Hyperheavy nuclei in axial relativistic Hartree-Bogoliubov calculations

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A Thesis
Submitted to the Faculty of
Mississippi State University
in Partial Fulfillment of the Requirements
for the Degree of Master of Science
in Physics
in the Department of Physics and Astronomy

Mississippi State, Mississippi

August 2018
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The existence of highest proton numbers at which the nuclear landscape cease to exist, the end of the periodic table of elements and the limits of the existence of the nuclei are some of the difficult questions to answer. To explore those questions, we investigated hyperheavy nuclei ($Z \geq 126$) using covariant density functional theory. We demonstrate the existence of three regions of spherical hyperheavy nuclei centered around ($Z \sim 138, N \sim 230$), ($Z \sim 156, N \sim 310$) and ($Z \sim 174, N \sim 410$). Also, we explored other properties of hyperheavy nuclei such as octupole deformation, alpha decay half lives, chemical potential, etc.

Key words: potential energy surface, ground state deformation, oblate deformation, octupole deformation, fission barriers, chemical potential, hexadecapole deformation, alpha-decay half-lives
DEDICATION

To my father Netra Prasad Gyawali, mother Yashoda Gyawali and brother Asim Gyawali
ACKNOWLEDGEMENTS

I would like to thank my supervisor Professor Anatoli Afanasjev for his guidance and support during my studies. He helped me to build my character as well as my academic skills. I would like to thank Sylvester Agbemava. He helped me in all aspects of research and was always there when I needed advice. Finally, I would like to thank Department of Physics and Astronomy at Mississippi State for all the resources I got, friends I made and the memories that I will cherish.
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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
**PES**  Potential Energy Surface
**SHE**  Super Heavy Element
**RHB**  Relativistic Hartree-Bogoliubov
CHAPTER I

INTRODUCTION

The investigation of superheavy elements (SHE) remains one of the most important sub-fields of low-energy nuclear physics [1]. The element Og with proton number \( Z = 118 \) is the highest \( Z \) element observed so far [2]. Although future observation of the elements in the vicinity of \( Z \approx 120 \) seems to be feasible, this is not the case for the elements with \( Z \) beyond 122. Considering also that the highest spherical shell closure in SHE is predicted at \( Z = 126 \) in Skyrme density functional theory (DFT) [3], it is logical to name the nuclei with \( Z > 126 \) as hyperheavy [4, 5]. The properties of such nuclei are governed by increased Coulomb repulsion and single-particle level density; these factors reduce the localization of shell effects in particle number [5].

Although hyperheavy nuclei have been studied both within DFTs [4, 5, 6, 7, 8, 9] and phenomenological [10, 11, 12] approaches, the majority of these studies have been performed only for spherical shapes of the nuclei. This is a severe limitation which leads to misinterpretation of the physical situation in many cases since there is no guarantee that spherical minimum in the potential energy surface exists even in the nuclei with relative large spherical shell gaps (see discussion in Ref. [13]). In addition, the stability of hyperheavy nuclei against spontaneous fission could not be established in the calculations
restricted to spherical shape. The effects of axial deformations in hyperheavy nuclei are considered only in Refs. [7, 14] (only few nuclei) and in Ref. [9], respectively. However, these studies are limited in the scope. Moreover, according to the present study, the deformation range employed in Ref. [9] is not sufficient for $Z \geq 130$ nuclei.

The investigation of hypernuclei is also intimately connected with the establishments of the limits of both the nuclear landscape and periodic table of elements. The limits of nuclear landscape at the proton and neutron drip lines and related theoretical uncertainties have been extensively investigated in a number of theoretical frameworks but only for the $Z < 120$ nuclei [15, 16, 17]. The atomic relativistic Hartree-Fock [18] and relativistic Multi-Configuration Dirac-Fock [19, 20] calculations indicate that the periodic table of elements terminates at $Z = 172$ and $Z = 173$, respectively. However, at present it is not even clear whether such nuclei are stable against fission. In addition, Refs. [18, 19, 20] employ phenomenological expression for charge radii and its validity for the $Z \sim 172$ nuclei is not clear.

To address these deficiencies in our understanding of hyperheavy nuclei the systematic investigation of even-even nuclei from $Z = 122$ up to $Z = 180$ is performed within the axial relativistic Hartree-Bogoliubov (RHB) framework employing the DD-PC1 covariant energy density functional [21]. This functional provides good description of the ground state and fission properties of known even-even nuclei [15, 22].
CHAPTER II

FORMALISM : RELATIVISTIC HARTREE-BOGOLIUBOV THEORY

2.1 The relativistic mean-field Lagrangian and the equations of motion

The nucleus is treated as a system of Dirac nucleons in relativistic mean field theory. These nucleons interact by the exchange of mesons within an electromagnetic field which can be described by an effective Lagrangian. The observable properties of the nuclei are described with the set of meson fields and electromagnetic field. The isoscalar scalar $\sigma$ meson, isoscalar vector $\omega$ meson, and the isovector $\rho$ meson are the smallest set of meson fields required to describe these properties [23, 24, 25, 26, 27].

The Lagrangian density for the Relativistic Hartree-Bogoliubov (RHB) model is given by

$$\mathcal{L} = \mathcal{L}_n + \mathcal{L}_m + \mathcal{L}_{int}$$

(2.1)

where $\mathcal{L}_n$ is the Lagrangian for free nucleons, $\mathcal{L}_m$ is the Lagrangian of the free meson and electromagnetic field, $\mathcal{L}_{int}$ is the Lagrangian due to interaction between the nucleons and the mesons.

Here, the Lagrangian for free nucleons is given by

$$\mathcal{L}_n = \bar{\psi}(i\gamma^\mu - m)\psi$$

(2.2)

where $m$ is the mass of the bare nucleon and $\psi$ is a Dirac spinor.
The Lagrangian for the free meson and electromagnetic field is given by

\[
\mathcal{L}_m = \frac{1}{2} \partial_{\mu} \sigma \partial^{\mu} \sigma - \frac{1}{2} m_{\sigma}^2 \sigma^2 - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_{\omega}^2 \omega_{\mu} \omega^{\mu} - \frac{1}{4} \tilde{R}_{\mu\nu} \tilde{R}^{\mu\nu} + \frac{1}{2} m_{\rho}^2 \tilde{\rho}_{\mu} \tilde{\rho}^{\mu} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}
\]

(2.3)

where \( m_{\sigma}, m_{\omega}, m_{\rho} \) are the corresponding masses and \( \Omega_{\mu\nu}, \tilde{R}_{\mu\nu}, F_{\mu\nu} \) are field tensors which are given by

\[
\Omega_{\mu\nu} = \partial_{\mu} \omega_{\nu} - \partial_{\nu} \omega_{\mu},
\]

\[
\tilde{R}_{\mu\nu} = \partial_{\mu} \tilde{\rho} - \partial_{\nu} \tilde{\rho},
\]

(2.4)

\[
F_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu},
\]

The Lagrangian for the interaction between meson fields and nucleons is given by

\[
\mathcal{L}_{\text{int}} = -\bar{\psi} \Gamma_{\sigma} \sigma \psi - \bar{\psi} \Gamma_{\omega}^{\mu} \omega_{\mu} \psi i - \bar{\psi} \Gamma_{\rho}^{\mu} \tilde{\rho}^{\mu} \psi - \bar{\psi} \Gamma_{e}^{\mu} A_{\mu} \psi
\]

(2.5)

with vertices \( \Gamma_{\sigma}, \Gamma_{\omega}^{\mu}, \Gamma_{\rho}^{\mu} \) and \( \Gamma_{e}^{\mu} \) represented by

\[
\Gamma_{\sigma} = g_{\sigma}, \quad \Gamma_{\omega}^{\mu} = g_{\omega} \gamma^{\mu}, \quad \Gamma_{\rho}^{\mu} = g_{\rho} \tilde{\gamma}^{\mu}, \quad \Gamma_{e}^{\mu} = e \frac{1 - \tau_3}{2} \gamma^{\mu}
\]

(2.6)

where \( g_{\sigma}, g_{\omega}, g_{\rho} \) are coupling constants and \( e \) is the electric charge.

Using the variational principle for Lagrangian density, we get the equation of motion in the form

\[
[\gamma^{\mu}(i \partial_{\mu} + V_{m} u) + m + S] \psi = 0
\]

(2.7)

Neglecting retardation effects for the meson fields [28], a solution is obtained when the mean field potentials

\[
S(r, t) = g_{\sigma} \sigma(r, t), \quad \text{and}
\]

\[
V_{\mu}(r, t) = g_{\omega} \omega_{\mu}(r, t) + e A_{\mu}(r, t) \frac{(1 - \tau_3)}{2}
\]

(2.8)
are calculated from the solution of the stationary Klein Gordan equations

\[-\nabla \phi_m + U'(\phi_m) = \pm <\bar{\psi} \Gamma_m \psi>\]  \hspace{1cm} (2.9)

where a '+' sign is for the vector field, a '-' sign is for the scalar field, and $m$ indicates mesons and photon with $\phi_m \equiv \{\sigma, \omega_\mu, \rho_\mu, A_\mu, \}$ and $U'(\phi_m)$ is the functional derivative of the corresponding potential with respect to the meson field.

In these calculations, retardation effects are omitted because of short range meson exchange forces. No sea approximation, where the Dirac sea is simply not considered, is used in the relativistic model for finite nuclei and nuclear matter [28].

### 2.2 Covariant density functional theory

The relativistic Hartree-Bogoliubov model is used to understand ground and excited states of nuclei. This self consistent mean field approach is an approximate application of Kohn-Sham density functional theory [29, 30]. Density functional theory uses a universal energy density functional and mean field model approximates the exact energy functional. All higher order corrections are contained in the exact energy functional. This functional has powers and gradients of nuclear densities. The effective field theory (EFT) of the energy density functional allows error estimation, providing power counting method which distinguishes long and short dynamics, thereby removing any model dependencies from the mean-field approach [28].
The total energy of the nuclear system in relativistic mean field theory is obtained from
the energy momentum tensor

\[ E[\psi, \bar{\psi}, \sigma, \omega^\mu, \bar{\rho}^\mu, A^\mu] = \sum_{i=1}^{A} \int \psi_i^*(\alpha \rho + \beta m) \psi_i d^3r + \int \frac{1}{2} (\nabla \sigma)^2 + U(\sigma) d^3r \]
\[ - \frac{1}{2} \int (\nabla \omega)^2 + m_\omega^2 \omega^2 d^3r - \frac{1}{2} \int (\nabla \rho)^2 + m_\rho^2 \rho^2 d^3r \]
\[ - \frac{1}{2} \int (\nabla A)^2 d^3r + \int [g_\sigma \rho \sigma + g_\omega \bar{\rho} \omega^\mu + g_\rho \bar{\rho} \rho^\mu + e_j \bar{\epsilon} A^\mu] d^3r \]

(2.10)

Using a relativistic single nucleon density matrix

\[ \hat{\rho}(r, r', t) = \sum_{i=1}^{A} |\psi_i(r, t)><\psi_i(r', t)| \]

(2.11)

the total energy as a function of meson fields and the density matrix \( \hat{\rho} \) is given as

\[ E_{RMF}[\hat{\rho}, \phi_m] = Tr[(\alpha p + \beta m)\hat{\rho}] \pm \int \frac{1}{2} (\nabla \phi_m)^2 + U(\phi_m) d^3r + Tr[(\Gamma_m \phi_m)\hat{\rho}] \]

(2.12)

An integration is done over coordinate space and summation is done in Dirac indices for
the trace operation in this equation. The index \( m \) again denotes mesons and photons. The
equations of motion (2.7) and (2.9) are obtained from the variational principle

\[ \delta \int_{t_1}^{t_2} dt \{ < \phi | i \partial_t | \phi > - E[\hat{\rho}, \phi_m] \} = 0 \]

(2.13)

For the density matrix, the equation of motion is

\[ i \partial_t \hat{\rho} = [\hat{h}(\hat{\rho}, \phi_m), \hat{\rho}] \]

(2.14)

The derivative of the energy with respect to the single particle density matrix gives the
generalized Hamiltonian for a particle, i.e.

\[ \hat{h} = \frac{\delta E}{\delta \hat{\rho}} \]

(2.15)
2.3 Covariant density functional theory with pairing

With pairing correlations considered, the energy functional will also depend upon a pairing tensor, in addition to density matrix $\hat{\rho}$ and the meson fields $\phi_m$. The total energy is then given by

$$E_{RHB}[\rho, \hat{\kappa}, \phi_m] = E_{RMF}[\hat{\rho}, \phi_m] + E_{pair}[\hat{\kappa}],$$  \hspace{1cm} (2.16)

where $E_{pair}[\hat{k}]$ is the pairing energy given by

$$E_{pair}[\hat{k}] = \frac{1}{4} Tr[\hat{k}^* V_{pp} \hat{k}]$$  \hspace{1cm} (2.17)

Here, $V_{pp}$ gives the pairing interaction for a two body problem. Now, for the generalized density matrix $\mathcal{R}$

$$i\partial_t \mathcal{R} = [H(\mathcal{R}), \mathcal{R}]$$  \hspace{1cm} (2.18)

The Hamiltonian $H$ is given by

$$H = \frac{\partial E_{RHB}}{\partial \mathcal{R}} = \begin{pmatrix} \hat{h}_D - m - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D^* + m + \lambda \end{pmatrix}$$  \hspace{1cm} (2.19)

The Dirac Hamiltonian is given by

$$\hat{h}_D = -i\alpha \nabla + V_0(r) + \beta(m + \delta(r))$$  \hspace{1cm} (2.20)

The pairing field in equation (2.19) is expressed as

$$\Delta_{ab}(r, r') = \frac{1}{2} \sum_{c,d} V_{abcd}^{pp}(r, r') \kappa_{cd}(r, r')$$  \hspace{1cm} (2.21)
where $a,b,c,d$ are quantum numbers for Dirac indices for the spinors and $V^{pp}$ are matrix elements for the pairing interaction for the two body problem.

The Hartree-Bogoliubov equation

$$
\begin{pmatrix}
\hat{h}_D - m - \lambda & \Delta \\
-\Delta^* & -\hat{h}_D^* + m + \lambda
\end{pmatrix}
\begin{pmatrix}
U_k(\vec{r}) \\
V_k(\vec{r})
\end{pmatrix} = E_k
\begin{pmatrix}
U_k(\vec{r}) \\
V_k(\vec{r})
\end{pmatrix}
$$

(2.22)

gives the solution for the stationary limit of equation (2.18) that describes the ground state of an open shell nucleus. The particle number subsidiary condition, which implies that the expectation value of the particle number operator in the ground state is equal to the number of nucleons, gives the chemical potential $\lambda$ [28]. The column vectors and $E_k$ are quasiparticle wave functions and quasiparticle energies respectively. The dimension of the Dirac equation is half of that of the relativistic Hartree-Bogoliubov matrix equation.

Every eigenvector $(U_k, V_k)$ for non-negative quasiparticle energy $E_k$ has a corresponding eigenvector $(U_k^*, V_k^*)$ for quasiparticle energy $-E_k$. Since simultaneous occupation of $E_k$ and $-E_k$ level is not allowed by commutation relations, only the eigenvectors with non-negative eigenvalue $E_k$ are considered for the solution of the ground state nucleus with even particle number [28].

The static Klein-Gordan equations for $\sigma, \omega, \rho$ mesons and the photon field are

$$
[-\Delta + m_\sigma^2] \sigma(\mathbf{r}) = -g_\sigma \rho_\sigma(\mathbf{r}) - g_2 \sigma^2(\mathbf{r}) - g_3 \sigma^3(\mathbf{r}),
$$

(2.23)

$$
[-\Delta + m_\omega^2] \omega^0(\mathbf{r}) = g_\omega \rho_\nu(\mathbf{r}),
$$

(2.24)

$$
[-\Delta + m_\rho^2] \rho^0(\mathbf{r}) = g_\rho \rho_3(\mathbf{r}),
$$

(2.25)

$$
-\Delta A^0(\mathbf{r}) = e \rho_p(\mathbf{r})
$$

(2.26)
The potentials are obtained from each of these equations which are used to solve the RHB equations. Only the isovector $\rho$-meson’s third component is taken into account due to charge conservation. The spatial components $\omega$, $\rho$, and $A$ of the vector fields disappear in the ground state for an even-even nucleus because of time reversal invariance [28].

The source terms $\rho_s$, $\rho_\nu$, $\rho_3$, $\rho_p$ are given by

$$\rho_s(r) = \sum_{k>0} V^\dagger_k(r) \gamma^0 V_k(r), \quad (2.27)$$

$$\rho_\nu(r) = \sum_{k>0} V^\dagger_k(r) V_k(r), \quad (2.28)$$

$$\rho_3(r) = \sum_{k>0} V^\dagger_k \tau_3 V_k(r), \quad (2.29)$$

$$\rho_{em}(r) = \sum_{k>0} V^\dagger_k(r) \frac{1-\tau_3}{2} V_k(r) \quad (2.30)$$

The no sea approximation applies for $\sum_{k>0}$. The ground state of a nucleus is given by the solution of Dirac-Hartree-Bogoliubov integro-differential and non-linear Klein Gordan equations. The eigenfunctions for an axially symmetric potential which is deformed is used for the expansion of nucleon spinors $U_k(r)$ and $V_k(r)$ and the meson fields in deformed nuclei [28].

The energies and pairing matrix elements are

$$\varepsilon_\mu = \langle \psi_\mu | \hat{h}_D - m | \psi_\mu \rangle, \quad \Delta_\mu = \langle \psi_\mu | \hat{\Delta} | \psi_\mu \rangle \quad (2.31)$$

The probabilities of occupation for single-nucleon states is

$$\nu^2_\mu = \frac{1}{2} \left( 1 - \frac{(\varepsilon_\mu - \lambda)}{\sqrt{(\varepsilon - \lambda)^2 + \Delta^2_\mu}} \right) \quad (2.32)$$

With these probabilities, the self consistent solution for the nuclear ground state has the BCS-state structure [31].
2.4 The details of numerical scheme of RHB equations

The charge quadrupole, octupole and hexadecapole moments are defined by

\[ Q_{20} = \int d^3r \rho(\vec{r})(2z^2 - r_\perp^2) \]  
\[ Q_{30} = \int d^3r \rho(\vec{r})z(2z^2 - 3r_\perp^2) \]  
\[ Q_{40} = \int d^3r \rho(\vec{r})(8z^4 - 24z^2r_\perp^2 + 3r_\perp^4) \]

with \( r_\perp^2 = x^2 + y^2 \). These values of moments can be directly compared with experimental data. However, expressing them in dimensionless deformation parameters is more convenient [32].

The deformation parameters \( \beta_2, \beta_3 \) and \( \beta_4 \) for quadrupole, octupole and hexadecapole deformations respectively are given by

\[ Q_{20} = \sqrt{\frac{16\pi}{5}} \frac{3}{4\pi} Z R_0^2 \beta_2 \]  
\[ Q_{30} = \sqrt{\frac{16\pi}{7}} \frac{3}{4\pi} Z R_0^3 \beta_3 \]  
\[ Q_{40} = 8 \sqrt{\frac{4\pi}{9}} \frac{3}{4\pi} Z R_0^4 \beta_4 \]

where \( R_0 = 1.2A^{1/3} \)

Most of the nuclei are axially and reflection symmetric in their ground states. Considering only axial and parity conserving intrinsic states, we can solve RHB equations in an axially deformed harmonic oscillator basis [33, 34]. For axial RHB equations, the computer code is based upon an expansion of the Dirac spinors and the meson fields in terms of the cylindrically symmetric harmonic oscillator wave function [15, 34]. The method of quadratic constraints is used for calculation by successive diagonalizations [31]. This
parallel version of the axial RHB code allows simultaneous calculations for large number of nuclei and deformation points in each nucleus [15].

For each nucleus, the minimization of the quantity

\[ E_{RHB} + \frac{C_{20}}{2} (\langle \hat{Q}_{20} \rangle - q_{20})^2, \]  

(2.39)

is done where \( E_{RHB} \) is the total energy and \( \langle \hat{Q}_{20} \rangle \) is the expectation value of the mass quadrupole operator

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

(2.40)

\( q_{20} \) is the constraint value of the multiple moment, and \( C_{20} \) is the corresponding stiffness constant [34]. For a converged solution of the multipole moment, the quantity \( q_{20} \) is replaced by \( q_{20}^{\text{eff}} \) which is automatically modified during the iteration such that [35]

\[ \langle Q_{20} \rangle = q_{20} \]  

(2.41)

The potential energy curve is calculated for each nucleus in a large deformation range by means of constraint on \( q_{20} \).

Similarly, for analysis of octupole deformation in the RHB-OCT code, the variation of the function

\[ E_{RHB} + \sum_{\lambda=2,3} C_{\lambda 0} (\langle \hat{Q}_{\lambda 0} \rangle - q_{\lambda 0})^2 \]  

(2.42)

is done. The method of quadratic constraints is used. \( E_{RHB} \) is the total energy and \( \langle \hat{Q}_{\lambda 0} \rangle \) is the expectation value of the quadrupole and octupole moments defined by

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

(2.43)

\[ \hat{Q}_{30} = z(2z^2 - 3x^2 - 3y^2) \]  

(2.44)
$C_{20}$ and $C_{30}$ in equation (2.42) are corresponding stiffness constants [34], while $q_{20}$ and $q_{30}$ are constrained values of the quadrupole and octupole moments. The quantity $q_{\lambda 0}$ is replaced by $q_{\lambda}^{\text{eff}}$ such that [35]

$$\langle Q_{\lambda 0} \rangle = q_{\lambda 0} \quad (2.45)$$

Also, in calculations with octupole deformation, the centre of mass of the nucleus is fixed at the origin with the constraint

$$\langle \hat{Q}_{10} \rangle = 0 \quad (2.46)$$

to keep away spurious centre-of-mass motion [32].
CHAPTER III

INVESTIGATION OF HYPERHEAVY NUCLEI.

3.1 Method of Axial RHB calculations

The CDFT calculations were performed within the relativistic Hartree-Bogoliubov framework [28] employing the state-of-the-art covariant energy density functionals for which the global performance with respect to the description of the ground state [13, 15, 36] and fission [22, 37, 38, 39] properties is well established. These functionals (DD-PC1 [21], DD-ME2 [40], PC-PK1 [41] and NL3* [42]) represent the major classes of covariant density functional models [15]. The absolute majority of the calculations employ the DD-PC1 functional which is considered to be the best relativistic functional today based on systematic and global studies of different physical observables [13, 15, 32, 36, 38, 39]. Other functionals are used to assess the systematic theoretical uncertainties in the predictions of the heights of fission barriers around spherical minima. To avoid the uncertainties connected with the definition of the size of the pairing window [43], we use the separable form of the finite-range Gogny pairing interaction introduced in Ref. [44].

The truncation of the basis is performed in such a way that all states belonging to the major shells up to $N_F$ fermionic shells for the Dirac spinors (and up to $N_B = 20$ bosonic shells for the meson fields in meson exchange functionals) are taken into account. The comparison of the axial RHB calculations with $N_F = 20$ and $N_F = 30$ shows that in
The truncation of basis at $N_F = 20$ provides sufficient accuracy for all deformations of interest. However, in hyperheavy nuclei the required size of the basis depends both on the nucleus and deformation range of interest. The $N_F = 20$ basis is sufficient for the description of deformation energy curves in the region of $-1.8 < \beta_2 < 1.8$. The deformation ranges $-3.0 < \beta_2 < -1.8$ and $1.8 < \beta_2 < 3.0$ typically require $N_F = 24$ (low-$Z$ and low-$N$ hypernuclei) or $N_F = 26$ (high-$Z$ and high-$N$ hypernuclei). Even more deformed ground states with $\beta_2 \sim -4.0$ are seen in high-$Z$/high-$N$ hypernuclei (see Figs. 3.1c and d for the $^{46}_{156}$ and $^{42}_{176}$ results); their description requires $N_F = 30$. Thus, the truncation of basis is made dependent on the nucleus and typical profile of deformation energy curves or potential energy surfaces.

For each nucleus under study, the deformation energy curves in the $-5.0 < \beta_2 < 3.0$ range were calculated in the axial reflection symmetric RHB framework [15]; such a large range of deformations is needed for a reliable definition of the ground states. The nuclei up to $Z = 138$ were calculated using the basis with $N_F$ up to 26. With the exception of the $^{46}_{156}$ and $^{42}_{176}$ nuclei, the $Z = 140 - 180$ nuclei were calculated with $N_F = 20$. The major goals of the calculations for the $Z = 140 - 180$ nuclei are (i) to define the type of the ground states, (ii) to find whether spherical or normal deformed states could be the ground states of these nuclei and (iii) to calculate the fission barriers around spherical states.

### 3.2 General structure of potential energy surfaces

Fig. 3.1 illustrates the dependence of the deformation energy curves, obtained in axial RHB calculations, on the nucleus. The $Z = 82$ $^{208}$Pb nucleus is spherical in the ground
state. The total energy of the nucleus is increasing rapidly with increasing oblate deformation. On the prolate side, it increases with the increase of quadrupole deformation up to $\beta_2 \sim 1.4$ and then stays more or less constant. This leads to the existence of high ($\sim 30$ MeV) and very broad fission barrier which is responsible for the stable character of this nucleus.

The $^{354}_{134}$ nucleus shows a completely different profile in the deformation energy curves (Fig. 3.1b). The ground state is located at $\beta_2 \sim -0.5$ and the deformation energy curves on the oblate side are more flat in energy as compared with $^{208}$Pb. The fission barrier for the $\beta_2 \sim -0.5$ minimum is rather high ($\sim 8.5$ MeV) and broad (Fig. 3.1b) which would suggest high stability for this nucleus against fission if the nucleus would stay axially symmetric. Note that at oblate shapes with deformation $\beta_2 < -1.5$ there are two solutions; the one shown by the solid line has hexadecapole deformation $\beta_4 \sim +0.67\beta_2$ and the other shown by a dotted line has $\beta_4 \sim -1.7\beta_2$. Both are characterized by the presence of an extremely deformed oblate minima at $\beta_2 \sim -2.5$. The $\beta_4 \sim -1.7\beta_2$ solution is lower in energy in axial calculations in a number of nuclei around the $^{354}_{134}$ nucleus, but it is unstable with respect to triaxial distortions. Thus, in considering oblate shapes with $\beta_2 < -1.5$, we focus on shapes with positive $\beta_4$ which are potentially stable with respect to triaxial distortions. In the $^{354}_{134}$ nucleus, an extremely deformed oblate minimum of this solution with $\beta_2 \sim -2.5$ is located at 4.2 MeV excitation energy with respect to the $\beta_2 \sim -0.5$ minimum.

Further increase in proton number leads to drastic modifications of the deformation energy curves. In the $^{466}_{156}$ and $^{426}_{176}$ nuclei, the minimum appears at extreme oblate defor-
mation of $\beta_2 \sim -4.0$. However, these minima are potentially unstable with respect to the transition to the prolate shape via $\gamma$-plane and subsequent fission since prolate shapes with corresponding quadrupole deformations are located at lower energies (compare dashed lines with solid ones in Figs. 3.1c and d). Note also that in the $^{466}_{156}$ nucleus there are excited local oblate (at $\beta \sim -1.2$) and spherical minima which could be potentially stable against fission.

The shapes appearing at these very large and extreme oblate deformations can be described as disk and toroidal-like structures, respectively [14]. Note, that toroidal nuclei are usually unstable against multifragmentation [14, 45].

Fig. 3.2 presents the systematics of ground state deformations obtained in axial RHB calculations for $Z = 122-138$ nuclei. Only a few spherical nuclei located around $Z \sim 130$, $N \sim 230$ are found in the calculations. Prolate deformed nuclei are seen only at $Z = 122$, 124 and $N = 218-236$. The rest of the nuclear chart is dominated by oblate shapes in the ground states. The deformations of the ground states depend on the combination of proton and neutron numbers. However, the general trend is that they increase with proton number. The calculations for nuclei beyond $Z = 138$ are extremely time-consuming due to the required increase in the fermionic basis up to $N_F = 30$. The scan of the deformation energy curves in axial RHB calculations with $N_F = 20$ for the $Z = 140-180$ nuclei located between two-proton and two-neutron drip lines does not show the presence of either prolate or spherical ground states (see Fig. 3.3). The ground states have extremely deformed oblate shapes with $\beta_2 < -1.4$. However, because of the limited size of the basis these values have to be considered as lower limits (in an absolute sense).
Deformation energy curves for $^{208}$Pb and selected even-even hyperheavy nuclei obtained in axial RHB calculations with the DD-PC1 functional and the $N_F = 30$ basis.

The insert in panel (c) shows the fission barriers around the spherical state in detail. Dashed lines show mirror reflection of the $\beta_2 > 0$ part of the deformation energy curve onto negative $\beta_2$ values.
Figure 3.2

Charge quadrupole deformations $\beta_2$ of the lowest in energy particle bound ground states obtained in axial RHB calculations.

The calculations were performed for each second even-even nucleus in the isotopic chain starting at approximately the two-proton drip line and ending at approximately the two-neutron drip line. The nuclei with ground state quadrupole deformations of $-0.8 < \beta_2 < 0.3$ are shown by squares; the colormap provide detailed information on their deformations. The nuclei with extremely deformed oblate ground states are shown by open black squares ($-2.0 < \beta_2 < -1.5$), solid dark blue circles ($-2.5 < \beta_2 < -2.0$), solid cyan triangles ($-3.0 < \beta_2 < -2.5$), solid dark green diamonds ($-3.5 < \beta_2 < -3.0$) and open black circles ($\beta_2 < -3.5$).

Figure 3.3

Ground state deformation for nuclei ranging from $z=138$ to 172. Most of the nuclei have deformed oblate shape.
3.3 Fission barriers and their dependence on the functionals, alpha-decay half-lives.

The analysis of the deformation energy curves obtained in axial RHB calculations reveals that hyperheavy nuclei could be stabilized at spherical shapes in some regions (see the insert to Fig. 3.1c). If the oblate minima in these nuclei are unstable against triaxial distortions or multifragmentation, these states represent the ground states. From our point of view, this is the most likely scenario. Otherwise, they are excited states frequently located at high excitation energies (Fig. 3.1c). It was verified that these spherical states are stable with respect to triaxial and octupole distortions. The largest island of stability of spherical hyperheavy nuclei is centered around $Z \sim 156, N \sim 310$ (Fig. 3.4a). In the calculations with the DD-PC1 functional the fission barriers reach 11 MeV for the nuclei located in the center of the island of stability. This is substantially larger than the fission barriers predicted in the CDFT for experimentally observed superheavy nuclei with $Z \sim 114, N \sim 174$ for which calculated inner fission barriers are around 4-5 MeV [39]. Smaller islands of stability for spherical hyperheavy nuclei are predicted at $Z \sim 138, N \sim 230$ and $Z \sim 174, N \sim 410$ (Fig. 3.4a). Since nuclei in these three regions have $N/Z \geq 1.64$ they cannot be formed in laboratory conditions. The only possible environment in which they can be produced is the ejecta from the mergers of neutron stars [46].

Additional calculations have been performed with the DD-ME2 [40], PC-PK1 [41] and NL3* [42] functionals in order to evaluate systematic theoretical uncertainties [47] in the predictions of fission barriers for spherical hyperheavy nuclei. The DD-ME2 functional provides predictions comparable with the DD-PC1 one (Fig. 3.4a,b). In contrast,
The heights of the fission barriers [in MeV] around spherical states.

The value of the fission barrier height is defined as the lowest value of the barriers located on the oblate and prolate sides with respect to the spherical state in the deformation energy curves (see insert in Fig. 3.1c) obtained in axial RHB calculations. The colormap indicates the height of the fission barrier. Only the nuclei with fission barriers higher than 2 MeV are shown.
The calculated $\alpha$-decay half-lives from the spherical states of hyperheavy nuclei forming the islands of stability shown in Fig.3.4.
the PC-PK1 and NL3* functionals predict lower fission barriers and smaller regions of stability (Fig. 3.4c,d). Note that the nuclear matter properties and the density dependence are substantially better defined for density-dependent (DD*) functionals as compared with non-linear NL3* and PC-PK1 ones [36]. As a consequence, DD* functionals are expected to perform better for large extrapolations from known regions. The large fission barriers obtained in the density-dependent functionals will lead to substantial stability for spherical hyperheavy nuclei against spontaneous fission. This stability is substantially lower for the NL3* and PC-PK1 functionals. Note that these spherical states are also relatively stable against $\alpha$-decay (see Fig. 3.5). The $\alpha$-decay half lives were computed using the phenomenological Viola-Seaborg formula [48]

$$
\log_{10} \tau_\alpha = \frac{az + b}{\sqrt{Q_\alpha}} + cZ + d
$$

with the parameters $a$, $b$, $c$ and $d$ from Ref. [49].

### 3.4 The end of the periodic table of elements

Existing atomic calculations suggest that the periodic table of elements ends at $Z \sim 172$ [18, 19, 20]. This takes place when the $1s$ electron binding energy dives below $-2mc^2$. However, these calculations employ the empirical formulas for the root-mean-square (RMS) nuclear charge radii. For example, the calculations of Ref. [18] employ the formula from Ref. [50] which underestimates the RMS nuclear charge radii as compared with the ones obtained in the RHB calculations. This is exemplified by the values of the RMS nuclear charge radii in the $^{368}138$, $^{466}156$ and $^{584}174$ nuclei which are 6.52 fm (6.91 fm), 7.10 fm (7.58 fm), 7.62 fm (8.31 fm) in the calculations with the empirical formula of Ref. [50] (the RHB calculations with DD-PC1). Note that these nuclei represent the cen-
ters of the islands of stability for spherical hypernuclei (see Fig. 3.4a). Unfortunately, the impact of nuclear size changes on atomic properties and thus on the end of periodic table of elements has not been investigated in Refs. [18, 19, 20]. However, these differences in the RMS nuclear charge radii are substantial and new atomic calculations are needed to see how they can affect the end of the periodic table of elements. In addition, there are other factors which could affect the existence of atoms at extreme $Z$ values. For example, the impact of neutron skin, which is quite large in the nuclei under study [0.193 fm, 0.291 fm and 0.433 fm in three above mentioned nuclei], on the atomic structure is unknown. Moreover, it is an open question on how extreme oblate deformations of nuclei, which will lead to the distortion of the central Coulomb field, could affect the atomic structure.

### 3.5 The impact of octupole deformation on fission

Fig. 3.6 shows potential energy surfaces of isotopes with atomic number $Z=122$. The arrow indicates the prolate minimum in each case. The fission barrier height calculated for $Z = 122$ and mass number 296, 300, 304 and 316 are 3.02, 3.07, 2.36 and 2.98 MeV respectively. This may indicate that these prolate minima are stable and could be the ground state of these nuclei. However, the calculations with octupole deformation show a different picture. To investigate the stability of such prolate minima, we calculated potential energy surfaces in the $(\beta_2, \beta_3)$ deformation plane which are shown in Fig. 3.7 and 3.8. The equipotential surfaces are in steps of 1 MeV. The octupole figures show that the fission barrier is very low (around 1 MeV) or none. For example, in $^{304}122$ (Fig. 3.7), the prolate minimum is located around $\beta_2 = 0.6$. Here, the fission path goes through octupole defor-
The potential energy surface of select $Z = 122$ hyperheavy nuclei in the axial RHB calculations with DD-PC1 functional. The arrow indicates prolate minimum with fission barrier height of more than 2 MeV.

and the barrier along the fission path is not high (around 1 MeV) which means that the octupole deformation is soft. Similarly, in $^{296}122, ^{300}122$ and $^{312}122$, the fission barrier is around 1 MeV. In the case of $^{316}122, ^{320}122, ^{316}124$ and $^{320}124$, the fission path for the prolate minimum via octupole deformation is washed out. Thus, the octupole deformation drives the system in such a way that it decays in that direction. The presence of octupole deformation eliminates the fission barrier and thus the system is unstable on the prolate side.
The potential energy surface of select $Z = 122$ nuclei in the $(\beta_2, \beta_3)$ plane calculated using the DD-PC1 functional. The colormap shows the normalized energies.
Figure 3.8

The potential energy surface of select $Z = 122$ nuclei in the $(\beta_2, \beta_3)$ plane calculated using DD-PC1 functional. The colormap shows the normalized energies.
3.6 Systematic result for the Z=138 isotope chain

Fig. 3.9 shows that as neutron number increases, the quadrupole deformation for the ground state becomes highly oblate. The fission barriers at the ground state are very high (10-30 MeV) indicating these ground states may be potentially stable. Thus, at high proton and neutron numbers, oblate shapes seems to be possible ground states for Z = 138.

Fig. 3.10 shows proton and neutron chemical potential for isotopes of Z = 138. When chemical potential is positive, the particle is unbound and when it is negative, the particle is bound. For the isotope with neutron number N = 186 in Fig. 3.10, proton chemical potential \( \lambda_p \) is positive in the deformation range \( \beta_2 \geq 1.6 \) and is negative for \( \beta_2 \leq -1.6 \). Here, the proton is unbound for \( \beta_2 \geq -1.6 \) and so the nucleus will have a tendency to lose proton. However, the neutron chemical potential \( \lambda_n \) is negative for the deformation range from -4 to 0 and hence the nucleus will not emit neutrons. From N = 190 to N = 210, a similar description can be given for chemical potential. From N = 214 up to N = 318, both \( \lambda_p \) and \( \lambda_n \) are negative in the deformation range from -4 to 0, implying nuclei are stable against particle emission in that deformation range. From N = 322, \( \lambda_n \) becomes positive for a number of deformation points and hence the nucleus will have tendency to loose neutrons at those deformations.

Fig. 3.11 shows how hexadecapole deformation \( \beta_4 \) of the lowest in energy solution varies with the change in quadrupole deformation \( \beta_2 \). The \( \beta_4 \) value varies parabolically with \( \beta_2 \) since increasing the absolute value of \( \beta_2 \) results in \( \beta_4 \) increasing.
Potential energy surfaces of isotopes with proton number $Z=138$. The figure shows nuclei starting from neutron number $N=186$ up to $326$. The figure is normalized in such a way that zero of energy scale starts from the ground state.
Figure 3.10

Proton and neutron chemical potential as a function of quadrupole deformation for $Z = 138$ isotopes. The blue dashed line indicates zero chemical potential.
Hexadecapole deformation as a function of quadrupole deformation for Z=138 isotopes.
CHAPTER IV

CONCLUSIONS

In summary, covariant density functional studies have been performed for superheavy and hyperheavy nuclei with proton numbers $Z = 122 - 180$. The nuclear landscape beyond $Z = 120$ is dominated by oblate shapes in axial calculations. The ground states of the $Z = 122 - 130$ nuclei typically have oblate deformation with $-1.0 < \beta_2 < -0.2$, but further increase of the proton number leads to a dominance of extreme oblate shapes representing disk-like and toroidal shapes. The calculations indicate three regions of potentially stable spherical hyperheavy nuclei centered around ($Z \sim 138, N \sim 230$), ($Z \sim 156, N \sim 310$) and ($Z \sim 174, N \sim 410$). However, theoretical systematic uncertainties in the predictions of their fission barriers are substantial. Furthermore, the current study suggests that only localized islands of stability can exist in hyperheavy nuclei.
REFERENCES


