ away from the neutron drip line.

- It has been found in axial reflection-symmetric calculations for superheavy nuclei with $Z \geq 106$ that the superdeformed minimum is frequently lower in energy than the normal deformed minimum [77, 78]. As long as triaxial [78] and octupole [77, 78] deformations are not included, this minimum is stabilized by the presence of an outer fission barrier. When including such deformations, however, it often turns out that this minimum becomes a saddle point, unstable against fission [77, 78]. Since these deformations are not included in the present calculations, we restrict our consideration to nuclei with $Z \leq 104$. The investigation of ground state properties of superheavy $Z \geq 106$ nuclei is inevitably connected with the studies of fission barriers; such investigations are currently in progress and their results will be reported in a forthcoming manuscript [3]. Of course, in the nuclear chart there exist also a small number of nuclei with stable octupole or triaxial deformations not considered here which we have to leave for future investigations.
The separable version of the finite range Brink-Booker part of the Gogny D1S force is used in the particle-particle channel. The strength variation across the nuclear chart is defined by means of the fit of rotational moments of inertia calculated in the RHB framework to experimental data. This has been discussed in more details in the Ref. [3].

The goals of the present study are as follows: (i) the systematic study of ground state observables for even-even nuclei within the relativistic Hartree-Bogoliubov (RHB) framework [61, 79] using several state-of-the-art CDFT parametrizations. My contribution toward the project was to calculate in DD-ME2, so most of the results in this chapter of the thesis are discussed with respect to DD-ME2.(ii) the estimated differences in the description of various observables on a global scale and especially in the regions of unknown nuclei and (iii) the comparison of the drip lines obtained in relativistic and non-relativistic DFT and thus the estimate of global theoretical errors.

3.3 Binding energies

In Table 3.1 are listed the rms-deviations $\Delta E_{\text{rms}}$ between theoretical and experimental binding energies for the global RHB calculations with the different CEDF’s. The masses given in the AME2012 mass evaluation [73] can be separated into two groups; one represents nuclei with masses defined only from experimental data, the other contains nuclei with masses depending in addition on either interpolation or extrapolation procedures. For simplicity, we call the masses of the nuclei in the first and second groups as measured and estimated. There are 640 measured and 195 estimated masses of even-even nuclei in the
Table 3.1

The rms-deviations $\Delta E_{\text{rms}}, \Delta (S_{2n})_{\text{rms}} \left( \Delta (S_{2p})_{\text{rms}} \right)$ between calculated and experimental binding energies $E$ and two-neutron(-proton) separation energies $S_{2n} \left( S_{2p} \right)$. They are given in MeV for the indicated CDFTs with respect to “measured” and “measured+estimated” sets of experimental masses.

<table>
<thead>
<tr>
<th>EDF</th>
<th>measured</th>
<th>measured+estimated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta E_{\text{rms}}$</td>
<td>$\Delta E_{\text{rms}}$</td>
</tr>
<tr>
<td>NL3*</td>
<td>2.96</td>
<td>3.00</td>
</tr>
<tr>
<td>DD-ME2</td>
<td>2.39</td>
<td>2.45</td>
</tr>
<tr>
<td>DD-MEδ</td>
<td>2.29</td>
<td>2.40</td>
</tr>
<tr>
<td>DD-PC1</td>
<td>2.01</td>
<td>2.15</td>
</tr>
</tbody>
</table>

AME2012 mass evaluation. One can see that to include the estimated masses leads only to a slight decrease in the accuracy in the description of experimental data.

To our knowledge, for relativistic density functionals, reliable\(^1\) global comparisons of experimental and theoretical masses have been performed so far only for the parametrizations NL3 [46], FSUGold [85], BSR4 [86] and TM1 [87] in the RMF+BCS approach using the constant gap approximation in Ref. [84] and for PC-PK1 [88] in the RMF+BCS approach with density-dependent pairing in Ref. [89]. Apart of BSR4 and PC-PK1 these CEDF’s were fitted more than ten years ago. The rms-errors for the masses found for these CEDF’s are 3.8 MeV for NL3, 6.5 MeV for FSUGold, 2.6 MeV for BSR4, 5.9 MeV for TM1 and 2.6 MeV for PC-PK1 (at the mean field level).

---

\(^1\)The masses were globally studied earlier in the RMF [80] or RMF+BCS [81, 82] formalisms. However, the pairing correlations have been completely ignored in the studies of Ref. [80]. The treatment of pairing via the BCS approximation in Refs. [81, 82] has to be taken with care in the region of the drip line since this approximation does not take into account the continuum properly and leads to the formation of a neutron gas [83] in nuclei near neutron drip line. In addition, these calculations use at most 14 fermionic shells for the harmonic oscillator basis, which according to our study and the one of Ref. [84] is not sufficient for a correct description of binding energies of actinides and superheavy nuclei and the nuclei in the vicinity of the neutron drip line.
One can see that the CEDF’s NL3*, DD-ME2, DD-MEδ, and DD-PC1 investigated in Ref. [3] provide an improved description of masses across the nuclear chart. The rms-deviations for the binding energies presented in Table ?? are more statistically significant than those of Refs. [84] and [89] since they are defined for 835 even-even nuclei. On the contrary, rms-deviations for binding energies for the NL3, FSUGold, BSR4 and TM1 CEDF’s are defined only for 513 (575 for PC-PK1) even-even nuclei in Refs. [84] and [89]. The extension of the experimental database to 835 nuclei may lead to further deterioration in the rms-deviations for these CEDF’s.

In Fig. 3.2, the errors in binding energies are summarized for all experimentally known even-even nuclei. If $E_{th} - E_{exp} < 0$, the nucleus is more bound in the calculations than in experiment. Here it is shown only for DD-ME2. Similar figures for other functionals can be found in Ref. [3]. This figure is prepared in the same style as Fig. 3 of Ref. [84]. This allows to comparison of the gross trends for the binding energy errors of the current and previous generations of the CEDF’s. In particular, old CEDF’s show in all cases a growing deviation from the zero line with increasing mass number (Fig. 3 in Ref. [84]). These deviations are especially pronounced for FSUGold and TM1, for which they reach 15 MeV for the highest measured masses. The deviations are smaller for the NL3 CEDF for which they reach 10 MeV for the highest measured masses, and quite moderate for the BSR4 parametrization. On the contrary, no such problems exist in the current generation of the CEDF’s. The accuracy of the description of the masses of heavy nuclei is comparable with or even better (as in the case of DD-PC1) than that of medium-mass and light nuclei (Fig. 3.2). The large deviation peaks seen in Fig. 3.2 are located in the vicinity of the
Figure 3.2

The difference between theoretical and experimental masses of 835 even-even nuclei investigated in RHB calculations with DD-ME2.
Figure 3.3

The relative accuracy in the description of experimental masses in DD-ME2. The same set of data as in Fig. 3.2 is used.

Figure 3.4

The binding energy spread as a function of proton and neutron number
doubly magic shell closures. For such nuclei, medium polarization effects associated with surface and pairing vibrations have a substantial effect on the binding energies [90].

Previous estimates of the rms-deviations for binding energies with these CEDF’s have been obtained only with restricted sets of experimental data. For example, the RHB(NL3*) results were compared with experiment only for approximately 180 even-even nuclei in Ref. [24]. However, no rms-deviations for binding energies were presented for this set. An rms-deviation of 2.4 MeV has been obtained in the analysis of 161 nuclei in the RMF+BCS calculations with DD-ME\(\delta\) using monopole pairing [21]. Note, however, that the binding energies of these nuclei were used in the fit of DD-ME\(\delta\). 93 deformed nuclei calculated in the RMF+BCS approach with the DD-PC1 CEDF were compared with experiment in Ref. [20]. The binding energies for the most of these nuclei deviate from experiment by less than 1 MeV, which is not surprising considering that 64 of these nuclei were used in the fit of the corresponding CEDF. However, much larger deviations have been reported for this CEDF in spherical nuclei [20]. Note that, so far, DD-PC1 is the only CEDF exclusively fitted to deformed nuclei. Theoretical binding energies of approximately 200 nuclei calculated in the RHB framework with the DD-ME2 CEDF and the Gogny D1S interaction in the pairing channel show an rms-deviation of less than 0.90 MeV from experiment [19].

Comparing these rms-deviations with the ones presented in Table ?? one can see that the increase in the size of the experimental data set leads to a deterioration in the average description of the binding energies. This clearly suggests that the experimental data sets used in the fits of the CEDF’s are not sufficiently large to provide an optimal localization of the model parameters in the parameter space and reliable extrapolation properties
of the CEDF’s with respect to binding energies. To our knowledge, so far, no attempt to create a “mass table” quality CEDF based on a fit to the full set of available experimental masses has been undertaken in CDFT. This is contrary to non-relativistic models where mass tables based on an extensive use of experimental data were generated in the macroscopic+microscopic model [91], the Skyrme [92] and the Gogny [93] DFT. We have to keep in mind, however, that the number of free parameters in such fits to thousands of experimental masses is considerably larger than that used in the CEDF’s investigated in this study. In particular, many of these fits include more or less phenomenological terms for the Wigner energy [94, 95] in $N \approx Z$ nuclei and for the rotational corrections in deformed nuclei.

One should also recognize the limitations of the description of masses at the mean field level. This is clearly visible in Fig. 3.3 where the relative errors are plotted as a function of mass number $A$. One can see that these errors are especially pronounced in light $A \leq 80$ nuclei for which the configuration mixing effects (which go beyond the mean field) are important [96, 97, 98]. In very light nuclei the clusterization effects can also be important [99] and for the nuclei in the $N = Z$ region the Wigner term [94, 95]. Such effects are not taken into account in these density functionals. For the heavier $A \geq 80$ nuclei, the relative error in the description of masses stays safely within the $\pm 0.5\%$ error band. In this context, it is interesting to mention that a similar level of error ($\sim 0.3\%$) in the description of binding energies is achieved in the DFT local density approximation in condensed matter physics [100].
Fig. 3.4 shows a color coded display of theoretical uncertainties $\Delta E(Z, N)$ in the description of binding energies where

$$\Delta E(Z, N) = |E_{\text{max}}(Z, N) - E_{\text{min}}(Z, N)|$$ (3.2)

Here $E_{\text{max}}(Z, N)$ and $E_{\text{min}}(Z, N)$ are the largest and the smallest binding energies for each $(N, Z)$-nucleus obtained with the four CEDF’s used in this study.

The comparison of Fig. 3.4 with Fig. 1 in Ref. [72] (which presents experimentally known nuclei in the nuclear chart), shows that the theoretical spread in the predictions of binding energies stays within 5-6 MeV for the known nuclei. This spread is even smaller (typically around 3 MeV) for the nuclei in the valley of beta-stability. However, the theoretical uncertainties for the masses increase drastically when approaching the neutron-drip line and in some nuclei they reach 15 MeV. This is a consequence of poorly defined isovector properties of many CEDF’s.

### 3.4 Two-proton dripline

Fig. 3.5 shows the calculated two-proton drip lines versus experimental data for the functional DD-ME2. Similar figures for other CEDFs can be found in Ref. [72]. For each isotope chain, the four experimentally known most proton-rich nuclei are shown by squares. Cyan shading of the squares is used for the nuclei located beyond the two-proton drip line ($S_{2p} < 0$). The experimental data are taken from Ref. [73]. The borderline between shaded and open squares delineates the known two-proton drip lines. Only in the case of the $Z = 4, 6, 8, 80, 82,$ and $84$ isotope chains, the location of two-proton drip
Figure 3.5

The calculated two-proton drip line versus experimental data for DD-ME2
line is firmly established since the masses of the nuclei on both sides of the drip line are
directly and accurately measured. The two-proton drip line is only tentatively delineated
for other isotope chains since either the masses of beyond the drip line nuclei are only
estimated in Ref. [73] or beyond the drip line nuclei are not known experimentally. The
red lines with small symbols show the calculated two-proton drip lines which go along the
last two-proton bound nuclei.

The proton drip line had been studied extensively more than a decade ago in the RHB
framework with the finite range Gogny pairing force D1S in Refs. [101, 102, 103, 104, 105,
106, 107]. However, the main emphasis was put on the one-proton drip line, for which,
at the time of these studies, experimental data was more available than that for the two-
proton drip line. In addition, only the NL3 parametrization [46] was used in these studies.
Therefore, no estimate of theoretical errors in the prediction of one- and two-proton drip
lines are available.

The experimental two-proton drip line is delineated firmly or tentatively up to $Z = 84$.
In the following discussion we concentrate on isotope chains containing proton unstable
nuclei since this provides the most reliable experimental information on the position of
two-proton drip line. One can see in Fig. 13 of Ref. [3] that NL3* tends to predict the
two-proton drip line at too low values of the neutron number $N$. Indeed, experimentally
known proton unstable nuclei at $Z = 8, 14, 16, 18, 20, 32, 34, 68, 76, 78, 80$, and 82
are predicted to be proton bound by NL3*. On the other side, the two-proton drip line is
predicted too early for the $Z = 52$ chain. Similar problems with the description of the
proton unstable $Z = 4, 8, 20, 32, 34, 76, 80$, and 82 nuclei exist for DD-ME2. Note also
that the two-proton drip line is predicted too early in the $Z = 26$ and 52 isotope chains in this CDFT parametrization.

The best reproduction of the two-proton drip line is achieved with DD-ME2 and DD-MEδ, which are characterized by the best residuals for two-proton separation energies $S_{2p}$ (Table ??). In general, the results of the calculations are very close to experimental data. This is because the proton-drip line lies close to the valley of stability, so that extrapolation errors towards it are small. Another reason is the fact the Coulomb barrier provides a rather steep potential reducing considerably the coupling to the proton continuum. This leads to a relatively low density of the single-particle states in the vicinity of the Fermi level.

According to Fig. 2 of Ref. [72], theoretical uncertainties in the predictions of the position of two-proton drip line are either very small (2 neutrons) or non-existent for isotope chains with $Z \leq 86$. These small uncertainties may be a source of observed discrepancies between calculations and experiment for a number of isotope chains (for example, the ones with $Z = 4, 14, 16, 18, 20, 26, 68, 76, 78$, and 80 in Fig. 2 of Ref. [72]). However, in a number of the cases (for example, in the $Z = 32$ and 34 isotopes chains) there is no uncertainty in the predicted position of the two-proton drip line (Fig. 2 in Ref. [72]). Thus, the observed discrepancies between theory and experiment may be due to the limitations of the model description at the mean field level. Indeed, it is well known that the Ge ($Z = 32$) [108] and Se ($Z = 34$) [97, 109] isotopes show prolate-oblate shape coexistence and/or $\gamma$-softness near the proton-drip line. A similar shape coexistence is also observed in heavier Kr [52, 96, 98, 110] and Rb [111] nuclei as well as in the $Z \sim 82$ proton-drip line nuclei [112, 113]. By ignoring the correlations beyond mean field, which are expected to
be most pronounced in light nuclei, we may introduce an error in the predicted position of two-proton drip line.

3.5 Two-neutron dripline

The landscape of bound even-even nuclei as obtained in the CDFT calculations.

Fig. 3.6 shows the nuclear landscape as obtained in the CDFT calculations. It is evident from Fig. 3.6 that the situation is different for the two-neutron dripline. Fig. 3.7 presents the compilation of known calculated two-neutron drip lines obtained with the state-of-the-art relativistic and non-relativistic EDF’s. They include four two-neutron drip lines obtained in the CDFT calculations of Ref. [72]. The predictions of the two-proton and two-neutron driplines for DD-ME2 are tabulated Table 3.2. The same for all other functionals can be found in the Ref. [3]. Non-relativistic results are represented by two-neutron drip lines obtained with the Gogny functional D1S [114] and with eight functionals of Skyrme
Figure 3.7

Two-neutron drip-lines obtained in state-of-the-art DFT calculations. The regions of well-defined localization of the two-neutron drip line are encircled.
type [28, 115]. In addition, the two-neutron drip line from the microscopic+macroscopic calculations of Ref. [91] is shown. One can see that with the exception of two encircled regions, the theoretical differences in the location of two-neutron drip line are much larger than the ones for the two-proton drip line. They are generally growing with increasing $Z$.

In most of the cases, the theoretical uncertainties in the location of the two-neutron driplines are much larger compared to that in the case of two-proton driplines and they are generally increasing with the increase in mass number. This is commonly attributed to poorly known isovector properties of the EDF [28]. Although this factor contributes, such an explanation is somewhat oversimplified from our point of view. That is because for some combinations of $Z$ and $N$ there is basically no (or very little) dependence of the predictions for the location of the two-neutron drip line on the CDFT parametrization. Such a weak (or vanishing) dependence is especially pronounced at spherical neutron shell closures with $N = 126, 184$ and $258$ around proton numbers $Z = 54, 80$ and $110$. It is interesting that the impact of shell structure at these particle numbers on the shape of the two-neutron drip line is more pronounced than that for the two-proton drip line due to $Z = 50$ and $82$ proton shell gaps.

However, moving away from these spherical shell closures the spread of theoretical predictions for the two-neutron drip line increases. This move also induces the deformation in the nuclei. Thus, there is a close correlation between the nuclear deformation at the neutron-drip line and the uncertainties in the prediction of the neutron-drip line; the regions of large uncertainties corresponds to transitional and deformed nuclei. This is caused by the underlying densities of the single-particle states. The spherical nuclei under discussion
are characterized by large shell gaps and a clustering of highly degenerate single-particle states around them. Deformation removes this high degeneracy of single-particle states and leads to a more equal distribution of the single-particle states with energy. Moreover, the density of bound neutron single-particle states close to the neutron continuum is substantially larger than that on the proton-drip line. As a consequence, inevitable inaccuracies in the DFT description of the deformed single-particle state energies which are present even in the valley of beta-stability [58] will lead to larger uncertainties in the predictions of the neutron-drip line.

The isovector properties of an EDF define the depth of the nucleonic potential with respect to the continuum and may affect the location of two-neutron drip line. The detailed discussion can be found in the Sec. VIII of the Ref. [3]. However, such uncertainties in the depth of the nucleonic potential exist also in known nuclei (see discussion in Sec. IVC of Ref. [116]). They cannot describe the observed features completely.

The shell structure effects are clearly visible in the fact that for some combinations of $Z$ and $N$ there is basically no (or very little) dependence of the predicted location of the two-neutron drip line on the CDFT parameterization. Such a weak (or vanishing) dependence, seen in all model calculations, is especially pronounced at spherical neutron shell closures with $N = 126$ and $184$ around the proton numbers $Z = 54$ and $80$, respectively. In addition, a similar situation is seen in the CDFT calculations at $N = 258$ and $Z \sim 110$. This fact is easy to understand because of the large neutron shell gap at the magic neutron numbers in all DFT’s.
Inevitable inaccuracies in the DFT description of single particle energies [58, 116] also contribute to increasing uncertainties in the prediction of the two-neutron drip line position when moving away from these spherical shell closures. This move induces deformation. The comparison of Figs. 3.7 and 3.8 shows that there is a close correlation between the nuclear deformation at the neutron-drip line and the uncertainties in their prediction. The regions of large uncertainties corresponds to transitional and deformed nuclei. Again this is caused by the underlying level densities of the single-particle states. The spherical nuclei under discussion are characterized by large shell gaps and a clustering of highly degenerate single-particle states around them. Deformation removes this high degeneracy of single-particle states and leads to a more equal distribution of the single-particle states with energy. This has been studied separately and has been discussed in detail in Ref. [117].

3.6 Nuclear Landscape and the comparison of the results obtained through CDFT and SDFT

Fig. 3.6 shows the nuclear landscape as obtained in the CDFT calculations. Experimentally known stable and radioactive nuclei are shown by black and green squares, respectively. The experimental data are from Ref. [73]. Two-proton and two-neutron drip lines calculated with different CEDF are shown by the lines of different color. The particle stability (and, as a consequence, a drip line) of a nuclide is specified by its separation energy, namely, the amount of energy needed to remove particle(s). Since our investigation is restricted to even-even nuclei, we consider two-neutron and two-proton separation energies.
Table 3.2

Two-proton and two-neutron drip lines predicted by DD-ME2. The neutron numbers $N$ corresponding to these drip lines are given for each even proton number $Z$.

<table>
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<th>Two neutron drip-line</th>
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Table 3.2
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<th>Two neutron drip-line</th>
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Fig. 3.1 presents the comparison between the theoretical CDFT uncertainties in the definition of the two-proton and two-neutron drip lines with the ones obtained in non-relativistic calculations by Skyrme density functional theory (SDFT)[118]. The shaded areas are defined by the extremes of the predictions of the corresponding drip lines obtained with different parametrizations. The blue shaded area shows the area where the CDFT and SDFT results overlap. Non-overlapping regions are shown by dark yellow and plum colors for SDFT and CDFT, respectively. The results of the SDFT calculations are taken from the supplement to Ref. [28]. The two-neutron drip lines obtained by microscopic+macroscopic (FRDM [91]) and Gogny D1S DFT [114] calculations are shown by red and blue lines, respectively. We have used so-called “Benchmark uncertainties” [118] obtained in Ref. [28] for Skyrme DFT employing six parametrizations.

One can see that the CDFT and SDFT uncertainties in the definition of two-proton drip line are small; they tightly overlap at \( Z \leq 70 \) while for higher \( Z \) the CDFT uncertainties are shifted slightly towards neutron deficient nuclei as compared with the SDFT ones. The uncertainties for two-neutron drip line are larger but still they are similar in the two models for many regions. In particular, the two-neutron drip line at \( Z \sim 54, N = 126 \) and \( Z \sim 82, N = 184 \) is well defined not only in the CDFT and SDFT calculations, but also in the mic+mac (FRDLM) and Gogny D1S calculations. This uniqueness is due to a corresponding well pronounced spherical shell closures in the model calculations.

The predictions of the DD-ME2, DD-ME\( \delta \) and DD-PC1 parametrizations are close to each other (Fig. 3.6) and are within the “2012 Benchmark uncertainties”. The NL3* parametrization typically shifts the two-neutron drip line to a higher \( N \)-value exceeding
in some regions “Benchmark uncertainties”. However, the same is true for recently fitted Skyrme TOV-min parametrization [118], the two-neutron drip line of which is very similar to the one obtained in the RHB(NL3*) calculations.

The biggest difference between CDFT and Skyrme DFT calculations appears at $N = 258, Z \sim 110$ (see Fig. 3.1) where the two-neutron drip line is uniquely defined in the CDFT calculations due to a large spherical gap at $N = 258$. This gap is also present in many Skyrme EDF but it does not prevent a significant spread in Skyrme DFT predictions for the two-neutron drip line in this region. This again underlines the importance of shell structure in the predictions of the details of the two-neutron drip line. A similar difference between CDFT and SDFT exists also in superheavy nuclei with $Z \approx 120 - 126, N \approx 172 - 184$ where different centers for islands of stability are predicted by these models [119, 120]. These results are contrary to the fact that both models generally agree for lighter $Z \leq 100$ nuclei.

### 3.7 Deformations

The solution of the variational equations of density functional theory yields values for the single particle density $\rho(r)$. Therefore density functional theory not only allows us to derive the binding energies of the system but in addition all quantities depending on $\rho(r)$. In this section we consider the charge quadrupole and hexadecupole moments:

$$Q_{20} = d^3 r \rho(r) (2z^2 - r_\perp^2),$$  \hspace{1cm} (3.3)

$$Q_{40} = d^3 r \rho(r) (8z^4 - 24z^2 r_\perp^2 + 3r_\perp^4).$$  \hspace{1cm} (3.4)
with \( r_\perp^2 = x^2 + y^2 \). In principle these values can be directly compared with experimental data. However, it is more convenient to transform these quantities into dimensionless deformation parameters \( \beta_2 \) and \( \beta_4 \):

\[
Q_{20} = 2 \frac{4\pi}{5} \frac{3}{4\pi} Z R_0^2 \beta_2, \tag{3.5}
\]

\[
Q_{40} = 8 \frac{4\pi}{9} \frac{3}{4\pi} Z R_0^4 \beta_4, \tag{3.6}
\]

where \( R_0 = 1.2A^{1/3} \). Eq. (3.5) is also used in the extraction of experimental \( \beta_2 \) deformation from measured data [121]. This justifies its application despite the fact that this simple linear expression ignores the contributions of higher power/multipolarity deformations to the charge quadrupole moment. Including higher powers of \( \beta_2 \), as in Ref. [122], yields values of \( \beta_2 \) that are \( \approx 10\% \) lower. In Fig. 3.8 we have shown the distribution of proton quadrupole \( \beta_2 \) for the CEDF DD-ME2. The similar figures for other functionals can be found in the Ref. [3].

![Figure 3.8](image)

Charge quadrupole deformations \( \beta_2 \) obtained in the RHB calculations with DD-ME2
Direct experimental information on the deformations of nuclei can be obtained from Coulomb excitation and lifetime measurements [121]. An alternative method is to derive a quadrupole moment from the $2^+ \rightarrow 0^+$ transition energy by using the Grodzins relation [123] or its later refinements [124]. However, these prescriptions are applicable only to well deformed nuclei. In general, it is estimated that experimental methods give an accuracy of around 10% [124] for the static charge quadrupole deformation $\beta_2$ in the case of well deformed nuclei. The error can be larger in transitional nuclei since in this case the deformation extracted from experimental data will contain also dynamic deformation resulting from zero-point oscillations of the nuclear surface in the ground state [125].

These considerations basically limit the possibilities of a comparison between calculated and experimental $\beta_2$ deformations to the well-deformed nuclei in the rare-earth and actinide regions. Although deformation exists also in the ground states of nuclei in many other regions, the potential energy surfaces of these nuclei are, in general, soft in $\beta_2$ or $\gamma$-deformation, leading to the phenomena of shape fluctuations, shape coexistence [126] and quantum phase transitions [127]. For such situations, the mean field description is not completely adequate, and, thus, a comparison between theoretical and experimental deformation properties is not conclusive.

A systematic comparison between calculated and experimental static charge quadrupole deformations $\beta_2$ has already been performed in each of these regions (with NL3* [56] in the actinides and with DD-ME2 and DD-PC1 [20] in the rare-earth region). They describe the experimental data well, typically within the experimental uncertainties.
The distribution of calculated static quadrupole deformations $\beta_2$ is similar in all four CEDF’s under consideration (see Fig. 3.8). The biggest difference between these results is related to the presence of two regions of oblate deformation at $(Z \sim 70, N \sim 160)$ and $(Z \sim 95, N \sim 230)$ in the calculations with NL3*. These regions are absent in the other CEDF’s. However, this is a consequence of the fact that the two-neutron drip line is located at higher $N$ values in NL3* as compared with other CEDF’s. As a result, these regions are neutron-unbound for DD-ME2, DD-MEδ, and DD-PC1.

The width of the gray region in Fig. 3.8 (the gray color corresponds to spherical and near-spherical shapes) along a specific magic number corresponding to a shell closure indicates the impact of this shell closure on the structure of the neighboring nuclei. Note that proton and neutron shell gaps act simultaneously in the vicinity of doubly magic spherical nuclei. Thus, the effect of a single gap is more quantifiable away from these nuclei. One can see in Fig. 3.8 that the neutron $N = 82, 126$ and $184$ shell gaps have a more pronounced effect on the nuclear deformations as compared with the proton shell gaps at $Z = 50$ and $Z = 82$. This feature is common for all the CEDF’s under investigation.

It is interesting to compare the RHB results with those obtained in non-relativistic models. The comparison of Fig. 3.8 with HFB results based on the Gogny D1S force in Fig. 3a of Ref. [114], with HFB results based on six Skyrme EDF’s in Fig. 2 of the Supplement to Ref. [28], and with the microscopic+macroscopic model in Fig. 9 of Ref. [91] show that the general structure of the distribution of charge quadrupole deformations $\beta_2$ in the nuclear chart is similar in all model calculations. Differences between models emerge mostly at the boundaries between the regions of different types of deformation, i.e.
in the transitional regions, where the energy surfaces are rather flat and static deformations are not well defined. There are boundaries between the regions of prolate and oblate shapes and between the regions of deformed and spherical shapes. This comparison also reveals that, similar to our relativistic results, also in non-relativistic calculations the neutron shell gaps with $N = 82, 126$ and $184$ have a more pronounced effect on the nuclear deformations than the proton shell gaps with $Z = 50$ and $Z = 82$.

![Proton quadrupole deformation spread $\Delta \beta_2$](image)

**Figure 3.9**

Proton quadrupole deformation spread $\Delta \beta_2(Z, N)$ as a function of proton and neutron numbers.

Fig. 3.9 shows proton quadrupole deformation spread $\Delta \beta_2(Z, N)$ as a function of proton and neutron number. $\Delta \beta_2(Z, N) = |\beta_2^{\text{max}}(Z, N) - \beta_2^{\text{min}}(Z, N)|$, where $\beta_2^{\text{max}}(Z, N)$ and $\beta_2^{\text{min}}(Z, N)$ are the largest and smallest proton quadrupole deformations obtained with the four employed CEDF for each $(Z, N)$. One can see that this spread is either non-existent or very small for spherical or nearly spherical nuclei as well as for well-deformed nuclei in
the rare-earth and actinide region. The largest uncertainties for predicting the equilibrium quadrupole deformations exist at the boundaries between regions of different deformations. They are extremely high in the regions of the prolate-oblate shape coexistence, indicating that the ground state in a given nucleus can be prolate (oblate) in one CEDF and oblate (prolate) in another CEDF. These uncertainties are more modest on the boundaries of the regions of spherical and deformed (oblate or prolate) shapes. It is well known that such nuclei are difficult to describe precisely at the mean field level [8, 126, 128]. Correlations going beyond mean field have to be taken into account [96, 97, 112, 129] and shape fluctuations do not allow a precise definition of deformation parameters. However, even if such correlations and fluctuations are taken into account properly by methods based on density functional theory and going beyond the mean field, there remain deficiencies of the current generations of the DFT models with respect of the description of single-particle energies [96]. Indeed, when we compare the profile of the potential energy surface (PES) as a function of the deformation in spherical or well-deformed nuclei with that in transitional nuclei, we find that this profile depends for transitional nuclei much more sensitively on the underlying single-particle structure than in the other two cases. However, it is well known that the single-particle energies (both spherical and deformed) are not very accurately described at the DFT level (see Refs. [58, 116] and references quoted therein). Considering that the PES’s obtained at the mean field level form the starting points of many beyond mean field calculations, further improvement in the description of the single-particle energies is needed in order to describe experimental data in transitional and shape-coexistent
nuclei reliably and consistently across the nuclear chart with a high level of predictive power by the methods going beyond the mean field.

### 3.8 Charge radii and neutron skin thickness.

Table 3.3

The rms-deviations between calculated and experimental charge radii, given in fm for the indicated CEDF’s. For the calculations of the rms-values, all experimental data are used in column 2, while the data on radii of He ($Z = 2$) and Cm ($Z = 96$) isotopes are excluded in column 3.

<table>
<thead>
<tr>
<th>CEDF</th>
<th>$\Delta r_{ch}^{\text{rms}}$ [fm]</th>
<th>$\Delta r_{ch}^{\text{rms}}$ [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NL3*</td>
<td>0.0407</td>
<td>0.0283</td>
</tr>
<tr>
<td>DD-ME2</td>
<td>0.0376</td>
<td>0.0230</td>
</tr>
<tr>
<td>DD-MEδ</td>
<td>0.0412</td>
<td>0.0329</td>
</tr>
<tr>
<td>DD-PC1</td>
<td>0.0402</td>
<td>0.0253</td>
</tr>
</tbody>
</table>

The charge radii were calculated from the corresponding point proton radii as

$$r_{ch} = \sqrt{\langle r^2 \rangle_p} + 0.64 \text{ fm} \quad (3.7)$$

Here we have neglected the small contributions to the charge radius originating from the electric neutron form factor and the electromagnetic spin-orbit coupling [130, 131] as well as the corrections due to the center of mass motion.

Fig. 3.10 presents the spread in the theoretical results on charge radii $\Delta r_{ch}(Z, N)$ which is given as follows:

$$\Delta r_{ch}(Z, N) = |r_{ch}^{\text{max}}(Z, N) - r_{ch}^{\text{min}}(Z, N)| \quad (3.8)$$
Figure 3.10

Charge radii spread $\Delta r_{ch}(Z, N)$ as a function of proton and neutron number.

where $r_{ch}^{\text{max}}(Z, N)$ and $r_{ch}^{\text{min}}(Z, N)$ are the largest and the smallest charge radii obtained with the four CDFTs for each $(Z, N)$ nucleus. The similarity of the results obtained in the calculation for all the CEDFs is clearly seen from Fig. 3.10 and Table 3.3. These comparisons are based on the latest compilation of experimental charge radii in Ref. [132], which includes charge radii for 351 even-even nuclei.

One can see that the calculations provide in general a good description of experimental data. However, there are four exceptions. First, there are very light nuclei He, Be and C (Fig. 23a in Ref. [3]), where the mean field description has obviously limitations. The discrepancy between theory and experiment is especially pronounced in the case of the He nuclei. Then there is a substantial discrepancy between theory and experiment for charge radii of Se, Kr and Sr isotopes at neutron numbers $N = 38 − 46$ (see Fig. 23b in Ref. [3]). The calculated ground state quadrupole deformations of these nuclei are predicted to
be either spherical or near-spherical (see Fig. 3.8). However, the potential energy surfaces are soft. This indicates that a proper description of their structure requires the inclusion of beyond mean field correlations. Next, the ground states of some proton-rich Hg and Pb isotopes are predicted to be oblate (or prolate) in contradiction with experiment. These earlier observed features \[133\] are in part due to incorrect position of the proton $1h_{9/2}$ spherical subshell \[57, 133\] and they are present in all the CEDF’s used here (see Fig. 3.8). When comparing theory with experiment we use for these nuclei the radii from the minimum of the potential energy surface corresponding to the experimental minimum, i.e. the spherical minimum for the $N = 104 – 114$ Pb isotopes and the oblate minimum for the $N = 100 – 108$ Hg isotopes. Finally, the last case is related to the unusual behavior of the charge radii in the U-Pu-Cm isotopes (see Fig. 23d in Ref. \[3\]). For a fixed neutron number, the increase of proton number leads in these isotopes to an increase of the calculated charge radius. However, in experiment the charge radii of the Cm ($Z = 96$) nuclei are lower than those of Pu ($Z = 94$) and U ($Z = 92$). This is the only case in the nuclear chart where such an inversion exists. Considering that both the ground state quadrupole deformations are very stable in this region, i.e. their variations with particle number are much less pronounced than in the rare-earth region, and that covariant density functional theory describes the experimental deformations in the actinides well \[56, 57\], it is impossible to understand this highly unusual behavior of charge radii in the Cm isotopes.
In neutron-rich nuclei the excess of neutrons over protons creates a neutron skin. The neutron skin thickness is commonly defined as the difference of proton and neutron root-mean-square (rms) radii

\[
r_{\text{skin}} = \sqrt{<r_n^2>^{1/2} - <r_p^2>^{1/2}}.
\] (3.9)

The neutron skin thickness is an important indicator of isovector properties. It is closely related with a number of observables in finite nuclei which are sensitive to isovector properties [26, 134, 135] and it affects the physics of neutron stars [26, 136, 137, 138].

The experimental data on the neutron skin thickness in $^{208}$Pb is contradictory. On the one hand, there is a large set of experiments which suggests that the neutron skin is around 0.2 fm or slightly smaller (see Table 1 in Ref. [139]). However, these experimental data are extracted in model dependent ways (see Ref. [140] and references quoted therein). For example, the neutron skin thicknesses $r_{\text{skin}} = 0.161 \pm 0.042$ [139] and $r_{\text{skin}} = 0.190 \pm 0.028$ [141] obtained from the energy of the anti-analogue giant dipole resonance rely on relativistic proton-neutron quasiparticle random-phase approximation calculations based on the RHB model. Another recent value of the neutron skin thickness of $r_{\text{skin}} = 0.15 \pm 0.03\text{(stat)}^{+0.00}_{-0.03}\text{(sys)}$ fm has been extracted from coherent pion photo-production cross sections [142]. However, the extraction of information on the nucleon density distribution depends on the comparison of the measured $(\gamma, \pi^0)$ cross sections with model calculations. On the other hand, a measurement using an electro-weak probe has very recently been carried out in parity violating electron scattering on nuclei (PREX) [143]. This experiment utilizes the preferential coupling of the exchanged weak...
boson to neutrons. The electro-weak probe has the advantage over experiments using hadronic probes in that it allows a nearly model-independent extraction of the neutron radius that is independent of most strong interaction uncertainties [144]. However, a first measurement at a single momentum transfer gave \( r_{\text{skin}} = 0.33 \pm 0.17 \) with a relatively large error bar [143]. A central value of 0.33 fm is particularly intriguing since it is around 0.13 fm higher than central values obtained in other experiments (see Table 1 in Ref. [139]). However, the analysis performed in Ref. [145] has found no compelling reason to rule out the models with large neutron skin in \(^{208}\text{Pb}\).

![Neutron skin thicknesses obtained in RHB calculations with DD-ME2](image)

**Figure 3.11**

Neutron skin thicknesses obtained in RHB calculations with DD-ME2

Fig. 3.11 shows calculated distributions of neutron skin thicknesses in the \((Z, N)\) chart for DD-ME2. Similar figures for other functionals can be found in Ref. [3] Neutron skin thicknesses are very similar for the DD-* CEDF’s. On the other side, the neutron skin thickness is larger for NL3*. In some nuclei it can reach 1.2 fm.
Neutron skin thickness spread as a function of proton and neutron number.

Fig. 3.12 shows the spreads of theoretical predictions $\Delta r_{\text{skin}}(Z, N) = |r_{\text{skin}}^{\text{max}}(Z, N) - r_{\text{skin}}^{\text{min}}(Z, N)|$ as a function of proton and neutron number. Here $r_{\text{skin}}^{\text{max}}(Z, N)$ and $r_{\text{skin}}^{\text{min}}(Z, N)$ are the largest and smallest proton hexadecapol deformations obtained with the four CDFTs for each $(Z, N)$ nucleus. The neutron skin thickness increases with isospin and become rather large in neutron-rich nuclei (reaching 0.25 fm in some cases). They are larger than those found in Skyrme calculations in Ref. [27]. This is a consequence of the use of NL3*, which contrary to DD-* of the present study and the Skyrme EDF’s used in Ref. [27], favors large neutron skins. As illustrated in Fig. 27 in Ref. [3], the spread in the neutron skin thicknesses become substantially smaller if we exclude NL3* from our consideration. This again stresses the importance of future PREX-II and CREX experiments. If PREX-II confirms the large neutron skin in $^{208}$Pb ($r_{\text{skin}} \sim 0.33$ fm) obtained in the first PREX experiment, the result would also require looking for density dependent CEDF’s
and Skyrme EDF’s with larger neutron skins. If this experiment leads to a smaller neutron skin thickness \( r_{\text{skin}} \sim 0.2 \text{ fm} \), then the EDF’s with large neutron skins (such as NL3*) should be excluded from further consideration. In either case, this experiment will lead to a substantial reduction of the uncertainty in the prediction of neutron skins in neutron-rich nuclei.

### 3.9 Pairing properties: a global picture

Fig. 3.13, Fig. 3.14, Fig. 3.15, Fig. 3.16 show the neutron pairing energies \( E_{\text{pairing}} \) obtained with the indicated CEDFs. In the region of known nuclei these energies are, in general, quite comparable. They are very similar in the RHB calculations with the three CEDF’s DD-ME2, DD-ME\( ^\delta \), and DD-PC1 CEDF’s with density dependent coupling constants and slightly higher (in absolute values) in the ones with the CEDF NL3*. This is examplified in Fig. 3.17. However, on approaching the two-neutron drip line, substantial
Figure 3.14

Neutron pairing energies $E_{\text{pairing}}$ obtained in the RHB calculations for DD-ME2.

Figure 3.15

Neutron pairing energies $E_{\text{pairing}}$ obtained in the RHB calculations for DD-MEδ.
Neutron pairing energies $E_{\text{pairing}}$ obtained in the RHB calculations for DD-PC1

Neutron pairing gaps $\Delta_{uv}$ and pairing energies $E_{\text{pairing}}$ of the Yb nuclei located between the two-proton and two-neutron drip-lines obtained in the axial RHB calculations with the indicated CEDF’s. The shaded yellow area indicates experimentally known nuclei. The ‘DD-PC1(scaled)’ curves show the results of the calculations in which the pairing strength is increased by 3.5%. 

69
differences develop between the pairing energies in the RHB calculations with these four CEDF’s. For DD-PC1 and DD-ME\(\delta\) the largest increase of neutron pairing energies is seen near the two-neutron drip line between \(N = 50\) and \(N = 126\), for other nuclei in the vicinity of the two-neutron drip line this increase is more modest. These increases in neutron pairing energy on approaching the two-neutron drip line become more pronounced in DD-ME2 (as compared with DD-PC1 and DD-ME\(\delta\)) and they are especially pronounced in NL3*. For the later CEDF, the absolute values of neutron pairing energies are by factor of 3-4 higher near the two-neutron drip line than those in known nuclei. This difference reduces to a factor 2 for the DD-ME2 CEDF and becomes even smaller for the DD-ME\(\delta\) and DD-PC1 CEDF’s. In this context we have to keep in mind, that the CEDF NL3* has no density dependence in the isovector channel. Therefore, as discussed in detail in Ref. [3] the symmetry energy and the slope of the symmetry energy at saturation is considerably larger in this case than in the other three cases.

Fig. 3.17 compares the evolution of the neutron pairing gaps \(\Delta_{uv}\) and pairing energies \(E_{\text{pairing}}\) as a function of the neutron number in the chain of the Yb isotopes with \(Z = 70\) for four different CEDFs. The pairing gaps and the pairing energies are given by:

\[
\Delta_{uv} = \frac{\sum_k u_k v_k \Delta_k}{\sum_k u_k v_k} \tag{3.10}
\]

\[
E_{\text{pairing}} = -\frac{1}{2} \text{Tr}(\Delta \kappa) = - \Delta_k u_k v_k \delta_{k>0} \tag{3.11}
\]
One can see that in the RHB calculations with the three density dependent sets DD-MEδ, DD-ME2 and DD-PC1 the pairing gaps $\Delta_{uv}$ in neutron-rich $N \geq 126$ nuclei have on average the same magnitude as pairing gaps in known nuclei (Fig. 3.17a). However, the absolute pairing energies are larger by a factor of about 2 in neutron-rich nuclei as compared with the ones in known nuclei. Note that both $\Delta_{uv}$ and $E_{\text{pairing}}$ are more or less constant in neutron-rich nuclei in the RHB calculations with DD-PC1 and DD-MEδ. On the contrary, a slight increase of the absolute values of these quantities is observed with increasing isospin in DD-ME2.

The situation is different for the CEDF NL3*. Its pairing correlations are only slightly stronger in known nuclei as compared with the density dependent CEDF’s. However, more pronounced differences are seen when the results in neutron-rich nuclei are compared with the ones in known nuclei. The pairing gaps $\Delta_{uv}$ are on average 25% larger in neutron-rich nuclei as compared with known ones and, in addition, they gradually increase with neutron number. The absolute values of the pairing energies rapidly increase with neutron number in neutron-rich $N \geq 126$ nuclei; near the two-proton drip line these energies are larger by a factor of 4 than average pairing energies in known nuclei.

Considering the existing differences in the $\Delta_{uv}$ and $E_{\text{pairing}}$ values obtained in the calculations with different CEDF’s in known nuclei (curves in the shaded area of Fig. 3.17), it is important to understand to which extent the minimization of these differences will also remove the differences in these quantities in neutron-rich nuclei. In order to address this question, the calculations with the DD-PC1 CEDF have been performed with a pairing strength increased by 3.5%. In the region of known nuclei, the $\Delta_{uv}$ values obtained in
these calculations are on average the same as the ones obtained in the calculations with NL3* CEDF (Fig. 3.17a). The pairing energies are also similar in both calculations (Fig. 3.17b). However, in the region of experimentally known nuclei the isospin dependences of the quantities $\Delta_{uv}$ and $E_{\text{pairing}}$ are slightly different in these calculations with NL3* and DD-PC1 CEDF’s. These differences increase with isospin; they are especially pronounced near the two-neutron drip line. This effect may be related to different density dependence of these two CEDF’s in the isovector channel.

The strong dependence of the predictions for neutron pairing on the underlying functional is also seen in the fact that Skyrme DFT calculations for the spherical nuclei with large proton gaps [146] show the reduction of neutron pairing towards the neutron drip line, which, however, is overcast by strong shell effects. This analysis is based on the $\Delta_{lcs}$ pairing gaps (for definition see Ref. [147] and Sect. IV of Ref. [3]) in even-even nuclei. However, it was found in Ref. [3] that the $\Delta_{uv}$ pairing gaps used in the present calculations reproduce the experimental odd-even mass staggerings in a considerably better way than the $\Delta_{lcs}$ pairing gaps.

3.10 Conclusions

The conclusions can be summerized as follows:

- A detailed and systematic survey of nuclear landscape and drip lines has been performed in the CDFT framework employing 4 different state-of-the-art CEDFs. They represent three classes of functionals which differ by basic model assumptions and fitting protocols.
The calculated two-proton drip lines are very close to experiment. The best reproduction of the two-proton drip line is achieved for the CEDF’s DD-ME2 and DD-MEδ, which are characterized by the best residuals for the two-proton separation energies \( S_{2p} \). Since the proton-drip line lies close to the valley of stability, the extrapolation errors towards it are small. In addition, the Coulomb barrier provides a rather steep potential reducing considerably the coupling to the proton continuum. This leads to a relatively low density of the single-particle states in the vicinity of the Fermi level, which helps to minimize the errors in the prediction of the two-proton drip line.

A detailed analysis of the sources of the spread in the predictions of the two-neutron drip lines existing in non-relativistic and covariant DFT has been performed. Poorly known isovector properties of the EDF’s, the underlying shell structure and inevitable inaccuracies in the DFT description of the single-particle energies contribute to these uncertainties. However, no clear correlations between the location of the two-neutron drip line and the nuclear matter properties of the corresponding EDF have been found.

The spread between the different models in the definition of the two-neutron drip line at \( Z \sim 54, N = 126 \) and \( Z \sim 82, N = 184 \) are very small due to the impact of the spherical shell closures at \( N = 126 \) and 184. The largest difference between covariant and Skyrme DFT exist in superheavy nuclei, where the first model (contrary to the second) consistently predicts a significant impact for the \( N = 258 \) spherical
shell closure. The spread of the theoretical predictions grows on moving away from these spherical closures. This is caused by the increasing deformation.

- A comparable level of accuracy (with a slightly better description by DD-ME2) is achieved by all the functionals under investigation for charge radii. Fig. 3.10 shows that the spread in predicting charge radii are not necessarily larger near the neutron drip line as compared with the valley of beta-stability.

- The experimental data on the neutron skin thickness $r_{\text{skin}}$ in $^{208}$Pb is somewhat contradictory. Hadronic probes give $r_{\text{skin}} \sim 0.2$ fm, whereas in the PREX experiment the electro-weak probe provides a central value of $r_{\text{skin}} = 0.3$ fm, however with very large error bars. The NL3* results come close to the central PREX value, while DD-ME2, DD-ME$\delta$ and DD-PC1 give much smaller neutron skins in the vicinity of $r_{\text{skin}} = 0.2$ fm. This can be understood by the fact that the last three functionals have a density dependence in the isovector channel, which leads to a smaller slope $L$ of the symmetry energy at saturation and, therefore, to larger values of the symmetry energy in the region of densities $\rho \sim 0.1$ fm below saturation (see Refs. [47, 134]). As a consequence, the neutrons are less bound to the protons in this region of densities. Globally, the spreads in the neutron skin thickness increase with isospin and become rather large in neutron-rich nuclei (reaching $r_{\text{skin}} = 0.25$ fm in some cases) reflecting the difference between NL3* and the DD CEDF’s. There is hope that these uncertainties can be reduced, if future PREX-II and CREX experiments provide neutron skin thicknesses in $^{208}$Pb and $^{48}$Ca with the required accuracy.
CHAPTER 4
SUPERDEFORMATION TO EXTREME DEFORMATION AND CLUSTERIZATION
IN THE $N \sim Z$ NUCLEI OF $A \sim 40$ MASS REGION.

4.1 Introduction

There is a considerable interest to the study of cluster structures and extremely deformed shapes in light nuclei [30, 34, 36, 37, 99, 148, 149, 150, 151, 152, 153]. Many of these structures are described in terms of clusters, the simplest one being the $\alpha$-particle [99, 150]. Providing a unique insight on the cluster dynamics inside of a nucleus, the initial assumptions about clusters represent a limitation of this type of models. Note also that many shell model configurations are beyond the reach of the cluster model. It is also important to remember that the cluster description does not correspond to clearly separated $\alpha$-particles, but generates the mean-field states largely by antisymmetrization [150]. In addition, the studies of molecular structures, which appear in many extremely deformed configurations, have gained considerable interest [99, 153, 154].

A systematic investigation for extremely deformed configurations, focused on the $N = Z$ and $N = Z + 2$ even-even S ($Z = 16$), Ar ($Z = 18$), Ca ($Z = 40$), Ti ($Z = 42$), Cr ($Z = 44$) (and also on $N = Z + 4$ $^{44}$Ca) and odd-odd $N = Z = 21$ $^{42}$Sc nuclei, have been undertaken in the framework of covariant density functional theory (CDFT). We have started with the $^{40}$Ca nucleus. This is a spherical doubly magic nucleus (in the
ground state) in which normal- and superdeformed configurations based on the 4 particle - 4 hole (4p-4h) and 8 particle - 8 hole (8p-8h) excitations, respectively, are observed at low excitation energies (Ref. [155]). In this mass region, superdeformation has already been observed in $^{40}$Ca ([155, 156]), $^{36}$Ar ([157, 158]), $^{35}$Cl ([159]), $^{40}$Ar ([160]) and probably $^{28}$Si [161]. Moreover, the SD bands have been seen up to very high spin of $I = 16\hbar$ in some of these nuclei. This is a quite important fact because according to the results obtained in the present study a further modest increase in the spin could lead to the population of extremely deformed structures in some of the nuclei. When populated such structures could be observed with the next generation of $\gamma$-tracking detectors such as GRETA and AGATA.

At low spin, these extremely deformed states are either generally unbound or lie at high excitation energies [37, 99]. Moreover, they are formed on the shoulder or in very
shallow minima of potential energy surfaces [39, 162]; thus, they are inherently unstable at low spin. The high density of nucleonic configurations at these energies and possible mixing among them is another factor hindering their observation with current and future generations of experimental facilities. In addition, the mechanisms of the reactions used in experimental studies frequently favor the population of yrast or near-yrast states [37].

The rotation of the nucleus can help to overcome these problems in experimental observation of extremely deformed structures. The reasons are as follows: First, very large deformation configurations (such as super- (SD), hyper- (HD) and megadeformed (MD) ones) are favored by rotation at high spins (see, the Refs. [38, 39]). Second, normal- and highly-deformed configurations, which are forming yrast or near-yrast structures at low and medium spins, have limited angular momentum content. As a consequence, only extreme deformation structures (SD, HD, or MD) exist and thus could be populated and observed above some specific spin values in the nuclei of interest.

In recent years, the investigations of exotic cluster configurations have been undertaken also in the density functional theory (DFT). The advantage of the DFT framework is the fact that it does not assume the existence of cluster structures; the formation of cluster structures proceeds from microscopic single-nucleon degrees of freedom via many-body correlations [152, 162]. As a result, the DFT framework allows simultaneous treatment of cluster and mean-field-type states [30, 32, 152, 162, 163]. It is important to mention that covariant (relativistic) energy density functionals (CEDFs) show more pronounced clustering of the density distribution as compared with non-relativistic EDFs because of deeper single-nucleon potentials [152]. The clustering phenomenon in light stable and ex-
otic nuclei was studied within the relativistic mean field (RMF) approach in Ref. [29] and within the Hartree-Fock (HF) approach based on the Skyrme energy density functionals (EDF) in Ref. [30]. Linear chain configurations of four \( \alpha \)-clusters in \(^{16}\)O and the relationship between the stability of such states and angular momentum were investigated using Skyrme cranked HF method in Ref. [31] and cranked RMF (further CRMF) in Ref. [32]. This is an example of a “rod shaped” nucleus. Another case of such structures is a linear chain of three \( \alpha \) clusters, suggested about 60 years ago [33]; it was recently studied in the CRMF theory in Ref. [34]. This exotic structure (“Hoyle” state) plays a crucial role in the synthesis of \(^{12}\)C from three \(^{4}\)He nuclei in stars [35]. The stability of rod-shaped structures in highly-excited states of \(^{24}\)Mg was studied in Ref. [36] in cranked Skyrme HF calculations.

Our study aims to do a systematic investigation of extremely deformed structures and clusterization within the CRMF framework in the nuclei shown in the Fig. 4.1 The main objectives of this study are as follows:

1. To understand at which spins the extremely deformed configurations are expected to become yrast (or come close to the vicinity of the yrast line). And to find the best candidates for experimental studies of such structures. This requires detailed knowledge of terminating configurations up to their terminating states since they form the yrast line at low and medium spins. However, the tracing of terminating configurations from low spin up to their terminating states is a non-trivial problem in density functional theories (see Sec. 8 in Ref. [7] and Ref. [164]). To our knowledge, such calculations have been done so far only in a few nuclei: \(^{20}\)Ne (in the cranked
Skyrme HF [165] and CRMF [10, 14] frameworks), $^{48}$Cr (in the HFB framework with Gogny forces [166]) and $^{109}$Sb (in the CRMF framework [7]). With appropriate improvements in the CRMF computer code we are able to perform such calculations for the majority of the configurations forming the yrast line at low and medium spins.

2. To calculate the basic properties (such as transition quadrupole moments, dynamic and kinematic moments of inertia) of the configurations of interest, which could be compared in the future with experimental data, are predicted.

3. To search for the fingerprints of the clusterization and molecular structures via a detailed analysis of the density distributions of the configurations under study.

4.2 The details of the theoretical calculations

The calculations have been done in the framework of cranked relativistic mean field theory (CRMF). The formalism and the applications of the CRMF theory to describe the rotating nuclei have already been discussed in the preceding chapter. For the present study we have adopted some formalism which are discussed as follows:

- The pairing correlations are neglected due to following reasons: The pairing correlations are quenched by rotation (Coriolis anti-pairing effect) [59, 167]. The presence of substantial shell gaps also leads to a quenching of pairing correlations [168]. Another mechanism of pairing quenching is the blocking effect which is active in many nucleonic configurations [59]. In a given configuration, the pairing is also very weak at the spins close to band termination [169]. Moreover, the pairing drastically de-
creases after paired band crossings in the proton and neutron subsystems [52]; at these spins the results of the calculations with and without pairing are very similar.

• The calculations for blocked configurations within the cranked Relativistic Hartree-Bogoliubov (CRHB) framework [63] are frequently numerically unstable [56]. This is a common problem for self-consistent Hartree-Bogoliubov or Hartree-Fock-Bogoliubov calculations which appears both in relativistic and non-relativistic frameworks [170]. However, these problems are much less frequent in unpaired CRMF calculations (see Ref. [39]). Even then it is not always possible to trace the configuration in the desired spin range. This typically takes place when (i) the local minimum is not deep enough for the solution (unconstrained in quadrupole moments) to stay in it during the convergence process and (ii) occupied and unoccupied single-particle orbitals with the same quantum numbers come close in energy and start to interact.

• Based on previous experience in $^{40}\text{Ca}$ (Ref. [155]), $^{48}\text{Cr}$ (Ref. [169]) and somewhat heavier $N \sim Z \ A = 58 - 80$ nuclei (Refs. [53, 52]), we estimate that the pairing becomes quite small and thus not very important above $I \sim 10\hbar$ in the nuclei of interest. This is exactly the spin range on which the current study is focused.

• We restricted ourselves to reflection symmetric shapes since previous calculations in the cranked Hartree-Fock approach with Skyrme forces [171] showed that odd-multipole (octupole, ...) deformations play a very limited role in extremely deformed configurations for the mass region under study.
• The CRMF equations are solved in the basis of an anisotropic three-dimensional harmonic oscillator in Cartesian coordinates characterized by the deformation parameters $\beta_0$ and $\gamma$ and oscillator frequency $\hbar\omega_0 = 41A^{1/3} \text{MeV}$, for details see Refs. [10, 51]. The truncation of basis is performed in such a way that all states belonging to the major shells up to $N_F = 14$ fermionic shells for the Dirac spinors and up to $N_B = 20$ bosonic shells for the meson fields are taken into account. This truncation scheme provides sufficient numerical accuracy (see Ref. [39] for details).

• The calculations have been performed with the NL3* functional [24] The details of this energy functional have already been discussed in Ref. [3].

The quadrupole deformation $\beta_2$ is defined in self-consistent calculations from calculated quadrupole moments using the simple relation [57, 172, 173]

$$\beta_2 = \frac{1}{XR^2} \frac{5\pi}{9} Q^X_0$$

(4.1)

where $R = 1.2A^{1/3} \text{fm}$ is the radius and $Q^X_0$ is a quadrupole moment of the $X$-th (sub)system expressed in $\text{fm}^2$. Here $X$ refers either to proton ($X = Z$) or neutron ($X = N$) subsystem or represents total nuclear system ($X = A$). However this expression neglects the higher powers of $\beta_2$ and higher multipolarity deformations $\beta_4, \beta_6, ...$ [122], which have an important role at very large deformations.

Because the definition of the deformation is model dependent [122] and deformation parameters are not experimentally measurable quantities, we prefer to use the transition quadrupole moment $Q_t$ for the description of deformation properties of the SD, HD and MD bands. This is an experimentally measurable quantity and thus in future our predic-
tions can be directly compared with the experimental results. The deformation properties of the yrast SD band in $^{40}$Ca [155] are used as a reference. The measured transition quadrupole moment of this band is $Q_{t}^{\exp} = 1.8^{+0.35}_{-0.29}$ eb [155]. Note that the CRMF calculations with the NL3* functional come close to experiment only slightly overestimating an experimental value (see Fig. 4.6 below). Thus we use $Q_{t}^{\exp} = 1.8$ eb in $^{40}$Ca as a reference point. Note that the SD band in $^{40}$Ca is the most deformed SD band among observed SD bands in this mass region.

Using this value we introduce the normalized transition quadrupole moment $Q_{t}^{\text{norm}}(Z, A)$ in the $(Z, A)$ system

$$Q_{t}^{\text{norm}}(Z, A) = \frac{ZA^{2/3}}{129.96} \text{ eb} \quad (4.2)$$

This is similar to what has been done in Ref. [39] in the analysis of the HD configurations in medium mass region. This equation is based on the ratio $Q_{t}^{\text{norm}}(Z, A)/Q_{t}(^{40}\text{Ca})$ calculated using Eq. (4.1) under the assumption that the $\beta_2$ values in the $(Z, A)$ system and in $^{40}$Ca are the same.

The band will be described as HD if its calculated $Q_t$ value exceeds $Q_{t}^{\text{norm}}(Z, A)$ by approximately 50%. This definition of HD is similar to the one employed in Ref. [39]. Following suggestion of Ref. [38], we describe even more deformed bands as megadeformed. The band is classified as MD when its calculated $Q_t$ value is approximately twice of $Q_{t}^{\text{norm}}(Z, A)$ or higher.

Single-particle orbitals are labeled by $\Omega[Nn_{z}\Lambda](r = \pm i)$ where $\Omega[Nn_{z}\Lambda]$ are the asymptotic quantum numbers (Nilsson quantum numbers) of the dominant component of the wave function at $\Omega_x = 0.0$ MeV and $r$ is the signature of the orbital.
Because the pairing correlations are neglected, the intrinsic structure of the configurations of interest can be described by means of the dominant single-particle components of the intruder states occupied. Thus, the calculated configurations will be labeled by shorthand \([n_1(n_2)(n_3),p_1(p_2)(p_3)]\) labels, where \(n_1, n_2\) and \(n_3\) are the number of neutrons in the \(N = 3, 4\) and 5 intruder/hyperintruder/megaintruder orbitals and \(p_1, p_2\) and \(p_3\) are the number of protons in the \(N = 3, 4\) and 5 intruder/hyperintruder/megaintruder orbitals. The \(N = 5\) megaintruder orbitals are not occupied in the HD configurations. As a consequence, the labels \(n_3\) and \(p_3\) will be omitted in the labeling of such configurations. Moreover, the \(N = 4\) and \(N = 5\) orbitals are not occupied in the SD configurations. So, in those configurations the \(n_2, n_3\) and \(p_2, p_3\) labels will be omitted. An additional letter \((a,b,c,\ldots)\) at the end of the shorthand label is used to distinguish the configurations which have the same occupation of the intruder orbitals (the same \([n_1(n_2)(n_3),p_1(p_2)(p_3)]\) label) but differ in the occupation of non-intruder orbitals.

4.3 The ⁴⁰Ca nucleus

We have started our study with ⁴⁰Ca. This is a doubly magic spherical nucleus in the ground state with 20 neutrons and 20 protons. The three lowest shells with \(N = 0, 1\) and 2 are occupied in its spherical ground state with \(I = 0^+\). Higher spin states are formed by particle-hole excitations from the \(N = 2\) shell into the \(f_{7/2}(N = 3)\) subshell across the respective \(Z = 20\) and \(N = 20\) spherical shell gaps. The particle-hole excitations form the high-spin level scheme which includes spherical states and deformed, terminating and
Energies of the calculated configurations in $^{40}$Ca relative to a smooth liquid drop reference, with the inertia parameter $A = 0.05$. 

Figure 4.2
Neutron single-particle energies (routhians) in the self-consistent rotating potential as a function of the rotational frequency $\Omega_{\pi}$.

Figure 4.3
The same as Fig. 4.3 but along the deformation path of the yrast HD configuration in $^{40}$Ca. The arrows indicate the particle-hole excitations leading to excited HD configurations.
Figure 4.5

The same as Fig. 4.3 but along the deformation path of the yrast MD [42,42] configuration in $^{40}\text{Ca}$.
superdeformed rotational structures [155, 156, 174]. Experimentally it has been found to extend up to the spin $I = 16\hbar$.

The results of the CRMF calculations for deformed configurations forming the yrast line are shown in the $(E - E_{RLD})$ plot in Fig. 4.2. This is the energies of the calculated configurations of $^{40}$Ca relative to a smooth liquid drop reference $AI(I + 1)$ plotted against spin. This way of the presentation of the results has clear advantages as compared with the energy versus spin plots, see Sec. 4.1 in Ref. [169] for details. Different types of configurations are shown by different types of lines. The SD, HD and MD configurations, which are yrast in respective deformation minima, are shown by thick lines with symbols. Also, different colors are used to indicate different classes of the bands. Note that low-spin spherical solutions are not shown here since we are interested in high-spin behavior of this nucleus.

The lowest deformed configuration [1,1] is based on simultaneous excitations of a proton and a neutron from the $d_{3/2}$ spherical subshell into the $f_{7/2}$ subshell across the $Z = 20$ and $N = 20$ spherical gaps. It has small quadrupole deformation of $\beta_2 \sim 0.16$ and $\gamma \sim -24^\circ$ at $I = 4\hbar$ and terminates at $I = 10\hbar$ in a state with the structure $\pi(f_{7/2})_{3,5}^{1}(d_{3/2})_{1,5}^{-1} \otimes \nu(f_{7/2})_{3,5}^{1}(d_{3/2})_{1,5}^{-1}$ and near-spherical shape. Additional excitations of the protons and neutrons across the $Z = 20$ and $N = 20$ spherical gaps lead to a more deformed [2,2] configuration which has $\beta_2 \sim 0.32$ and $\gamma \sim -30^\circ$ at $I = 10\hbar$. It is expected to terminate at $I_{max} = 20\hbar$ with the terminating state built at high energy cost and located high above the yrast line. However, we were not able to trace this configuration up to termination in the calculations. Next excitations of protons and neutrons across the
$Z = 20$ and $N = 20$ spherical gaps lead to even more deformed $[3,3]$ configurations which are located close to each other up to spin $I = 16\hbar$ (see Fig. 4.2). The configuration which terminates at spin $I = 18\hbar$ is located in positive $\gamma$ minimum of potential energy surfaces and has $\beta_2 \sim 0.47$ and $\gamma \sim 21^\circ$ at $I = 12\hbar$. The structure of the terminating state is $\pi(f_7/2)^3_7(d_3/2)^{-3}_{1.5} \otimes \nu(f_7/2)^3_7(d_3/2)^{-3}_{1.5}$. Another $[3,3]$ configuration is located in the negative $\gamma$ minimum in the potential energy surfaces and is expected to terminate at $I = 24\hbar$. Similar to the $[2,2]$ configuration, we were not able to trace it up to the terminating state which is expected to be located high above the yrast line.

Neutron single-particle energies (routhians) in the self-consistent rotating potential of $^{40}$Ca as a function of the rotational frequency $\Omega_x$ are presented in Fig. 4.3, Fig. 4.4 and Fig. 4.5. They are calculated along the deformation path of the yrast SD, HD and MD configurations, respectively. Long-dashed, solid, dot-dashed and dotted lines indicate $(\pi = +, r = +i)$, $(\pi = +, r = -i)$, $(\pi = -, r = +i)$ and $(\pi = -, r = -i)$ orbitals, respectively. At $\Omega_x = 0.0$ MeV, the single-particle orbitals are labeled by the asymptotic quantum numbers $\Omega[Nn\Lambda]$ (Nilsson quantum numbers) of the dominant component of the wave function. Solid (open) circles indicate the orbitals occupied (emptied). These diagrams form the basis for understanding the microscopic structure of the configurations of interest. Particle-hole excitations shown by arrows in Fig 4.3, result in the formation of excited superdeformed rotational bands. For example, the yrast SD configuration $[4,4]$ is characterized by large SD shell gap at particle number 20 both in the proton and neutron subsystems (Fig. 4.3). All single-particle states below these gaps are occupied in the $[4,4]$ configuration. Note that apart of the Coulomb shift in energy the proton routhian diagram
is similar to the neutron one shown in Fig. 4.3. The [4,4] configuration is only yrast at \( I = 22\hbar \); it is located above the yrast line at lower spin in agreement with the experiment [155].

Starting from the yrast SD configuration [4,4] there are two ways to build excited configurations. The first one is by exciting particles from the \( 3/2[321](r = \pm i) \) orbitals into the \( 1/2[200](r = \pm i) \) orbitals; they are shown by the arrows as the S1–S4 excitations in Fig. 4.3. The combination of proton and neutron excitations of this type leads to the [3,3] configurations. If the proton (neutron) excitations of this type are combined with the neutron (proton) configuration of the yrast SD band, the [3,4] and [4,3] configurations are created. These configurations are excited with respect to the yrast [4,4] SD configuration; some of them are shown by red lines in Fig. 4.2. Note that due to the similarity of the proton and neutron routhian diagrams some of these excited configurations are degenerated (or nearly degenerated) in energy. In addition, we show only some of highly excited SD configurations for the sake of clarity. An important feature is a quite large energy gap between the yrast [4,4] and lowest excited [3,3]d SD configurations. Such a situation favors the observation of the yrast SD band since the feeding intensity is concentrated on it (see discussion in Refs. [39, 175]).

Alternatively, one can excite the particle from either the \( 5/2[202](r = -i) \) or \( 5/2[202](r = +i) \) orbital to the lowest in energy hyperintruder \( 1/2[440](r = -i) \) orbital emerging from the hyperintruder \( N = 4 \) shell; the occupation corresponding to such a configuration is shown on left side of Fig. 4.4. The combination of the proton and neutron excitations of this kind leads to four-fold degenerate [41,41] HD configurations. This degeneracy is due
to very small signature splitting of the configurations built on opposite signatures of the \(5/2[202]\) orbitals and the combination of proton and neutron configurations of this kind.

At first glance this statement is in contradiction with Fig. 4.4 where there is a substantial energy splitting between the \(r = -i\) and \(r = +i\) branches of the \(5/2[202]\) orbital which are almost parallel in rotational frequency. This feature is the consequence of non-pairwise occupation of the opposite signatures of some orbitals which leads to the presence of nucleonic currents at rotational frequency \(\Omega_x = 0.0\) MeV (see Sec. IVA in Ref. [11]).

The occupied orbital is always more bound than its unoccupied time-reversal counterpart. So the change in the signature of the occupied \(5/2[202]\) state (from \(r = -i\) in Fig. 4.4 to \(r = +i\)) will only inverse the relative positions of both signatures of this orbital so that the total energy of the configurations built on the holes in the \(5/2[202](r = -i)\) and \(5/2[202](r = +i)\) orbitals will be almost the same. The \([41,41]\) configurations are the lowest in energy among the HD configurations at spins above \(I = 24\hbar\) (Fig. 4.2). The excited HD configurations \([31,31]\)a and \([31,31]\)b (Fig. 4.2) are formed as the combination of the H1 and H2 excitations (shown in Fig. 4.4) in the proton and neutron subsystems. The \([31,41]\)a and \([31,41]\)b configurations are based on the H1 and H2 excitations in the neutron subsystem and the proton configuration of the yrast \([41,41]\) HD configuration. The \([41,31]\)a and \([41,31]\)b configurations (not shown in Fig. 4.2), based on the H1 and H2 excitations in the proton subsystem and the neutron configuration of the yrast \([41,41]\) HD configuration, are located at the energies which are similar to the ones of the \([31,41]\)a and \([31,41]\)b configurations. The HD configurations never become yrast in \(^{40}\)Ca. How-
ever, such configurations compete with megadeformed ones for yrast status in neighbouring nuclei. That was a reason for a quite detailed discussion of their structure.

The additional occupation of the $N = 4$ proton and neutron orbitals leads to the $[42,42]$ MD configuration which is yrast at spin above $I = 23\hbar$ (Fig. 4.2). It is characterized by large (around 3 MeV) MD $Z = 20$ and $N = 20$ shell gaps (Fig. 4.5). Thus, this configuration can be considered as a doubly magic megadeformed configuration. Indeed, excited MD configurations (such as $[42,51]$, $[51,51]$, $[51,42]$ etc) are located at excitation energy of more than 2 MeV with respect to the yrast MD configuration (Fig. 4.2). The fact that the yrast MD configuration $[42,42]$ is separated from the excited configurations by such a large energy gap should make its observation in experiment easier. This is because of the concentration of feeding intensity on the yrast MD configuration in such a situation (see discussion in Refs. [39, 175]).

Calculated transition quadrupole moments $Q_t$ and $\gamma$-deformations of the normal- and highly-deformed triaxial, SD, HD and MD configurations are shown in Figs. 4.6 and 4.8. The configurations which are yrast in local deformation minima, namely, SD $[4,4]$, HD $[41,41]$ and MD $[42,42]$ have the largest transition quadrupole moment among the calculated SD, HD, and MD configurations, respectively. This is because particle-hole excitations leading to excited configurations reduce the number of occupied deformation driving orbitals.

Note that most of the calculated SD configurations have $\gamma \sim -12^\circ$. The only exception is the unusual $[31,31]$a configuration which has large positive $\gamma$-deformation rapidly increasing with spin. It has some similarities with the HD configurations. First, it involves
Calculated transition quadrupole moments $Q_t$ and $\gamma$-deformations of the yrast and excited SD and HD configurations in $^{40}$Ca.
The same as Fig. 4.6 but for the normal and highly-deformed triaxial configurations in $^{40}\text{Ca}$. 
Figure 4.8

The same as Fig. 4.6 but for the megadeformed configurations in $^{40}$Ca.
Figure 4.9

The self-consistent proton density distributions for the yrast SD configurations in $^{40}$Ca.

Figure 4.10

The self-consistent proton density distributions for the yrast HD configurations in $^{40}$Ca.
The self-consistent proton density distributions for the yrast MD configurations in $^{40}\text{Ca}$.

The $N = 4$ proton and neutron. Second, its slope in the $E - E_{RLD}$ plot is similar to the one of the HD configurations (see Fig. 4.2). However, it has substantially smaller $Q_t$ values as compared with the HD configurations.

The colors of the lines for different types of configurations roughly correspond to those used in Fig. 4.2. Red and orange (black and dark brown) are used for the SD (HD) configurations. While the calculated $Q_t$ and $\gamma$ values cluster for the SD configurations (Figs. 4.6a and c), they are scattered for the HD configurations (Figs. 4.6b and d). This suggests that the potential energy surfaces are much softer in the HD minimum as compared with the SD one. Indeed, in the HD minimum a single particle-hole excitation induces much larger changes in the $Q_t$ and $\gamma$ values than in the SD one. On the contrary, the MD configurations show the clusterization of the calculated $Q_t$ and $\gamma$ values which is similar to the one observed in the SD minimum (Fig. 4.8).
The most deformed HD configuration ([41,41]) has $Q_t$ values which are roughly 40% larger than the ones for most deformed SD configuration ([4,4]) (Fig. 4.6a and c). Yrast MD configuration [42,42] has the $Q_t$ values which are larger by roughly 45% and 105% than the ones for most deformed HD and SD configurations (compare Fig. 4.8a and Fig. 4.6a and c).

The self-consistent proton densities $\rho_p(y, z)$ as a function of $y$ and $z$ coordinates for the yrast SD, HD and MD configurations in $^{40}$Ca are shown in Fig. 4.9, Fig. 4.10 and Fig. 4.11 at indicated spin values. The equidensity lines are shown in steps of 0.01 fm$^{-3}$ starting from $\rho_p(y, z) = 0.01$ fm$^{-3}$. The stretching of nuclear shape is definitely more pronounced in the HD [41,41] and especially in the MD [42,42] configurations. Indeed, the semi-major to semi-minor axis ratio is 2.05, 2.27 and 2.9 for the densities of the SD [4,4], HD [41,41] and MD [42,42] configurations. Note that the changes in the semi-axis ratio on going from one type of configuration to another are substantially smaller than the relevant changes in the $Q_t$ values discussed above. The densities of the [41,41] HD configuration show some indications of the development of neck and these indications become much more pronounced in the MD [42,42] configuration.

4.4 The $^{42}$Sc nucleus

The next nucleus considered here is $^{42}$Sc, this is only odd-odd nucleus in the present study. It is formed by addition of one proton and one neutron to $^{40}$Ca. The configurations forming the yrast line of $^{42}$Sc are shown in Fig. 4.12. The [1,1] configuration is built in valence space; it terminates at $I = 7h$. The [2,2] configuration is an analog of the [1,1]
configuration in $^{40}$Ca but with an extra proton and extra neutron placed into the orbitals emerging from the $f_{7/2}$ spherical subshell. As a consequence, it has substantially larger deformation and maximum spin within the configuration than the $[1,1]$ configuration in $^{40}$Ca. At spin $I = 4\hbar$, the deformation of the $[2,2]$ configuration is $\beta_2 \sim 0.27$ and $\gamma \sim -15^\circ$. It terminates at $I = 15\hbar$ in a terminating state with the structure $\pi (f_{7/2})^2_{6,0} (d_{3/2})^{-1}_{1.5} \otimes \nu (f_{7/2})^2_{6,0} (d_{3/2})^{-1}_{1.5}$ and near-spherical shape with $\beta_2 \sim 0.05$.

Additional excitations of the proton and neutron across the $Z = 20$ and $N = 20$ spherical gaps lead to a more deformed $[3,3]$ configuration which has $\beta_2 \sim 0.37$ and $\gamma \sim -31^\circ$ at $I = 10\hbar$. It is expected to terminate at $I_{\text{max}} = 23\hbar$ with the terminating state built at high energy cost and located above the yrast line. However, we were able to trace this configuration in the calculations only up to $I \approx 22\hbar$ (one $\hbar$ short of termination).
Figure 4.13

The same as Fig. 4.6 but for $^{42}$Sc.

Figure 4.14

The self-consistent proton density distributions $^{42}$Sc. for the indicated configuration.
Figure 4.15

The self-consistent proton density distributions $^{42}$Sc. for the indicated configuration.

Figure 4.16

The self-consistent proton density distributions $^{42}$Sc. for the indicated configuration.
The self-consistent proton density distributions $^{42}$Sc. for the indicated configuration.

The lowest four SD configurations $[4,4]$ in $^{42}$Sc are formed from the yrast SD configuration $[4,4]$ in $^{40}$Ca by addition of the proton and neutron to the $1/2[200](r = \pm i)$ orbitals located above the $Z = 20$ and $N = 20$ SD shell gaps (see Fig. 4.3). Their deformation properties are summarized in Fig. 4.13. Similar to the SD bands in $^{40}$Ca, they are located in the $\gamma \sim -12^\circ$ minimum of the potential energy surface. Note that the lowest $[4,4]$ SD configuration undergoes unpaired band crossing (due to the crossing of the $1/2[400](r = -i)$ and $1/2[200](r = -i)$ orbitals seen in Fig. 4.3) which leads to the $[41,41]$ HD configuration.

At spin above $I = 22\hbar$, the HD configuration $[41,41]$ becomes the lowest in energy. In this configuration, all single-particle states below the $Z = 21$ and $N = 21$ HD shell gap (Fig. 4.4) are occupied. So contrary to the yrast HD bands in $^{40}$Ca, which are degenerate in energy, the yrast HD line in $^{42}$Sc is represented by a single strongly decoupled branch of the $[41,41]$ configuration.
At even higher spin (above $I = 30\hbar$), the yrast line is formed by the megadeformed configuration $[421,421]$ (Fig. 4.12). This configuration contains the proton and neutron in the lowest megaintruder $N = 5$ orbital above the unpaired band crossing at $\Omega_x \sim 1.80$ MeV (above $I = 31\hbar$). At lower spin the structure of this MD configuration is $[52,52]$; this is a result of unpaired band crossing emerging from the interaction of the lowest megaintruder ($N = 5$) $(r = +i)$ orbital with the $1/2[321](r = +i)$ orbital taking place at $\Omega \sim 1.8$ MeV (Fig. 4.5). Note that this band crossing is blocked in the closely lying $[52,52]$ MD configuration, shown by a solid blue line in Fig. 4.12, in which the 21st proton and 21st neutron are placed into the $1/2[321](r = -i)$ orbital located above the $Z = 20$ and $N = 20$ MD shell gaps.

Table 4.1

The semi-axis ratios of the density distributions of the indicated configurations at given spin. The semi-axis ratios are extracted at $\rho_p = 0.04$ fm$^{-3}$ which roughly corresponds to half of the proton density in the central part of the nucleus.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Configuration, spin</th>
<th>Type</th>
<th>Semi-axis ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{40}$Ca</td>
<td>$[4,4], I = 12$</td>
<td>SD</td>
<td>2.05</td>
</tr>
<tr>
<td>$[41,41], I = 24$</td>
<td>HD</td>
<td>2.27</td>
<td></td>
</tr>
<tr>
<td>$[42,42], I = 25$</td>
<td>MD</td>
<td>2.90</td>
<td></td>
</tr>
<tr>
<td>$^{42}$Sc</td>
<td>$[41,41], I = 22$</td>
<td>HD</td>
<td>2.23</td>
</tr>
<tr>
<td>$[52,52], I = 25$</td>
<td>MD</td>
<td>2.65</td>
<td></td>
</tr>
<tr>
<td>$[421,421], I = 31$</td>
<td>MD</td>
<td>3.40</td>
<td></td>
</tr>
<tr>
<td>$[421,421], I = 40$</td>
<td>MD</td>
<td>3.64</td>
<td></td>
</tr>
<tr>
<td>$^{50}$Cr</td>
<td>$[62,62], I = 31$</td>
<td>HD</td>
<td>2.27</td>
</tr>
<tr>
<td>$^{32}$S</td>
<td>$[2,2], I = 12$</td>
<td>SD</td>
<td>2.09</td>
</tr>
<tr>
<td>$[21,21], I = 31$</td>
<td>HD</td>
<td>2.15</td>
<td></td>
</tr>
</tbody>
</table>
Proton density distributions for the HD configuration [41,41] and MD configurations [52,52] and [421,421] are shown in Fig. 4.14, Fig. 4.15, Fig. 4.16 and Fig. 4.17. The major semi-axis ratio of the proton density distribution increases only moderately (from 2.23 to 2.65 [see Table 4.1]) on going from the [41,41] configuration to the [52,52] one. However, this transition triggers a drastic change in the transition quadrupole moment \( Q_t \); it is increased from \( Q_t \sim 2.65 \, \text{eb} \) for the [41,41] configuration to \( Q_t \sim 4.5 \, \text{eb} \) for the [52,52] configuration (see Fig. 4.13). The occupation of the megaintruder proton and neutron \( N = 5 \) orbitals leading to the MD [421,421] configuration creates both additional elongation of the proton density and neck in this density distribution. The [421,421] configuration is the most elongated structure in the present study. A three-dimensional representation of this density distribution is shown in the Fig. 1(a) of the Supplemental Material of Ref. [176]. This density distribution has a large semi-axis ratio of 3.40 at \( I = 31\hbar \) which is increasing with spin (Table 4.1). In part, this large value is a consequence of the development of the neck which leads to a small semi-axis in the direction perpendicular to elongation. Note that despite large difference in the semi-axis ratio (3.40 for the [421,421] configuration and 2.65 for the [52,52] one), the \( Q_t \) value of the [421,421] configuration (\( Q_t \sim 5.2 \, \text{eb} \) at \( I = 31\hbar \)) is only by 15% larger that the one for the [52,52] configuration (see Fig. 4.13). These examples clearly indicate that there is no simple relation between the semi-axis ratio of the proton density distribution and the transition quadrupole moments.
Table 4.2

The maximum spin (in $\hbar$) which could be built within the configuration of given type. The asterisk is used to indicate the configurations which involve the hole(s) in the $d_{5/2}$ orbital(s). The SD configurations are not included into this table.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>valence space</th>
<th>2p-2h</th>
<th>4p-4h</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{40}\text{Ca}$</td>
<td>[0,0], $I_{\text{max}} = 0$</td>
<td>[1,1], $I_{\text{max}} = 10$</td>
<td>[2,2], $I_{\text{max}} = 20^*$</td>
</tr>
<tr>
<td>$^{42}\text{Sc}$</td>
<td>[1,1], $I_{\text{max}} = 7$</td>
<td>[2,2], $I_{\text{max}} = 15$</td>
<td>[3,3], $I_{\text{max}} = 23^*$</td>
</tr>
<tr>
<td>$^{50}\text{Cr}$</td>
<td>[6,4], $I_{\text{max}} = 14$</td>
<td>[7,5], $I_{\text{max}} = 16^*$</td>
<td></td>
</tr>
<tr>
<td>$^{32}\text{S}$</td>
<td>[0,0], $I_{\text{max}} = 12^*$</td>
<td>[1,1], $I_{\text{max}} = 20^*$</td>
<td></td>
</tr>
</tbody>
</table>

4.5 The general features of high-spin spectra

Table 4.2 illustrates how the maximum spin, which could be built within the configuration, changes when particle-hole excitations across the spherical $Z = 20$ and $N = 20$ spherical shell gaps are involved. Here 2p-2h configurations are defined as the configurations which involve the excitations of one proton and one neutron across the respective shell gaps. The excitations of two protons and two neutrons across these gaps lead to the 4p-4h configurations. One can see that these excitations increase drastically the maximum spin within the configurations of $^{40}\text{Ca}$.

The analysis of the $^{40}\text{Ca}$ and $^{42}\text{Sc}$ nuclei clearly indicates that subsequent particle-hole excitations lead to the yrast or near-yrast SD, HD and MD configurations at the spins which are either similar to the maximum spins which could be built within the 2p-2h and 4p-4h configurations or slightly above them. Note that the nuclei in these 2p-2h and 4p-4h configurations could at most be described as highly-deformed.

The importance of these 2p-2h and 4p-4h configurations lies in the fact that at low and medium spins they dominate the yrast line and thus are expected to be populated in
experiment with high intensity. The observation of the SD, HD and MD configurations requires that these bands are either yrast or close to yrast at the spins where the feeding of the bands takes place. This is especially critical for the HD and MD bands since in most of the nuclei they have completely different slope in the $E - E_{RLD}$ plots as compared with the bands of smaller deformation. As a result, their excitation energies with respect to the yrast line grow up very rapidly with decreasing spin below the spins where the HD and MD bands are yrast or near yrast. This factor will limit the spin range in which they can be observed in future experiments to the spin range in which these bands are either yrast or close to yrast and few states below this spin range.

Note that the results discussed in this section only illustrate the general features of rotating nuclei and provide some crude estimates of the competition of terminating and extremely deformed configurations. Indeed, detailed calculations are needed to define the properties of such bands and the spins at which extremely deformed configurations become yrast. For the sake of simplicity, we also do not discuss here possible excitations across the spherical $N = 28$ and $Z = 28$ shell gaps.

The examples of the $^{40}$Ca and $^{42}$Sc nuclei discussed above once more confirm that rotating nuclei are the best laboratories to study shape coexistence. Indeed, starting from either spherical or weakly deformed ground states by means of subsequent particle-hole excitations one can build any shape (prolate, oblate, triaxial, super-, hyper- and megadeformed as well as cluster and/or molecular structures [see Sec. 4.7 below for a discussion of latter structures/shapes]) in the same nucleus.
4.6 Other nuclei in the neighbourhood of $^{40}$Ca

Similar to $^{40}$Ca and $^{42}$Sc, analysis has also been performed for the other nuclei shown in Fig. 4.1. Detailed results can be found in the Ref. [176]. Here we focus on $^{28}$Si, $^{32}$S and $^{50}$Cr which are the lightest and the heaviest nuclei in our study.

Note that, in the calculations of terminating structures at low and medium spins we concentrate on the configurations which define the general structure of the yrast line and the spins at which the transition to extremely deformed configurations takes place. The main focus of this section is on the super-, hyper- and megadeformed rotational configurations and, in particular, on the ones which potentially show the features of clusterization and molecular structures.

4.6.1 $^{28}$Si nucleus

The detailed analysis of $^{28}$Si can be found in the Ref. [177]. Fig. 4.18 shows the calculated configurations in the yrast and near yrast region. At low spin, the [0,0]-obl configuration is yrast up to $I \sim 10\hbar$. It has an oblate shape in agreement with experimental findings [178]. The angular momentum content of this configuration is quite limited and it terminates at $I = 12\hbar$. The yrast line starting at $I \sim 10\hbar$, is built on the superdeformed [1,1]b configuration which terminates at spin $I = 18\hbar$. At higher spin, the hyperdeformed (HD) [2,2] configuration becomes yrast. The transition quadrupole moments $Q_t$ and $\gamma$-deformations of the plotted configurations are presented in Fig. ???. The density distributions of the configurations of interest are presented in Fig. 4.19, Fig. 4.20, Fig. 4.21 and Fig. 4.22 for selected spin values.
The energies of the calculated configurations in $^{28}\text{Si}$ relative to a smooth liquid drop reference $AI(I + 1)$, with the inertia parameter $A = 0.05$.

The self-consistent proton density distributions $^{28}\text{Si}$. for the indicated configuration.
Figure 4.20

The self-consistent proton density distributions $^{28}$Si for the indicated configuration.

Figure 4.21

The self-consistent proton density distributions $^{28}$Si for the indicated configuration.
The self-consistent proton density distributions $^{28}\text{Si}$ for the indicated configuration.

The [0,0]-pr configuration is characterized by substantial quadrupole and hexadecapole deformations and shows the indications of the development of a neck. However, present calculations do not suggest that it could be described as a cluster of two nuclei since the maximum of the density is seen in the central part of the nucleus (Fig. 4.19). This configuration rather well describes both the excitation energies (compare Fig. 4.18 with left panel of Fig. 7 in [179]) and the moments of inertia at experimental prolate bands; the latter is $J^{(1)} \sim 4 \hbar^2/\text{MeV}$ both in experiment [179] and theory.

Based on the comparison of experimental and calculated moments of inertia, the observed $4\hbar$ and $6\hbar$ SD states are most likely associated with the [2,2] configuration. The calculated kinematic moment of inertia of this configuration $J^{(1)} \sim 6.68 \hbar^2/\text{MeV}$, which is nearly constant for a large spin range, is only slightly above the experimental value ($J^{(1)} \sim 6 \hbar^2/\text{MeV}$ [178]). Note that there are large similarities in the predictions of the
properties of oblate, prolate and SD bands obtained in present CRMF calculations and the ones within the antisymmetrized molecular dynamics model of [179]

4.6.2  $^{32}$S nucleus

The SD configurations were predicted in $^{32}$S a long time ago in Refs. [180, 181]. The SD bands built on such structures have been studied both in non-relativistic cranked DFTs based on the Gogny [182, 183] and Skyrme [184, 185] forces and in the CRMF calculations with the NL3 CEDF in Ref. [186]. The detailed structure of the yrast spectra in this nucleus has also been investigated in the cranked Nilsson-Strutinsky (CNS) approach in Ref. [186]. Note that contrary to more microscopic studies which are limited to collective structures, this CNS study considers also terminating/aligned states along the yrast line which is important for a proper description of the yrast line at low and medium spins.

Fig. 4.23 shows the high-spin structures in $^{32}$S. The lowest SD configuration with the structure [2,2] is yrast above spin $I = 10\hbar$. The same result has also been obtained in other models quoted above. Above spin $I = 24\hbar$, the occupation of the lowest $N = 4$ hyperintruder proton and neutron orbitals leads to the HD [21,21] configuration. Note that this induces an unpaired band crossing the consequence of which is the impossibility to trace in the calculations the SD band above $I \sim 23\hbar$ and the HD band below $I \sim 27\hbar$. This problem could be avoided if diabatic orbitals were built using the approach of Ref. [169]; the expected diabatic continuations of the SD [2,2] and HD configurations [21,21] are shown by dotted lines in Fig. 4.23. Note that the CNS calculations of Ref. [186] also suggest that the lowest HD configuration has the [21,21] structure and becomes yrast at
The same as Fig. 4.2 but for $^{32}$S. Dotted lines show expected diabatic continuations of the [2,2] and [21,21] configurations beyond the spin range where the convergence has been obtained similar spins. The same HD configuration has also been obtained in the cranked Skyrme HF calculations of Ref. [184], where the HD band becomes yrast around $I \sim 25\hbar$ in the calculations with SIII and SkM* Skyrme forces.

At spin $I = 0$, the calculated $Q_t$ values for the [2,2] SD configuration are 50% larger than $Q_{t \text{norm}}$ (Fig. 4.24). Therefore, this band would be described as HD. However, at this spin the [2,2] SD configuration is located around 10 MeV above the ground state which prevents its observation. The rotation and the limited angular momentum content in low deformation configurations brings this SD configuration to the yrast line. However, it also triggers the decrease of the collectivity (as measured by $Q_t$) so this configuration is more properly described as SD in the spin range where it is yrast. The occupation of
Figure 4.24

The same as Fig. 4.6 but for $^{32}$S.
the lowest \( N = 4 \) proton and neutron orbitals leading to the [21,21] HD configuration triggers a substantial increase in \( Q_t \); at spin \( I = 31\hbar \) it is 60% larger than \( Q_t^{\text{norm}} \). Density distributions of the [2,2] and [21,21] configurations at spins of interest are shown below.

Note that many [1,1] configurations are of transitional type; they are SD only at very low spins (Fig. 4.24) and are only highly-deformed at higher spins. Truly SD configurations are obtained with additional occupation of the \( N = 3 \) orbital leading to either [2,1] or [1,2] configurations (Fig. 4.24).

Present calculations indicate a large gap between the yrast SD [2,2] configuration and excited configurations in the spin range \( I = 16 - 22\hbar \) (Fig. 4.23). Although this would favor the population of this configuration, all experimental attempts to observe this band undertaken in the beginning of the last decade have failed.

### 4.6.3 \( {}^{50}\text{Cr} \) nucleus

The calculated configurations are shown in Fig. 4.25. Below spin \( I = 14\hbar \), the yrast line is built from the valence space [6,4] configuration. Higher spin terminating configurations ([51,4], [51,31] and [51,41]) are build by means of particle-hole excitations across the \( Z = 28 \) and \( N = 28 \) spherical shell gaps. They dominate the yrast line up to \( I = 31\hbar \). At even higher spin closely lying HD [62,62] and [72,62] configurations are either yrast or close to yrast. Transition quadrupole moments \( Q_t \) and \( \gamma \)-deformations of the calculated configurations are summarized in Fig. 4.26. An example proton density distribution is shown in Fig. 4.27 for the HD [62,62] configuration at \( I = 31\hbar \). Note that neither superde-
formed nor megadeformed configurations show up in the vicinity of the yrast line in this nucleus in the spin range of interest.

![Graph](Figure 4.25)

The same as Fig. 4.2 but for $^{50}\text{Cr}$

### 4.7 Clusterization and molecular structures

One of the main goals of the present study is the search for possible candidates showing clusterization and molecular structures in the near-yrast region of the nuclei under study. Different single-particle states have different spatial density distributions which are dictated by the underlying nodal structure of their wavefunctions (see Fig. 9 in Ref. [14]); the centers of the density distribution are found at the nodes and peaks of the oscillator eigenfunctions. The total density distribution is built as a sum of the single-particle density distributions of occupied single-particle states. Thus, for specific occupations of the single-
Figure 4.26

The same as Fig. 4.6 but for $^{50}$Cr
The self-consistent proton density distributions \(^{50}\text{Cr.}\) for the indicated configuration.

Particle states at some deformations one may expect the effects in the density distributions which could be interpreted in terms of clusterization and molecular structures. Note that the structure of the wavefunctions of the single-particle orbitals is affected by rotation (see discussion in Sec. V of Ref. [14]); this could lead to a modification of the single-particle density distributions (see Fig. 9 in Ref. [14]). For some of the orbitals the effect of rotation on single-particle density distributions is quite substantial, while it has very little impact on the single-particle density distributions for others. This could lead either to the destruction or the emergence/enhancement of the clusterization and molecular structures with rotation.

In the mass region under study, a well-known case of molecular structure is the superdeformed configuration [2,2] in \(^{32}\text{S}\). We can see the development of a neck in its density distribution. According to Refs. [150, 154] the wavefunction of this band contains significant admixture of the molecular \(^{16}\text{O}+^{16}\text{O}\) structure. A similar neck also exists in the HD [21,21] configuration of \(^{32}\text{S}\), but the presence of density depressions at \(z \sim \pm 2\) fm
Figure 4.28

Systematics of the most interesting configurations showing the features of extreme deformation and clusterization.
may suggest more complicated structure than the pair of two $^{16}$O. In addition, the neck is also present in the density distribution of the [31,21] configuration in $^{34}$S but this configuration is characterized by an unusual density distribution with density depression in the highly elongated central region which is surrounded by the region of maximum density (Ref. [176]). Note that the SD configurations, which have the structure of $^{16}$O+$^{16}$O+two valence neutrons in molecular orbitals, have recently been predicted in the AMD+GCM calculations of Ref. [153].

The present study also reveals a number of other interesting molecular structures, as discussed below. We were able to trace some such configurations in an extended spin range starting from spin zero (or from very low spin), at which they are located at 20 – 30 MeV excitation energy above the ground state, up to very high spin where they are either yrast or close to the yrast line. These are the [42,31] and [42,22] MD configurations in $^{38}$Ar, the [31,31] and [41,41] MD configurations in $^{36}$Ar, the [42,42] MD configuration in $^{40}$Ca (Fig. 4.2), the [62,42] MD configuration in $^{42}$Ca, the [62,62] MD configurations in $^{44}$Ti and [52,52] and [421,421] MD configurations in $^{42}$Sc (Fig. 4.12). These examples allowed us to study the impact of rotation on clusterization.

The molecular structures become well pronounced in the [31,31] and [41,41] MD configurations of $^{36}$Ar which are characterized by a well established neck. Figures and details of the discussions can be found in the Ref. [176]. They are also seen in the [42,31] configuration of $^{38}$Ar. Note that in this case the rotation increases the separation of the fragments and makes the neck much more pronounced.
In $^{40}$Ca, the density distribution of the MD [42,42] configuration at spin zero shows a triple-humped structure (top panel of Fig.34 in Ref. [176]). A similar configuration has been analyzed in Ref. [150] and it was concluded that an $\alpha$-cluster interpretation becomes quite fuzzy. Alternatively, one may consider this configuration as a $^{12}$C+$^{16}$O+$^{12}$C chain built of distorted $^{16}$O and $^{12}$C nuclei. The validity of such an interpretation should be verified in the future by comparison with the results of the cluster and/or antisymmetrized molecular (AMD) calculations similar to the ones presented in Ref. [150]. The comparison of the density distribution for this configuration at $I = 0\hbar$ and $I = 25\hbar$ shows that the rotation hinders the tendency for clusterization as seen from the density distributions. Indeed, the central hump becomes less pronounced and the depressions in the density distributions develop in central parts of the left and right segments at $I = 25\hbar$ (bottom panel of Fig.34 in Ref. [176]).

Similar effects are also seen in the MD [42,22] configuration of $^{38}$Ar which could be considered as the MD [42,42] configuration of $^{40}$Ca with two proton holes in the $N = 3$ orbitals. The addition of two neutrons to the MD [42,42] configuration of $^{40}$Ca creates the MD [62,42] configuration in $^{42}$Ca which has the features in the proton density distribution (see Figs. 33(c) and 33(d) in the Ref. [176]) similar to the ones seen in Fig.34 of Ref. [176].

These results show that in the few configurations discussed above the rotation tries to suppress the features of the density distribution which could be attributed to the clusterization. However, the density modifications induced by rotation definitely depend on the nucleonic configuration. For example, the density distribution of the [62,62] configura-
tion in $^{48}$Cr is modified only modestly by rotation. Note that this configuration does not show the features typical for clusterization. On the other hand, with increasing spin the separation of the fragments becomes larger and the neck becomes more pronounced in the [42,31] configuration of $^{38}$Ar and the [421,421] configuration of $^{42}$Sc.

Another interesting case of possible clusterization is the [62,62] MD configuration in $^{44}$Ti. Three fragments are clearly seen in the density distribution at $I = 0\hbar$ indicating possible $^{16}$O+$^{12}$C+$^{16}$O chain of nuclei. Note that with rotation the central fragment dissolves but two outer segments became slightly more pronounced. It is interesting that a similar three-fragment structure survives in the [52,52] MD configuration up to very high spins in $^{42}$Sc. This configuration could be considered as built from the [62,62] one in $^{44}$Ti by creating proton and neutron holes in the $N = 3$ orbital.

A very interesting case of molecular structures is seen in the example of the [421,421] MD configuration in $^{42}$Sc (top panel of Fig. 1(a) in the supplemental Material of Ref. [176]). This system could probably be described as a combination of two prolate deformed $^{20}$Ne cores located in tip-to-tip arrangement with an extra proton and neutron.

It is necessary to understand that suggested interpretations of molecular structures are based on the consideration of only density distributions. Their validity should be verified in future by the analysis of the wavefunctions of the underlying configurations (and their overlaps with mean field solutions) obtained in the cluster and/or antisymmetrized molecular calculations similar to the ones presented in Refs. [150, 154].
Figure 4.29

Kinematic ($J^{(1)}$) and dynamic ($J^{(2)}$) moments of inertia of typical SD, HD and MD configurations in indicated nuclei.
4.8 Rotational properties of extremely deformed configurations

The important physical observables characterizing the SD, HD and MD structures are kinematic \( J^{(1)} \) and dynamic \( J^{(2)} \) moments of inertia and transition quadrupole moments \( Q_t \). However, only \( Q_t \) gives direct information on the deformation of the charge distributions and therefore can reveal the true nature of the band. The experimental investigation of the SD bands clearly shows that the \( Q_t \) quantity is measured in dedicated experiments and thus it is available only for a small fraction of the SD bands. Thus in future experiments it will be easier to obtain the information on rotational properties of the bands which are described in terms of kinematic and dynamic moments of inertia using the expressions

\[
J^{(1)}(\Omega_x) = J \left( \frac{dE}{dJ} \right)^{-1} = \frac{J}{\Omega_x}, \tag{4.3}
\]

\[
J^{(2)}(\Omega_x) = J \left( \frac{d^2E}{dJ^2} \right)^{-1} = \frac{dJ}{d\Omega_x}, \tag{4.4}
\]

where

\[
\Omega_x = \frac{dE}{dJ}, \tag{4.5}
\]

defines the rotational frequency and \( E \) and \( J \) are total energy and the expectation value of total angular momentum on the axis of rotation, respectively. Their experimental counterparts are extracted from the observed energies of the \( \gamma \)-transitions within a band according to the prescription given in Sec. 4.1 of Ref. [169]. Note that the kinematic moment of inertia depends on the absolute values of spins, while only the differences \( \Delta I = 2 \) enter the definition of dynamic moment of inertia.

The SD bands observed in the \( A \sim 40 \) mass region are linked to the low-spin level scheme. Thus their spins are known which is exceptional to the majority of the SD bands.
in the nuclear chart. It is quite likely that some SD bands which will be observed in this mass region in the future will follow this pattern. On the contrary, it is expected that the spins of the HD and MD bands will be difficult to define in future experiments. For such bands, only the dynamic moment of inertia will be available for comparison with the results of calculations.

The kinematic and dynamic moments of inertia of the (typically lowest in energy) SD, HD and MD bands are shown in Fig. 4.29 for each nucleus under consideration. The calculated $J^{(1)}$ and $J^{(2)}$ values are shown by solid and open symbols, respectively. Red circles, black squares and blue triangles are used for the SD, HD and MD configurations, respectively. For a majority of the SD and HD bands it is evident that the condition $J^{(1)} \geq J^{(2)}$ is satisfied at medium and high frequencies. As discussed in Ref. [169] this condition is valid for the rotational bands in the unpaired regime. This condition is not valid in the region of unpaired band crossing with weak interaction where $J^{(2)}$ grows rapidly with increasing rotational frequency. This takes place at the highest calculated frequencies in the [2,2] SD configuration of $^{32}$S (Fig. 4.29a), [4,4] SD configuration in $^{40}$Ca (Fig. 4.29e), and [62,62] HD configuration in $^{48}$Cr (Fig. 4.29k). Note also that such a situation is seen at medium spin in the [31,21] HD configuration of $^{34}$S (Fig. 4.29b) and the [51,4] SD configuration of $^{44}$Ca (Fig. 4.29g).

The moments of inertia of the MD bands show three different patterns of behavior. Some of the MD bands undergo a centrifugal stretching that results in an increase of the transition quadrupole moments $Q_t$ with increasing rotational frequency. This process also reveals itself in the moments of inertia: the kinematic moments of inertia are either nearly
constant or slightly increase with increasing rotational frequency, whereas the dynamic moments of inertia show two patterns of behavior. In the first the dynamic moment of inertia is almost the same as the kinematic one at low to medium rotational frequencies while in the second, as rotation increases \( J^{(2)} \) becomes bigger than \( J^{(1)} \) and the difference between them gradually increases with frequency. These are the MD configurations shown in Figs. 4.29e, f, g and i. The pattern of the behavior of the [421,421] MD configuration in \(^{42}\)Sc is very different (Fig. 4.29h); both moments increase with increasing rotational frequency but \( J^{(2)} \geq J^{(1)} \) at all calculated frequencies. Note that this configuration has the most elongated density distribution among those studied here with clear indication of molecular structure (see Sec. 4.3.) The rotational properties of above discussed MD bands are very similar to the HD ones in the \( Z = 40 – 58 \) mass region investigated in Refs. [39, 175]. On the other hand, the [31,31] MD configuration in \(^{36}\)Ar (Fig. 4.29c) and [42,31] MD configuration in \(^{38}\)Ar (Fig. 4.29d) show the relative properties of the two moments similar to the ones seen in the majority of the SD and HD bands shown in Fig. 4.29.

The examples shown in Fig. 4.29 clearly indicate strong dependence of the calculated \( J^{(1)} \) and \( J^{(2)} \) values on the nucleonic configuration and frequency. In most of the cases, at medium and high rotational frequencies there is a correlation between the moments of inertia and deformation so that the moments of inertia increase with increasing deformation. However, there are exceptions to this observation. For example, the dynamic moments of inertia of the [4,4] SD and [41,41] HD configurations in \(^{42}\)Sc are quite similar (see Fig. 4.29h) despite a substantial difference in the transition quadrupole moments (see Fig.
4.13a). An even more striking example is the similarity of the dynamic moments of inertia for the [3,3] SD and [31,31] MD configurations in $^{36}$Ar (Fig. 4.29c). Such similarities are also seen for the kinematic moments of inertia as illustrated by the case of the [52,52] SD and [62,62] HD bands in $^{48}$Cr (Fig. 4.29k). Thus, the decision on the nature of the band (SD, HD or MD) observed in experiment cannot be based solely on the measured values of dynamic or kinematic moments of inertia; only the measurement of the transition quadrupole moment can reveal the true nature of the band.

4.9 Conclusions

A systematic investigation for extremely deformed structures in the $N \sim Z, A \sim 40$ nuclei has been performed in the framework of covariant density functional theory. The goal of this study is to define at which spins such structures become yrast, their properties and to find the configurations showing the fingerprints of clusterization and molecular structures. The conclusions are as follows.

1. Our calculations reveal that the $N = Z$ nuclei are better candidates for the observation of extremely deformed structures as compared with the nuclei which have an excess of neutrons over protons. This result agrees to the studies in the Ref. [39, 175].

2. Because the normal and highly-deformed configurations forming the yrast line at low and medium spins have limited angular momentum content, the extremely deformed structures inevitably become yrast with increasing spin in the nuclei under study. The most important question is at which spin the transition from terminating to extremely deformed configurations takes place, this is basically defined by the maximum spin
which could be built in terminating configurations with a limited number of particle-hole excitations across the respective spherical shell gaps. This spin is quite limited for particle-hole excitations across the proton $Z = 20$ and neutron $N = 20$ spherical shell gaps. As a result, the nuclei most favored for the observation of extremely deformed structures are located in the vicinity of $^{36}$Ar and $^{40}$Ca. For example, present calculations suggest that in $^{36}$Ar the increase of spin above the measured $I = 16\hbar$ state is only possible by the population of the hyperdeformed band. On the contrary, the configurations built on particle-hole excitations across the spherical $N = 28$ and $N = 28$ gaps, which bring a substantial amount of angular momentum, dominate the yrast line at medium spin (up to $I \sim 30\hbar$) in the Cr nuclei. As a result, only at higher spins do extremely deformed configurations become yrast.

3. The underlying single-particle structure of nucleonic configurations with specific nodal structure of the single-particle density distribution leads to a clusterization in the form of molecular structures. The calculations suggest that in some nuclei such structures are either yrast or close to yrast at high spin. Thus, it would be possible to observe these structures with the new generation of $\gamma$-tracking detectors such as GRETA and AGATA in the near future. The calculations with cluster or/and antisymmetrized molecular dynamics models are definitely needed in order to establish the weights of those clusters in the structure of the total wavefunction.

4. The impact of rotation on the density distribution and clusterization (molecular nature) depends sensitively on the nucleonic configuration. The density distributions of
some configurations are weakly affected by rotation. The features for clusterization, present at zero spin, are washed away by rotation in other configurations. However, the clusterization is enhanced by rotation in some specific configurations; with increasing spin the separation of the fragments becomes larger and the neck becomes more pronounced.

5. There is a strong dependence in the calculated kinematic and dynamic moments of inertia on the configuration and frequency. In most of the cases the moments of inertia increase with increasing deformation at medium and high rotational frequencies. However, there are exceptions to this observation. As a result, the decision on the nature of the band (SD, HD or MD) observed in experiment cannot be based solely on the measured values of dynamic or kinematic moments of inertia. The true nature of the band can be given only by the measurement of transition quadrupole moments.
CHAPTER 5

ASSESSING THEORETICAL UNCERTAINTIES IN FISSION BARRIERS OF
SUPERHEAVY NUCLEI

5.1 Introduction

There is a considerable interest in both experimental and theoretical studies of super-heavy elements (SHE), which are characterized by the extreme values of proton number $Z$ (see Refs. [40, 41, 42] and references therein). Currently available experimental data have reached the proton number $Z = 118$ [187, 188] and dedicated experimental facilities such as the Dubna Superheavy Element Factory will hopefully allow to extend the region of SHE up to $Z = 120$ and for a wider range of neutron numbers for lower $Z$ values.

The stability of SHEs is defined by the fission barriers. The experimental studies of SHEs are based on the observation of $\alpha$-decays. As a consequence, only SHEs with spontaneous fission half-lives $\tau_{SF}$ longer than the half-lives $\tau_{\alpha}$ for the $\alpha$-decays could be observed in experiment. An additional limit is set up by the fact that only $\alpha$-decays longer than $10 \mu s$ can be observed in an experiment. Therefore it is important to study the fission barriers in SHEs. The height of the fission barrier, $B_f$, which is the difference in the energies of the respective saddle in the potential energy surface (PES) and the ground state, is one of most important quantities. It defines the survival probability of SHEs synthesized in heavy-ion reactions and impacts the spontaneous fission half-lives. The later is impor-
tant for an understanding of the competition between the fission process and $\alpha$ particle emission.

Fission barriers have been extensively studied in different theoretical frameworks; these studies have been reviewed in Refs. [40, 189]. The theoretical frameworks used are the microscopic+macroscopic method [190], non-relativistic density functional theories (DFT) based on finite range Gogny [191] and zero range Skyrme forces [5], and covariant density functional theory (CDFT) [7]. A systematic investigation of the fission barriers in the $Z = 112 – 120$ SHE has been performed in the triaxial relativistic mean field plus BCS (RMF+BCS) framework with the NL3* functional in Ref. [78] and potential energy surfaces in the $(\beta, \gamma)$ plane for the even-even isotopes in the $\alpha$-decay chains of the $^{208}120$ and $^{300}120$ nuclei have been calculated in the triaxial relativistic Hartree-Bogoliubov approach with the DD-PC1 functional in Ref. [192]. Theoretical investigations require an estimate of theoretical uncertainties. This becomes especially important when one deals with the extrapolations beyond the known regions, as for example in particle number or deformation. This issue has been discussed in detail in Refs. [26, 193] and in the context of global studies within CDFT in the introduction of Ref. [3]. In the CDFT framework, the studies of theoretical uncertainties have so far been restricted to the ground state properties. Systematic theoretical uncertainties and their sources have been studied globally for the ground state physical observables in Refs. [3, 42, 72, 117, 194, 195].

We have undertaken the systematic investigation of the fission barriers in $Z = 112–120$ nuclei in the framework of covariant density functional theory. In my study, I have considered also the systematic theoretical uncertainties in the description of fission barriers.
They emerge from the underlying theoretical approximations. In the DFT framework, there are two major sources of these approximations, namely, the range of interaction and the form of the density dependence of the effective interaction [5, 23]. In the relativistic case point coupling and meson exchange models have an interaction of zero and of finite range, respectively [7, 19, 20, 24]. The density dependence is introduced either through an explicit dependence of the coupling constants [19, 20, 25] or via non-linear meson couplings [23, 24]. This ambiguity in the definition of the range of the interaction and its density dependence leads to several major classes of the covariant energy density functionals (CEDF) which were discussed in Ref. [3] and in the Chapter 1 of this dissertation.

As a consequence, in the present study, we focus on the uncertainties related to the choice of the energy density functional. We have defined the theoretical uncertainty for a given physical observable (which we call in the following “spreads”) via the spread of theoretical predictions as [3]

$$\Delta O(Z, N) = |O_{max}(Z, N) - O_{min}(Z, N)|,$$

(5.1)

where $O_{max}(Z, N)$ and $O_{min}(Z, N)$ are the largest and smallest values of the physical observable $O(Z, N)$ obtained within the set of CEDFs under investigation for the $(Z, N)$ nucleus. Note that these spreads are only a crude approximation to the systematic theoretical errors discussed in Ref. [193] since they are obtained with a very small number of functionals which do not form an independent statistical ensemble. Also, these systematic errors are not well defined in unknown regions of the the nuclear chart or deformation.
since systematic biases of theoretical models could not be established in these regions in the absence of experimental data and/or an exact theory.

The state-of-the-art energy density functionals which we have considered for our study are: NL3*[24], DD-ME2 [19], DD-MEδ [21], DD-PC1 [20] and PC-PK1 [88]. An additional source of theoretical uncertainties is related to the details of the fitting protocol of these functionals such as the choice of experimental data and the selection of adopted errors. It applies only to a given functional and the related theoretical uncertainties are called statistical [193, 196].

We have restricted our investigation to inner fission barriers. There are several reasons behind this choice. A systematic investigation of Ref. [78] within the RMF+BCS framework with the NL3* CEDF has shown that the fission barriers of many SHEs have a double-humped structure in axial reflection-symmetric calculations. The inclusion of octupole and triaxial deformations lowers outer fission barriers by 2 to 4 MeV so that they are only around 2 MeV in height with respect to the superdeformed minimum. A similar situation exists also in Gogny DFT calculations (Ref. [197]). In addition, similar to actinides (Ref. [198]) symmetry unrestricted calculations which combine octupole and triaxial deformations simultaneously could further reduce the heights of outer fission barriers. These low barriers would translate into a high penetration probability for spontaneous fission such that most likely these superdeformed states are metastable and that outer fission barriers do not affect substantially the fission process in total. Note also that outer fission barriers do not exist in most of the SHEs with $Z \geq 110$ in Skyrme DFT calculations [77, 199]. An accurate description of outer fission barriers would require the use of a symmetry unrestricted
RHB code. Unfortunately, the computational cost for such an investigation of theoretical uncertainties in the description of outer fission barriers is prohibitively high. On the other hand, it is reasonable to expect that theoretical uncertainties in the description of outer fission barriers have to be of similar magnitude to the ones for inner fission barriers.

Despite these limitations this investigation provides for a first time a systematic analysis of theoretical uncertainties in the description of fission barriers within the CDFT framework. It also gives an understanding about which observables/aspects of many-body physics can be predicted with a higher level of confidence than others for density functionals of the given type. Moreover, it is expected that they will indicate which aspects of the many-body problem have to be addressed with more care during the development of next generation EDFs. This study also represents an extension of our previous studies of theoretical uncertainties in the global description of the ground state properties of the nuclei from the proton to neutron drip lines [3, 72, 117, 195], superheavy nuclei [42], and rotating nuclei [56].

5.2 The details of numerical calculation

In the present study we have used the triaxial relativistic Hartree-Bogoliubov (TRHB) framework to study the fission barriers and related theoretical uncertainties. The numerical details are as follows:

- TRHB equations are solved in a parity conserving Cartesian oscillator basis [63, 75] using five CEDFs NL3* [24], DD-ME2 [19], DD-MEδ [21], DD-PC1 [20] and PC-PK1 [88]. These state-of-the-art functionals represent the essential types of CEDFs
used in the literature (for more details see the discussion in Sect. II of Ref. [3] and the introduction to Ref. [42]). Moreover, their performance and the related theoretical uncertainties have recently been analyzed globally in Refs. [3, 89, 195, 194] and in particular in superheavy nuclei in Ref. [42]. They are characterized by an improved accuracy of the description of experimental data as compared with the previous generation of CEDFs.

• In order to avoid uncertainties connected with the size of the pairing window, we use the separable form of the finite range Gogny pairing interaction introduced by Tian et al.[68]. As follows from the RHB studies with the CEDF NL3* of odd-even mass staggerings, moments of inertia and pairing gaps, the Gogny D1S pairing and its separable form work well in the actinides (Refs. [3, 56, 170]). The weak dependence of its pairing strength on the CEDF has been seen in the studies of pairing and rotational properties of deformed actinides in Refs. [56, 57], of pairing gaps in spherical nuclei in Ref. [3] and of pairing energies in Ref. [117]. Thus, the same pairing strength is used also in the calculations with DD-PC1, DD-ME2, DD-MEδ, and PC-PK1.

• TRHB calculations are enormously time consuming when compared to the axial RHB calculations. Thus, we restricted the TRHB calculations to a selected set of the \( Z = 112 - 120 \) nuclei. These nuclei are located mostly in the region where extensive experimental studies have already either been performed or will be performed in a foreseeable future. Even then the calculations of full potential energy surfaces (PES)
are numerically prohibitive for the $N_F = 20$ fermionic basis. However, the topology of the PESs obtained in the TRHB calculations with the truncation of the fermionic basis at $N_F = 16$ and $N_F = 20$ is the same. Thus, full PESs have been calculated only with the $N_F = 16$ fermionic basis. These results define the positions and the energies of axial and triaxial saddles. Afterwards, they are corrected for the $N_F = 20$ fermionic basis by performing the TRHB calculations with the $N_F = 20$ fermionic basis in the spherical/normal deformed minimum and at a few grid points near the saddle points.

5.3 Systematic theoretical uncertainties in the description of inner fission barriers in triaxial RHB calculations.

![Figure 5.1](image)

Potential energy surfaces of the $^{300}_{120}$ nucleus as obtained in TRHB calculations with indicated CEDF.
Figure 5.2
Potential energy surfaces of the $^{300}120$ nucleus as obtained in TRHB calculations with indicated CEDF.

Figure 5.3
Potential energy surfaces of the $^{300}120$ nucleus as obtained in TRHB calculations with indicated CEDF.
Figure 5.4

Potential energy surfaces of the $^{300}_{120}$ nucleus as obtained in TRHB calculations with indicated CEDF.

Figure 5.5

Potential energy surfaces of the $^{300}_{120}$ nucleus as obtained in TRHB calculations with indicated CEDF.
The systematic investigation of the heights of inner fission barriers in superheavy nuclei performed within the RMF+BCS approach with the NL3* CEDF in Ref. [78] has revealed that triaxial deformation lowers the heights of the inner fission barriers in a number of nuclei; this is especially pronounced in the vicinity of $Z = 120$ and $N = 184$ particle numbers (see Table V in Ref. [78]).

We concentrate on the selected set of the $Z = 112 - 120$ superheavy nuclei which will be in the focus of experimental studies within the next few decades. In the selection of nuclei we focus on the nuclei in which the triaxial saddle is expected to be the lowest in energy in the region of interest. According to systematic studies in the RMF+BCS framework with the CEDF NL3* of Ref. [78], these are the nuclei in the vicinity of the $Z = 120$ and $N = 184$ lines. On the contrary, the axial saddles are the lowest in energy in the nuclei which are away from these lines. For example, this takes place for $N \leq 174$ in the $Z = 112, 114, 116$ nuclei (see Ref. [78]). Triaxial RHB calculations for the $(Z = 112, N = 164), (Z = 112, N = 172), (Z = 114, N = 166)$ and $(Z = 114, N = 172)$ nuclei confirm this observation of Ref. [78] for all CEDFs employed in the present study.

The dependence of the potential energy surfaces on the CEDF is illustrated in Fig. 5.1, Fig. 5.2, Fig. 5.3, Fig. 5.4 and Fig. 5.5 for $^{300}120$ nuclei. The similar for $^{284}112$ nuclei are illustrated in the Fig. 5.6, Fig. 5.7, Fig. 5.8, Fig. 5.9 and Fig. 5.10. These PES are characterized by a complicated topology. The PES are shown in the order of decreasing height of the inner fission barrier. The energy difference between two neighboring equipotential lines is equal to 0.5 MeV. The PES reveals some typical triaxial saddles. In the figures the
Figure 5.6

Potential energy surfaces of the $^{284}_{112}$ nucleus as obtained in TRHB calculations with indicated CEDF.

Figure 5.7

Potential energy surfaces of the $^{284}_{112}$ nucleus as obtained in TRHB calculations with indicated CEDF.
Figure 5.8
Potential energy surfaces of the $^{284}_{112}$ nucleus as obtained in TRHB calculations with indicated CEDF.

Figure 5.9
Potential energy surfaces of the $^{284}_{112}$ nucleus as obtained in TRHB calculations with indicated CEDF.
Potential energy surfaces of the $^{284}_{112}$ nucleus as obtained in TRHB calculations with indicated CEDF.

Ax, Ax-Tr, Tr-A and Tr-B saddles are shown by blue/red circles, diamonds, triangles, and squares, respectively.

For example, in the nucleus $^{300}_{120}$, the saddles are located at $(\beta_2 \sim 0.32, \gamma \sim 21^\circ)$, $(\beta_2 \sim 0.43, \gamma \sim 33^\circ)$, and $(\beta_2 \sim 0.49, \gamma \sim 24^\circ)$ for the functionals DD-ME2, PCPK1, NL3* and DD-PC1. The later two are also visible in the CEDF DD-ME$\delta$. However, the first one is shifted to smaller $\beta_2$ and $\gamma$ deformations, namely, to $(\beta_2 \sim 0.20, \gamma \sim 15^\circ)$.

For all functionals except DD-ME$\delta$ the axial saddle is higher in energy by roughly 0.5 MeV than the triaxial saddle at $(\beta_2 \sim 0.32, \gamma \sim 21^\circ)$ and by approximately 1.5 MeV than the triaxial saddles at $(\beta_2 \sim 0.43, \gamma \sim 33^\circ)$ and $(\beta_2 \sim 0.49, \gamma \sim 24^\circ)$. The PES of the DD-ME$\delta$ functional has a completely different topology. Although the $(\beta_2 \sim 0.20, \gamma \sim 15^\circ)$ saddle is lower in energy than the axial saddle by approximately 1 MeV, the axial
saddle is located only $\sim 0.2$ MeV below the triaxial saddles at $(\beta_2 \sim 0.33, \gamma \sim 25^\circ)$ and $(\beta_2 \sim 0.45, \gamma \sim 33^\circ)$.

The presence of these saddles leads to several fission paths which have been discussed in detail in Ref. [78]. Although this discussion is based on RMF+BCS results with NL3*, we found that it is still valid for the TRHB results with DD-ME2, PCPK1, NL3* and DD-PC1. This is because for a given functional the topology of PES obtained in triaxial RMF+BCS and RHB calculations is similar. The situation is different for DD-ME$\delta$ which has an axial saddle located at $\beta_2 \sim 0.13$. Thus, the fission path will proceed from the oblate minimum via the triaxial saddle at $(\beta_2 \sim 0.20, \gamma \sim 0.15)$ which has a low excitation energy of only 3 MeV.

As shown in Ref. [78], the axial saddle becomes energetically more favored as compared with triaxial saddles on moving away from the particle numbers $Z = 120$ and $N = 184$. This is clearly seen in the nucleus $^{284}_{112}$, in which the axial saddle at $\beta_2 \sim 0.32$ is lower in energy than the triaxial saddles located around $(\beta_2 \sim 0.38, \gamma \sim 34^\circ)$ and $(\beta_2 \sim 0.47, \gamma \sim 26^\circ)$. This feature is also seen in Fig. 4 of Ref. [78] which compares the results for selected $Z = 112, 114$, and 116 nuclei obtained in the RMF+BCS calculations with NL3*.

To simplify the further discussion we follow the notation of Ref. [78] and denote the axial saddle as ‘Ax’, the triaxial saddle with $(\beta_2 \sim 0.3, \gamma \sim 10^\circ)$ as ‘Ax-Tr’, the triaxial $(\beta_2 \sim 0.4, \gamma \sim 35^\circ)$ saddle as ‘Tr-A’ and the triaxial saddle with $(\beta_2 \sim 0.5, \gamma \sim 22^\circ)$ as ‘Tr-B’. Although the positions of these saddles move somewhat in the deformation plane.
with the change of proton and neutron numbers, they appear in the majority of nuclei under study.

Fig. 5.11 summarizes the results of the calculations for the inner fission barrier heights. The DD-ME2 and DD-MEδ functionals provide the highest and the lowest fission barriers among those obtained in the calculations with five CEDFs. The results of the calculations with the CEDFs NL3*, DD-PC1 and PC-PK1 are located in between of these two extremes. Note that these three functionals have been benchmarked in the actinides in Refs. [78, 192, 198, 200] where they provide a good description of experimental data.

![Figure 5.11](image)

The heights of inner fission barriers as obtained in the TRHB calculations with indicated CEDFs.
Fig. 5.11 clearly shows that different functionals are characterized by different isotopic and isotonic dependencies for the inner fission barrier heights. As a result, the functionals, which give similar results in one part of the \((Z, N)\) plane, could provide substantially different results in another. This leads to the spreads in the predictions of the inner fission barrier heights which are presented in Figs. 5.12, Figs. 5.13, Figs. 5.14, Figs. 5.15 and 5.16, 5.17, 5.18, 5.19. The spread is defined as

\[
\Delta E^S(Z, N) = |E^S_{\text{max}}(Z, N) - E^S_{\text{min}}(Z, N)|
\]  

(5.2)

where, for given \(Z\) and \(N\) values, \(E^S_{\text{max}}(Z, N)\) and \(E^S_{\text{min}}(Z, N)\) are the largest and smallest energies of the saddles obtained with the set of functionals NL3*, DD-ME2, DD-MEδ, DD-PC1, and PC-PK1.

The strongest correlation between these spreads is observed for the ‘Ax’ and ‘Ax-Tr’ saddles; this is seen both for the set of four (Fig. 5.12 and Fig. 5.13) and the set of three (Fig. 5.16 and Fig. 5.17) functionals. This is because these saddles are closely located in the deformation plane so that the change in the energy of the ‘Ax’ saddle affects in a similar way the energy of the ‘Ax-Tr’ saddle. The correlations in the spreads of the energies of the ‘Ax’ saddle on one hand and the ‘Tr-A’ and ‘Tr-B’ saddles on the other hand depends on how many functionals are used in the analysis. On average, they are strongly correlated for the set of the DD-PC1, NL3* and PC-PK1 functionals (compare Fig. 5.16, Fig. 5.18 and Fig. 5.19) which have large similarities in the topology of PESs and for which the \(\Delta E^S\) spreads are typically below 2 MeV. Note that these three functionals successfully describe
experimental fission barriers in the actinides [192, 200, 201]. These correlations decrease with the addition of the functionals DD-ME$\delta$ and DD-ME2; the $\Delta E^s$ spreads are typically smaller for the ‘Tr-A’ and ‘Tr-B’ saddles as compared with the ‘Ax’ one (compare Fig. 5.12, Fig. 5.14, Fig. 5.15).

Figure 5.12

The spreads of the energies of triaxial saddles for a selected set of nuclei as a function of $Z$ and $N$.

It is important that the spreads for the axial ‘Ax’ saddles and the lowest in energy saddles are strongly correlated (compare Fig. 5.12 and Fig. 5.15 with Fig. 5.16 and Fig. 5.19). This also suggests that for other regions of the nuclear chart, not covered by the present TRHB calculations, the spreads in inner fission barrier heights obtained in the axial RHB calculations could be used as a reasonable estimate of the spreads which would be obtained in the calculations with triaxiality included.
Figure 5.13
The spreads of the energies of triaxial saddles for a selected set of nuclei as a function of $Z$ and $N$.

Figure 5.14
The spreads of the energies of triaxial saddles for a selected set of nuclei as a function of $Z$ and $N$.

Figure 5.15
The lowest in energy saddles for a selected set of nuclei as a function of $Z$ and $N$. 

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Spreads of the inner fission barrier heights [MeV]

Figure 5.16
The same as in Fig. 5.12 excluding DD-ME2 and DD-MEδ CEDFs.

Figure 5.17
The same as in Fig. 5.13 excluding DD-ME2 and DD-MEδ CEDFs.

Figure 5.18
The same as in Fig. 5.14 excluding DD-ME2 and DD-MEδ CEDFs.
5.4 Comparison of fission barriers in different models

Fig. 5.20 shows the heights of inner fission barriers of the $Z = 112 - 120$ superheavy nuclei for various relativistic and non-relativistic models. Note that the TRHB results in a few $N \sim 166$ and $N = 172$ nuclei and the trends of the evolution of PES with particle number allow to firmly establish the axial symmetric nature of the lowest saddle in the $Z = 112$ and 114 nuclei (as well as in $Z = 116$ nuclei for the NL3* and DD-ME2 functionals) for neutron numbers between 164 and 172. For some of these nuclei, we use axial RHB results when the TRHB results are not available. The position of the inner fission barrier saddle in deformation space varies as a function of particle number. Thus, the lowest saddles are labelled by ‘Ax’, ‘Ax-Tr’, ‘Tr-A’ and ‘Tr-B’. The results of triaxial RMF+BCS calculations are taken from Ref. [78]. The results of Skyrme DFT calculations with SkM* have been taken from Ref. [199]. The results of the MM calculations are taken from Ref. [202] (labeled as ‘MM (Möller)’) and Ref. [203] (labeled as ‘MM (Kowal)’). While providing similar predictions in the actinides, they do extrapolate in very different ways.
to the superheavy region. Their predictions vary significantly and the inner fission barrier heights found within these models can differ by up to 6 MeV. The substantial differences in the predictions of the two macroscopic + microscopic (MM) calculations are in particular surprising. Unfortunately, at present, there are only very few experimental data unless available on fission barriers in superheavy elements and they are not reliable enough to distinguish between theoretical predictions of the various models (see discussion in Ref. [78]).

![Figure 5.20](image)

**Figure 5.20**

Inner fission barrier heights $B_f$ as a function of the neutron number $N$.

Fig. 5.20 also compares the energies of the lowest inner fission barriers obtained in tri-axial RMF+BCS (Ref. [78]) and RHB (present study) calculations with the CEDF NL3*. Pairing correlations are treated in these two calculations in a very different way. Monopole
pairing with a finite pairing window is used in the RMF+BCS calculations of Ref. [78]. Its strength is adjusted to the “empirical” pairing gaps of Ref. [204]. In the RHB calculations, the separable form of the finite range Gogny pairing interaction [68] is used. The differences in the calculated inner fission barriers seen in Fig. 5.20 are (i) due to different extrapolation properties of these two types of pairing on going from actinides to the superheavy region and (ii) due to the dependence of fission barrier heights on the pairing window used for the monopole force [205]. Because of these reasons the inner fission barriers are found to be roughly 1 MeV higher in the RHB results than in the RMF+BCS calculations for \( N \leq 174 \) \((N > 176)\). For these neutron numbers, the RHB results come closer to the mic-mac model predictions ‘MM (Kowal)’. However, the difference between the TRHB and RMF+BCS results decreases at higher \( N \). Note that for the \( Z = 118 \) and 120 nuclei the TRHB results are close to the ‘MM (Kowal)’ results. The present analysis based on a set of the state-of-the art CEDFs as well as the comparison with other models (shown in Fig. 5.20) indicates substantial theoretical uncertainties in isotopic and isotonic trends for the inner fission barriers, even for the functionals which are benchmarked in the actinides. In addition, these uncertainties have a “chaotic” component which randomly changes from nucleus to nucleus. These uncertainties will definitely affect the calculated spontaneous fission half-lives by many orders of magnitude. This fact is important not only for our understanding of SHE’s but also for fission recycling in neutron star mergers [206]. The later process will be definitely affected by the increased (as compared with the actinides) uncertainties of the inner fission barrier heights seen in neutron-rich nuclei.
5.5 Conclusions

The systematic investigation of theoretical uncertainties in the predictions of inner fission barrier heights in SHEs have been carried out using state-of-art covariant energy density functionals, namely NL3*, DD-ME2, DD-MEδ, DD-PC1, and PC-PK1. The conclusions of the study are as follows:

- Systematic theoretical uncertainties in the predictions of inner fission barriers and their propagation towards unknown regions of higher $Z$ values and of more neutron-rich nuclei have been quantified. These uncertainties are substantial in SHEs. It is clear that the differences in the basic model assumptions such as a range of the interaction and the form of the density dependence together with the different fitting protocols based only on nuclear matter and bulk properties data lead to these uncertainties.

- Systematic theoretical uncertainties in the inner fission barrier heights do not form a smooth function of proton and neutron numbers; there is always a random component in their behavior. This is a consequence of the fact that fission barrier height is the difference in the energies between the ground state and saddle point. Any differences in the predictions of their energies, which are not acting coherently as a function of proton and neutron numbers, will lead to this random component.

- Benchmarking of the functionals to the experimental data on fission barriers in the actinides allows reduction of the theoretical uncertainties for the inner fission barriers of unknown SHEs. However, even then they increase on moving away from
the region where benchmarking has been performed. This feature is seen not only for different CEDFs but also for different classes of the models such as microscopic+macroscopic and non-relativistic DFTs. The resulting uncertainties in the heights of inner fission barriers will result in uncertainties of many orders of magnitude for spontaneous fission half-lives. The increased theoretical uncertainties in the fission barriers of neutron-rich SHEs could have a substantial impact on fission recycling modeling in r-process simulations of neutron-star mergers.

- Comparing different functionals one can see that the results (including the topology of the PES) obtained with DD-MEδ differ substantially from the results of other functionals. The heights of the inner fission barriers obtained with this functional are significantly lower than the experimental estimates in the $Z = 112 - 116$ nuclei and the values calculated in all other models. In addition, this functional does not lead to octupole deformation in those actinides which are known to be octupole deformed [194]. Thus, this functional is not recommended for future investigations in the actinides and superheavy nuclei in spite of the fact that it provides a good description of masses and other ground state observables in the $Z \leq 82$ nuclei [3].

The analysis of the description of fission barrier heights is frequently performed in terms of the parameters which are related to bulk properties (see, for example, the discussion in Ref. [189]). However, this is only part of the physics which affects the heights of fission barriers. Indeed, it is well known that in actinides the lowering of the inner and outer fission barriers due to triaxial and octupole deformations is caused by relevant
changes in the single-particle density which affect the shell correction energy [78, 202]. Substantial differences in the predictions of the ground state deformations by the state-of-the-art CEDFs along the $Z = 120$ and $N = 184$ lines (see Ref. [42]) are also caused by the differences in the underlying single-particle structure. The differences among the models in the single-particle structure of superheavy nuclei are substantially higher than in the region of known nuclei [42, 207]. It is clear that this is one of the major contributors to the systematic theoretical uncertainties in the description of inner fission barriers. A further improvement in the description of the single-particle energies within DFT is needed in order to reduce the systematic theoretical uncertainties in the description of fission barriers.
CHAPTER 6
CONCLUSIONS

In this dissertation, covariant density functional theory (CDFT) has been applied to different physical properties of ground and excited states in atomic nuclei. The major conclusions of the three projects are:

- In the first project, CDFT has been applied to axially symmetric systems. The aim of this project is the global assessment of the accuracy of the description of the ground state properties of even-even nuclei and the estimate of \textit{systematic theoretical uncertainties} in known regions of the nuclear chart and their propagation towards the neutron drip line. Large-scale axial relativistic Hartree-Bogoliubov (RHB) calculations were performed for all $Z \leq 104$ even-even nuclei between the two-proton and two-neutron drip lines with the four modern covariant energy density functionals NL3*, DD-ME2, DD-ME$\delta$ and DD-PC1. The physical observables of interest include the binding energies, two-particle separation energies, charge quadrupole deformations, isovector deformations, charge radii, neutron skin thicknesses and the positions of the two-proton and two-neutron drip lines. The detailed comparison with available experimental data has been performed and the predictions and uncertainties for neutron-rich systems have been quantified.
In the second project, CDFT has been applied to rotating systems. A systematic search for extremely deformed and clustered structures in the $N \sim Z$ nuclei of the $A \sim 40$ mass region has been performed for the first time in the framework of covariant density functional theory. At spin zero such structures are located at high excitation energies which prevents their experimental observation. The rotation acts as a tool to bring these exotic shapes to the yrast line or its vicinity so that their observation could become possible with a future generation of $\gamma$–tracking (or similar) detectors such as GRETA and AGATA. The major physical observables of such structures such as transition quadrupole moments as well as kinematic and dynamic moments of inertia, the underlying single-particle structure and the spins at which they become yrast or near yrast are defined. The search for the fingerprints of clusterization and molecular structures is performed and the configurations with such features are discussed. The best candidates for observation of extremely deformed structures are identified in Ref. [176].

Finally, in the third project, CDFT has been applied to triaxial systems. Theoretical uncertainties in the predictions of inner fission barrier heights in superheavy elements have been investigated in a systematic way for a set of state-of-the-art CEDFs. The systematic uncertainties have been quantified and they are substantial in superheavy elements and their behavior as a function of proton and neutron numbers contains a large random component. The benchmarking of the functionals to the experimental data on fission barriers in the actinides allows to reduce the systematic theoretical uncertainties for the inner fission barriers of unknown super-
heavy elements. However, even then they on average increase on moving away from
the region where benchmarking has been performed. In addition, a comparison with
the results of non-relativistic approaches is performed in order to define full system-
atic theoretical uncertainties over the state-of-the-art models. Even for the models
benchmarked in the actinides, the difference in the inner fission barrier height of
some superheavy elements reaches $5 - 6$ MeV. This uncertainty in the fission barrier
heights will translate into huge (many tens of the orders of magnitude) uncertainties
in the spontaneous fission half-lives.
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