# STRUCTURE OF DRIP-LINE AND SUPERHEAVY NUCLEI IN EFFECTIVE RELATIVISTIC AND NONRELATIVISTIC INTERACTIONS

A THESIS SUBMITTED FOR THE DEGREE OF **Doctor of Philosophy** IN THE PHYSICAL SCIENCE

by

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## Abstract

The main objective of this proposed work is to probe the structural properties has led to the discovery of several unexpected features that provide new challenges for nuclear theory and our current models. Such features include the structural and decay properties of superheavy nuclei, internal substructure (clustering) of intermediate and light nuclei, nuclear halos, neutron skins, prediction of new magic number beyond <sup>208</sup>Pb, Island of inversion for few selective region of nuclear chart and the evolution of shell structure which leads to the changes in the magic numbers away from the region of stability etc. The discovery of these phenomena has led to the development of the models to describe these crucial and interesting nuclear properties, which may be a substantial progress have been made in the areas of low-energy nuclear theory. The recent and most successful widely used theoretical developments in the field of nuclear many body systems is the selfconsistent mean-field theory (MFT), which provides an elegant and economic framework for calculation of nuclear system for a widely extrapolated region. The present thesis based on the structural study of exotic nuclei including superheavy using MFT and their development. Which will lead to some unique calculations as well as predictions, being as follows:

- 1. A brief discussion on the development of these formalisms will be included in the present work. Addition to these, a short discussion will be covered about the newly develop microscopic of origin nucleon-nucleon potential from relativistic mean field theory and its application on the study of cluster radioactivity.
- 2. The well known and quite successful models such as Relativistic Mean Field Theory,

Effective Field Theory motivated RMF and Skyrme Hartee-Fock will be used for the calculation of ground and intrinsic excited state properties of various nuclei through out the mass table.

- 3. Special attention will be given for exotic nuclei including super-heavy elements. A crucial and extensive calculation will be carried out for finding the island of stability in the super-heavy valley.
- 4. The internal sub-structure like clusters inside a nuclei will be studied for lighter and intermediate regions of the nuclear chart. One most important first time attempt in this calculation is to count the number of nucleons inside the cluster (s) region.
- 5. The calculated results will be compared with the existing experimental data and extensive theoretical prediction will be made.

Basically, the whole effort in the present thesis is devoted in the development of nuclear models, pursuing few new ideas and explaining the structural properties of dripline nuclei including super-heavy. In this context, we have applied the well established as well as widely used non-relativistic Skyrme Hartee-Fock (SHF), relativistic mean field (RMF), and effective field theory motivated relativistic mean field (E-RMF) to explain the interesting phenomena such as decay properties of superheavy nuclei, the island of stability in the superheavy valley, the clustering inside the parent nucleus i.e the evolution of nuclear sub-structure inside a parent nucleus, and their decay probabilities. As a large number of experiments are being planned to study the existence and the decay behavior of superheavy nuclei, our theoretical predictions on the superheavy nuclei are extremely useful for future analysis and investigation. The prediction of clustering is most interesting phenomenon in the intermediate and light mass region, our work corresponding to this study are one step forward in the nuclear structure physics. Based on these important and interesting works, the thesis brief symmetrization of the thesis is given bellow.

First of all **Chapter 1** represents an introduction, which contains a brief descriptions of the nuclear models for nuclear structure, which have been developed since the earliest days of nuclear physics. The main aim of these models are gaining deeper insights into the nuclear force and becoming closer to answering some of the most fundamental questions about the physical world. For example, where are the limits of existence for nuclei?, what are the heaviest elements that can be made?, how does the ordering of quantum states change in exotic nuclei and what can our understanding of the nuclear force tell us about the way the heavy and super-heavy elements are synthesized through collision processes in stars?. To answer these questions it is essential to develop nuclear models to be able to accurately describe the structure properties of nuclei across the full landscape. Based on the fundamental questions, the main focus is directed towards nuclear interactions and their prospectives. Few models such as macroscopic approach (Liquid Drop Model), macroscopic-microscopic approach (Finite-Range-Droplet-Model), quite successful microscopic models (Relativistic mean field, realistic calculations, Shell model, Gogny, Skryme etc) and most fundamental model (ab initio methods) are included for discussions. The merit of each models and their limitations are also discussed in this chapter. Additional correlations beyond mean fields are also looked out in this section, which are important to achieve higher precision or to describe larger set of data. A deep look is forwarded towards the recent development in the experimental as well as corresponding theoretical progress.

In Chapter 2, we have presented both non-relativistic (Skryme-Hartree-Fock) and relativistic (Relativistic mean field) models in detail. The Skyrme Hartee-Fock (SHF) model is generated by the interactions between all the constituent nucleons in the nucleus as described by the nucleon-nucleon force. This leads to the ansatz for the Hartree-Fock approximation that the ground-state trial wavefunction of a nucleus containing A nucleons is written as a Slater determinant, or antisymmetrised product of occupied states. The full many-body Hamiltonian, written in terms of an one-body kinetic energy and a two-body force of nucleons. The expectation value of the total Hamiltonian with respect to the Hartree-Fock wavefunction gives an approximation to the ground-state energy. In case of relativistic mean field theory, the interaction between the nucleons introduced by different mesons. The Lagrangian density that introduces nucleon field  $\psi$ , isoscalar scalar meson field  $\sigma$  resonance states of  $\pi$ - mesons, isoscalar vector meson field  $\omega$  ( $3\pi$ resonance state), isovector vector meson field  $\rho$  ( $2\pi$  p-state) and isovector scalar meson
field  $\delta$ . The Euler-Lagrange equation reproduced the field equations for different fields
and these are solved self-consistently. The total energy of the nucleus comes from the energy contribution from nucleons and mesons. The BCS pairing correlation also discussed
in this sections. The fixation of parameters as well as different forces are also discussed in
this chapter. This chapter contains all mathematical derivations and parametrizations,
which are used in the calculation and further predictions in the subsequent chapters.

In Chapter 3, we have discussed microscopic origin of nucleon-nucleon (NN) potential derived from linear and nonlinear relativistic mean field theory (RMFT). The NN potential obtained from RMFT is entitled as R3Y (L-R3Y and N-R3Y for linear and nonlinear, respectively), which could replace the phenomenological M3Y NN-interaction for most of the calculations of nuclear observables. The R3Y is presented eloquently in terms of the well-known inbuilt RMF theory parameters. In other word, the potential can be expressed in terms of meson masses  $(m_{\sigma}, m_{\omega}, m_{\rho} \text{ and } m_{\delta})$  and their coupling constants  $(g_{\sigma}, g_{\omega}, g_{\rho} \text{ and } g_{\delta})$  for different fields. The results obtained from different force parameters are compared with M3Y potentials. To show the applicability of the R3Ypotential, we have studied the cluster radioactivity. This makes a bridge between R3Y and the phenomenological M3Y in terms of optical potential and explaining the cluster decay property the nuclei. At present, the NN-potential derived from linear and nonlinear Lagrangian density, the improvement of the R3Y interaction for use of the E-RMF Lagrangian is straightforward. The generation of different types of microscopic origin NN-potential as well as an additional improvement in the present interaction is a motivation in the nuclear structure theory. Exploring such R3Y potential from RMF theory being considered as a unified formalism for studying a number of nuclear phenomena or, at least one step forward in our understanding of NN-interaction.

In Chapter 4, we have studied the nuclear structure for ground and intrinsic excited (or isomeric) states of superheavy nuclei in the frame work of relativistic and non-relativistic effective interactions. The axially deformed relativistic mean field and

non-relativistic Skryme-Hartree-Fock theory are employed to investigate the bulk properties of recently synthesized or planned to be synthesized super-heavy nuclei such as Z=115, 117, 120 and 122 and their isotopic chains. First of all, the potential energy surfaces (PES) is calculated by using both the RMF and SHF theories in a constrained calculation, i.e., instead of minimizing the ground state Hamiltonian  $H_0$ , we have minimized  $H = H_0 - \lambda Q_2$ , with  $\lambda$  as a Lagrange multiplier and  $Q_2$ , the quadrupole moment. Thus, we get the solution at a given quadrupole deformation and the PES is a function of quadrupole deformation parameter  $\beta_2$  for a given nucleus. From, the curve, one can find the ground as well as the intrinsic excited state solution of the nucleus. The gross properties, such as binding energy (BE), root mean square charge radius  $r_{ch}$ , proton radius  $r_p$ , neutron radius  $r_n$ , matter radius  $r_m$  and quadrupole deformation parameter  $\beta_2$  are calculated using various forces (NL3,NL3\* for RMF and SkI4,Sly4 for SHF). From the calculated binding energy, we also estimated the two-neutron separation energy  $S_{2n}$  for the isotopic chain. The pairing energy  $E_{pair}$  and the shape co-existence  $\Delta E$  are evaluated for all atomic nuclei. From the binding energy per particle (BE/A) analysis, we found the most stable isotope correspond to N=172 and 182 or 184, for all the atomic nucleus. Some shell structure are also observed in the calculated quantities at N = 172 or 184 for RMF and at N = 182186 for SHF calculations for the various isotopes of the Z = 115, 117, 120 and 122. We found spherical and super-deformed or hyper-deformed ground state solution for Z=115, 117 and Z=120,122, respectively. The  $\alpha$ -decay observables such as  $\alpha$ -decay energy  $Q_{\alpha}$ , half-life time  $T_{\alpha}$  and mean-life  $\tau$  are also estimated for <sup>287,288</sup>115,  $^{293,294}117$ ,  $^{292,304}120$  and  $^{292}122$  series. Our predicted observables for  $\alpha$ -decay chains agree nicely with the FRDM calculations and available experimental data for all the isotopic series are considered in the thesis. Both SHF and RMF formalisms are employed to see the force dependence of the results. We found qualitatively similar predictions in both techniques and independent to the force parameters use.

In Chapter 5, we have extended our calculation in the superheavy valley to found the next magic nuclei beyond Z=82 and N=126. According to the previous calculation (Chapter-3), we found a shell structure at N=172, 182 or 184 for all atomic nuclei, which increase our curiosity to find a suitable combination of neutron and proton number at superheavy island with magic properties. The main aim of this work is to identify the next double closed shell nucleus beyond <sup>208</sup>Pb, which may be a possible candidate for the experimentalists to look for. For this, we have used two well established distinct approaches such as non-relativistic SHF and relativistic mean field formalism for various force parameters (FITZ, SIII, SkMP, SLy4 for SHF and NL-Z2, NL3, G1, G2 for RMF). Here we are concentrated on the well understood and settled magic characteristics as follows:

- The average pairing gap  $\Delta$  for nucleon is minimum (~ 0) at the magic number.
- The binding energy per particle is maximum compared to the neighboring one in an isotopic chain.
- There must be a sudden decrease (jump) in two nucleon separation energy  $S_{2N}$ (N = n, p) just after the magic number in an isotopic or isotonic chain.
- The shell correction energy  $E_{shell}$  is maximum for magic nuclei.
- A pronounced energy gap in the single-particle levels  $\epsilon_{n,p}$  appears at the magic number.

Based on the above four important characteristics, first we have tested these observables for a well known and experimentally verified double closed Pb isotopes. For this, we have taken the isotonic chain of Z=78-82 with isotopic series N=120-140 and calculate average pairing gap (for proton  $\Delta_p$  and neutron  $\Delta_n$ ), two neutron separation energy  $S_{2n}$ and single-particle energy spectra  $\epsilon_{n,p}$ . And found, all the physical quantities exhibit the magic properties at Z=82 and N=126, which make a lightening path for our aim of the present study. In the second phase, we scanned a wide range of nuclei starting from the proton-rich to the neutron-rich region in the superheavy valley (Z=112-130). The average pairing gap ( $\Delta_p$  and  $\Delta_n$ ),  $S_{2n}$ ,  $E_{shell}$  and  $\Delta \epsilon_{n,p}$  are analyzed for these nuclei. To our knowledge, this is one of the first such extensive and rigorous calculation in both SHF and RMF models using a large number of parameter sets. The recently developed effective field theory motivated relativistic mean field forces G1 and G2 are also involved. Although the results depend slightly on the forces used, the general set of magic numbers beyond <sup>208</sup>Pb are Z=120 and N=172, 182/184. The highly discussed proton magic number Z = 114 in the past (last four decades) is found to be feebly magic in nature. It is well accepted that the sequence of the magic number for exotic system is much different from that of the normal nuclei, which is quite normal in superheavy region.

In Chapter 6, we extend the idea of nuclear structure to sub-structure, i.e. the internal configuration (clustering) of a nucleus. The aim of this work is to discuss the possibility of existence (preformation) of cluster (s) inside the parent nucleus and identify them. It is well known that the clustering phenomena is an interesting and crucial mode of decay in intermediate region of the nuclear chart. The recently observation GANIL for the decays of  $^{118,122}Ba^*$  nuclei produced in  $^{78,82}Kr+^{40}Ca$  reactions at a lower incident energy, and the recent prediction from cluster-decay-model (DCM) motivate us to study such interesting clusters for the ground and/ or excited states of Ba nuclei with well developed and microscopic model. Here, we have taken relativistic mean-field formalism with successful NL3 force for the present study. First of all, we have calculated the gross nuclear properties like binding energy, deformation parameter  $\beta_2$ , the charge radius  $r_c$  and the nucleon density distributions  $\rho_{n,p}$  for the isotopic chain  $^{112-122}$ Ba using the deformed relativistic mean field (RMF) theory. The bulk properties obtained from RMF show qualitative as well as quantitative similarity to the experimental values. The internal configuration of a nucleus directly influence by the nucleonic density distributions. From the density analysis, we get the internal sub-structure or clusters in Ba isotopes. The most important and tedious calculation is directed to identify the cluster (s) of a nucleus. Here we are using a straight forward method to found the number of nucleons (proton and neutron separately) for a cluster region. Using this method, we find the prolate ground and first-excited oblate states of some Ba isotopes, specifically, the <sup>112,114,116</sup>Ba and  ${}^{118,120,122}$ Ba, respectively, to consist of  ${}^{12}C$  cluster. The ground-state (g.s.) solutions also support the cluster configurations of other light and the relatively heavier nuclei such

as H, N, Cl, Ar and Ca. Some g.s. solutions also contain light particles like  $^{1,2,3}H$ . This is an interesting result of the RMF(NL3) technique for nuclear structure physics. It is relevant to mention here that, the above results on clustering are not expected to change much by changing of the RMF parametrization. For example, the clustering phenomenon remains almost similar with NL3 and another forces, which shows these results are more apparent and universal. However, the cluster structure of a nucleus remained unaffected as long as the solution for that nucleus existed. As already pointed out, clustering is also important for the decay of excited compound nuclei formed in nuclear reactions. Todate, the decay of <sup>116,118,122</sup>Ba<sup>\*</sup> compound nuclei in to only the intermediate mass fragments (IMFs), and symmetric and near-symmetric fission fragments are measured, and the fusion-evaporation residues are not yet identified. The  ${}^{12}C$  as one of the IMFs measured with the largest yield, is shown in RMF(NL3) calculation to arise from the interior of Ba nuclei, and not from the outer region. Further going to the lighter mass region of nuclear landscape, it is observed and well verified that the  ${}^{12}C$  and  ${}^{16}O$  nuclei contains 3- and 4-  $\alpha$  particles in their ground state. One can observed, the most possible decaying clusters are <sup>4</sup>He, <sup>8</sup>Be, <sup>12</sup>C, <sup>16</sup>O, <sup>20</sup>Ne, <sup>24</sup>Mg and <sup>28</sup>Si having N = Z, which are integral multiple of the  $\alpha$ -cluster  $(n \cdot \alpha)$ . In other word, the possible and most probable clusters emitted are integral multiple of  $\alpha$ -cluster with n = 1, 2, 3... To see such interesting phenomena in the lighter mass region, we have chosen Mq isotopes for our study. It is worth mentioning that, the methods of calculation and the formalism for this work is similar to the Ba-clustering study. The only difference is that, here we have used  $NL3^*$  and NL075 force parameters instead of NL3. The results for nuclear bulk properties from our calculation show qualitative and quantitative similarity with the experimental datas. We found, the deformed prolate ground states of Mq isotopes, which are consistent with the experimental data. The ground state solution consists of  $^{16}O + 2 \cdot \alpha$  cluster along with the excess neutrons. To test the pairing effect on the clustering, we have we have plotted the counter plot of the density profile of <sup>24</sup>Mg with and without pairing. We find almost identical structures in both the cases. This implies, there is no or a very little effect of pairing on clustering of a nucleus. These confirms

the power of RMF theory for cluster prediction. These are some of the interesting result of the RMF (NL3,NL3\* and NL075) techniques for nuclear structure and sub-structure physics. Finally, the present RMF model, used for the calculation of clustering structure in nuclei, has still some scope to take into account the parity reflection symmetry in the formalism, which may at present be a limitation.

In concluding this thesis we would like to say that, the main objective behind the present effort has been to see how far the effective interaction can account the diverse properties of nuclei in normal as well as exotic situations. The reasons behind the choice of the SHF and RMF theory for the study of nuclear properties are manifold. One of the important reasons, is the simplicity and self-consistent solution involved in calculations. These approaches become feasible over nuclear chart including superheavy nuclei. It has been possible to describe successfully many important observables like binding energy, root mean square charge and matter radius, quadrupole deformation parameter, single particle energy, pairing energy, average pairing gap for nucleons, the shell correction energy, single particle energy levels and other related properties with popular set of forces such as FIT-Z, SIII, SKMP, SKI4, SLY4 (for SHF) and NL-SH, NL3, NL3<sup>\*</sup>, NL075, G1 and G2 (for RMF).

**Future Prospects:** The studies of nuclei far from the valley of stability broaden the opportunities of research in the area of both nuclear structure and reaction physics. This is also an indirect impact to the atomic physics as well as in astrophysics and material science. In nuclear physics there are a number of exciting and crucial topics to be addressed. Some of the topics which we are intending to pursue in immediate future are as follow:

The nuclear structure near the drip-line is one of the excited research topics in present day nuclear physics. A lot of exotic phenomena like halo and skin structure exhibit due to the large isospin in such nuclei. A detail analysis is needed within the available nuclear models taking into account the necessity of the problem. This can also be extended to superheavy nuclei, which is again a virgin area. More explanations are needed to understand the superdeformed / hyperdeformed (β<sub>2</sub> ~

0.5) ground state in case of exotic nuclei including superheavy. Further substantial modification in the method of calculation of half-life  $t_{1/2}^{\alpha}$  and mean-life  $\tau^{\alpha}$  of nucleus is needed.

- In the intermediate region, the nuclei far away from the β -stable region or near to drip-line showing some magicity, i.e. the half-life of these nuclei higher in magnitude than that of the neighbor. This implies, exploring such special features are important topic at the present status of nuclear physics. Further more explanation needed for the crucial feature such as Island of Inversion in some specific region of the nuclear chart.
- The experimental proton drip-line is known up to Z=82. However, to reach the neutron drip-line experimentally is much more tricky, and the present experimental status to reach the theoretical prediction of neutron drip-line is up to the Mg-isotopes. Many interesting physics has been evolved in recent past near the proton and neutron drip lines. The proton and neutron halo and skin is one among the exciting discoveries. More work in this direction are needed.
- The application of these models in nucleon-nucleus and nucleus-nucleus reaction also plays significant roles to understand the observables like differential reaction cross-section dσ/dΩ, total reaction cross-section σ<sub>t</sub>, analyzing power A<sub>y</sub> and the spin rotation parameter. We have already dedicated some efforts in this directions but more clarification and deep understanding is essential.
- We have already undertaken some modification in the relativistic mean field Lagrangian i.e. a complete Lagrangian. At present, we have introduced some extra terms like the cross-coupling of  $\omega$  and  $\rho$  with new coupling constant  $\Lambda_v$  in effective field theory motivated relativistic mean field theory (E-RMF) and applied this to the study of nuclear matter. The extension of this modified Langagian to the study of finite nuclei under rudimentary stage.

Here we have mention some work, which are already taken care in our plan for the current or near future study. Also, there are so many highly interesting and crucial work are already there to explore in the nuclear structure study. Again, an unified description

both for nuclear matter under extreme conditions and the properties of finite nuclei starting from the beta stable to drip-line and superheavy nuclei using simple effective interaction is one step forward in nuclear physics, which already in progress.

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### STRUCTURE OF DRIP-LINE AND SUPERHEAVY NUCLEI IN EFFECTIVE RELATIVISTIC AND NONRELATIVISTIC INTERACTIONS

A THESIS SUBMITTED FOR THE DEGREE OF Doctor of Philosophy IN THE PHYSICAL SCIENCE

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by

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JUNE 2013

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## Vita

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# Keywords

- 21.30.-x Nuclear forces
- 21.60.-n Nuclear models
- *21.65.Jk* Mesons
- *14.20.-c* Baryons
- 13.75.Gx Nucleon-meson interactions
- 13.75.Cs Nucleon-nucleon interactions
- 21.10.Dr Nuclear binding energy
- 21.10.Ft Nuclear charge distributions
- 21.10.Gv Nucleon distribution and halo features
- 21.10.Hw Spin and parity
- 21.10.Sf Nuclear Coulomb effects
- 21.10.-k Nuclear energy levels
- 23.20.Lv Level energies
- 21.10.Ma Level density
- 21.10.Tg Lifetimes, widths
- 21.10.Pc Single-particle levels
- 36.40.-c Clusters in nucleus

Note: These are standard classification for keywords, such as, ACM Computing Classification, JEL Classification, AMS Classification etc.

# Notation and Abbreviations

 $\psi$  spinor wave function describing nucleons

- $\phi$  the meson mediating finite range attractive interaction among nucleons
- $\omega$  the meson mediating finite range repulsive interaction among nucleons
- $\rho\,$  the meson that takes care of asymmetry of nucleons
- $g_s$  coupling constant for  $\sigma$ -mesons
- $g_v$  coupling constant for  $\omega$ -mesons
- $g_{\rho}$  coupling constant for  $\rho$ -mesons

 $\eta_1; \eta_2$  non-linear coupling constant for  $\sigma$  and  $\omega$ -mesons

- $\kappa_3; \kappa_4$  non-linear self coupling constant for  $\sigma$ -mesons
  - $\zeta_0\,$  non-linear self coupling constant for  $\omega\text{-mesons}$
  - $\eta_\rho\,$  non-linear coupling constant for  $\sigma$  and  $\rho\text{-mesons}$
  - $\tau\,$  Pauli matrices
  - $\beta_2$  deformation parameter
  - $\alpha$  Dirac matrix
  - $\beta$  Dirac matrix
  - $A_{\mu}$  the photon-field

# Chapter 1

# Introduction

The existence of the atomic nucleus was revealed by *Rutherford* in 1911 by the celebrity  $\alpha$ -particle scattering experiment, i.e. the bombardment of a gold-foil with an  $\alpha$ -particles. The isotopes of an atomic nucleus and their weight or mass was explored by *J. J. Thom*son. The neutron was discovered in 1932 by *Chadwick*, together with proton appearing to be the basic constituent of nucleus. It was the first fundamental interest to expose the essential interaction, which binds the protons and neutrons in a nucleus. Since that time it has been one of the basic problems and tasks of nuclear physics to understand its nature and principle, and, consequently, to describe the structure and properties of atomic nuclei.

Nowadays, it is generally accepted that the fundamental challenges for theoretical nuclear physics is to understand the properties of finite systems with many degrees of freedom in terms of their interactions between the individual components. In the case of self-bound many-body systems governed by non-relativistic quantum mechanics, significant simplifications must be incorporated into the theoretical models. As the nucleus is highly correlated with many-body system, in order to render the many-body problem [1], which is exactly the case for describing the structure and dynamical properties in nuclear physics [2, 3, 4]. In case of atomic nucleus, the structure is defined in terms of the interactions between its constituents (nucleons). The dimension of the mathematical equations describing these interactions is directly proportional to the system size (i.e.

number of particles). In other word, the dimensions of the mathematical equations grow rapidly with size of the system, which cannot be solved analytically. To find the exact solution of the equation, we have to follow the numerical technique, which is applicable for very simplest nuclei (containing few particles). But in case of higher mass (hundred(s) of nucleons), it is ideal to take an approximations to the model in such a way that the microscopic objects behave and interact with each other, based on the underlying nuclear force [5]. Our understanding of the key components of this force between nucleons, the residual strong force, has been gained through studying even the most basic properties of nuclei and has led to the development of a set of theoretical models that successfully describe the trends and detailed properties of a wide range of systems [6]. However, our understanding of the underlying many-body interactions is not yet complete.

A land mark progress was achieved in 1937, the muon interpreted as a particle was found in cosmic radiation proposed by Yukawa and the incorrectness of this assumption revealed later, it had supported the interest in Yukawas idea. Finally, the real meson, pion ( $\pi - meson$ ) was discovered in cosmic background in 1947 and soon after also in Berkeley. In this direction, the heavier mesons ( $\omega$ -meson at Berkeley and  $\rho$ -meson at Brookhaven) are found, which cover the nature of strong interaction. In earlie 1970, a re-normalizable field theory of baryons and mesons is developed, which is characterized by finite number of coupling constants and masses [7, 8]. This theory is calibrated to the nuclear observables and further it is possible to extrapolate in high density and high temperature regions without any additional parameters. As baryons and mesons are used as relevant degrees of freedom, the theory has been known as quantum hydrodynamics (QHD). Here also, relativistic nucleon motion must be considered with increasing density as well as causal constraints.

The recent advancements both in the theoretical and experimental nuclear physics and astro-nuclear physics, it is necessary to modify or improve the models describing such systems. Now-a-days the techniques using radioactive ion beam facilities have provided significant opportunities for the exploration of the exotic nuclei that populate the majority of nuclear chart. Again, the new accelerator facilities produce nuclei with high isospin asymmetry and nuclear matter at high densities and developing astrophysical observations of compact objects. The aim of this work is to probe their internal structure properties, which has led to the discovery of several unexpected features that provide new challenges for nuclear theory and our current models. Such features include structural and decay properties of superheavy elements [9, 10, 11, 12], internal substructure (clustering) of intermediate and light nuclei [13, 14], nuclear halos [15], neutron skins [16], prediction of new magic number beyond <sup>208</sup>Pb [17] and the evolution of shell structure which leads to the changes in the magic numbers away from the region of stability [18]. The discovery of these phenomena has led to the development of the models to describe these crucial and interesting nuclear properties, which may be a substantial progress that has been made in the areas of low-energy nuclear theory.

### 1.1 Nuclear Structure Theories

The aim of the nuclear models to be used in the present thesis is to gain deep perception to the nuclear forces and attempt to answer some of the fundamental questions about the nucleus. These includes:

- Whether there is a limit for nucleus that can co-exist either in nature or can be produced from artificial synthesis by using modern techniques ?
- What is the maximum number of protons and neutrons that of a nucleus ?
- How does the ordering of single particle level / the magic number changes in an exotic nuclei ?
- What can our understanding of nuclear force to explain the formation of superheavy nuclei in astrophysical objects ?
- What is the next double shell closure nucleus beyond <sup>208</sup>Pb ?
- What is the internal configuration of a nuclei?
- If, clustering is there in the nucleus then what are the constituents of a cluster(s).

To find the solution of these problems, it is necessary for nuclear models to accurately describe the structural properties of nuclei across the nuclear landscape. The basic properties includes nuclear binding energy, shape of the nucleus, root mean square radius, the precise shell structure and the single-particle spectra with splitting levels, of a nucleus in its ground as well as in intrinsic excites states. Several models are available for above defined purpose but the most fundamental is *ab initio* method, described from the nucleon-nucleon (NN) scattering data [19] and obtained from low energy QCD [20, 21, 22] or from diagrammatic techniques [23, 24]. This formalism is used to compute the equation of state for nuclear matter, or to the description of finite nuclei. This approach can reproduce the basic properties of nuclei upto a precision of ~5% (with two-body forces) and a precision of ~1% (with three-body forces) for finite nuclei upto mass number  $A \sim$ 20 [25, 26]. Although the microscopic origin of this force is not well understood since the nucleon-nucleon interaction is modified with increasing nucleon number in a complicated way. Hence, this models is not computationally made for large scale nuclear structure calculations at present.

In other hand, the usually used nuclear theories are the macroscopic approaches, which are based on the liquid drop model [27, 28, 29]. The total energy of a nucleus is expressed in its basic properties such as volume, surface, coulomb, asymmetry and pairing energy. The constants of these models are called as free parameters and determined by fitting phenomenologically to the nuclear data [30]. These models are able to explain the nuclear bulk properties for nuclei on or near  $\beta$ - stable region of the nuclear chart. However, some of the crucial finite nucleus observables like shell-correction energy, single-particle spectra and single-particle potential are generally included to the model by phenomenological adjustment [31]. The macroscopic-microscopic theory has been highly successful in described the nuclear properties [32], which constitutes a microscopic description with added shell correction by hand. The main demerits of these models are unable to explain the exotic nuclei i.e. the uncertainty arises when extrapolating the prediction to the unknown region of the nuclear landscape. A direct connection of micro-macroscopic and self-consistent mean-field theory is obtained by means of semi-classical approximations. The simplest one is the Thomas-Fermi model or extended Thomas-Fermi model [33]. In this method, one can reproduce many local features of self-consistent mean-field theories. References on many relativistic and extended Thomas-Fermi works can be found in Ref. [34].

### **1.2** Recent Developments

The recent theoretical developments in the field of nuclear many body systems can be grouped into three different approaches: (1) *ab initio* methods; (2) self-consistent meanfield (MFT) and shell-model theories; and (3) macroscopic models with microscopic shell corrections. The *ab initio* method is started with the aim to explain the nucleon-nucleon scattering data by using a given nucleon-nucleon potential. The potential characterized by a strong repulsive core, thus the nuclear matter behaves like a strongly correlated quantum liquid. To explain such quantized liquid system, we needs a highly sophisticated many-body theories (for example, Dirac-Brueckner-Hartree-Fock) [8, 35], which results the direct connection of two-nucleon problem and nuclear matter properties. However, due to this complexity it is not applicable to finite nuclei calculations at present. For this incapability to perform full *ab initio* calculation over the nuclear chart of finite nuclei, one employs effective interactions.

The intermediate level between *ab initio* and macroscopic-microscopic approaches [2, 3, 4] are the microscopic models based on effective interactions. There are mainly two different microscopically origin approaches: (1) Shell model and (2) the self-consistent mean-field models. The shell model [36] aims to explain the mean field descriptions for ground state and intrinsic excited properties of finite nuclei. This model is built from wave functions of a phenomenological single particle basis, such as the harmonic oscillator. The many-body states are constructed from the basis states around the Fermi energy by configuration mixing [37, 38]. However, the dimensions of these calculations grow rapidly with the size of the system, requiring the use of Monte Carlo methods to study heavier nuclei [39, 40].

Due to the present incapability to perform full *ab initio* and shell model calculation over the nuclear chart of finite nuclei, one employs effective interactions. In other way, the mean-field theories (MFT) are based on effective interactions and concentrate on selfconsistent determination of the nuclear mean field. The forces of the MFT consists of few numbers of parameters and these are adjusted by fitting to the nuclear structure data. The mean-field potential well of nucleons are computed from the nucleonic wave functions at Hartree-Fock level. The theories are somewhat inadequate for the description of the finite nuclear properties of a nuclear system, which are strongly influenced by pairing correlations. The concept of pairing field is included into the mean-field to take these correlations into account. Generalization of the mean-field concept with the Hartree-Fock-Bogoliubov (HFB) equations [41], and the widely used BCS approximation for time-reversal-invariant systems are two different formalisms for the calculation of pairing energy in the mean-field theory.

### **1.2.1** Effective Interactions

Presently, three standard models used in the nuclear mean field are the *zero* range Skryme interaction [42], the finite range Gogny [43] and the relativistic mean-field theory [7].

In case of Skryme interaction, the total energy evaluated from Skyrme-Hartree-Fock approach constitutes the kinetic energy, energy from effective nucleon-nucleon interaction (the Skyrme energy functional), the Coulomb energy, the pair energy and corrections for spurious center-of-mass motion. The local approximation in the Skyrme energy functional has several technical advantages. The direct and exchange terms of the Skyrme-Hartree-Fock have same structure, which significantly reduce the number of integrations required for solutions of field equations. There are two different methods to evaluate the Skyrme energy functional. The first technique belongs to the derivation from the Hartree-Fock expectation value of the zero-range momentum dependent two-body force introduced by Skyrme. The pairing properties are unrealistic for all the Skyrme forces in this method. For this reasons, this strict approach is thus rarely used, and the contributions to the pair energy are dropped. Moreover, it introduces many dependencies among the coupling constants that make so many difficulties in finding the solution. Also there exist a spin instability in the infinite nuclear matter and finite nuclei, because of the usual parametrization of a three-body force which was used in some early parametrizations and the problem still persists even in recent parametrizations. In other one, the energy functional is parametrized directly without reference to an effective two-body force. These free parameters are coupling constants of the energy functional, which are not fixed by global symmetries. The *particle-hole* and *particle-particle* pairing channels of the interactions are decoupled, which make free from all previous mentioned difficulties. The only disadvantage is that the additional coupling constants have to be adjusted on the observed nuclear data. A flexible isospin structure in the spin-orbit interaction is an interpretation for the energy density functional in the earlier Skryme interactions. The new forces [44] are constructed to reproduce the shell structure of the exotic nuclei and are different from the standard Skyrme forces. The importance of the spin-orbit force in Skryme forces are not only isospin dependence but also density dependence, which is not the case in standard relativistic mean field theory. The Skyrme Hartree-Fock method uses strictly point couplings, whereas the standard relativistic mean-field model has finite range couplings through exchange of mesons. The gradient term with the zero-range two-body force into a finite-range two-body coupling shows the variant of the Skyrme force. An alternative concept has been developed [45], where the Skyrme functional can be viewed as a systematic expansion in derivatives up to second order with usually simple density dependence. In this alternative method, the functional omits the terms containing derivatives except for the spin-orbit interaction and employs much more elaborate density dependence for all remaining terms.

The Gogny force employs a finite range interaction, unlike than that of the Skryme interaction. However, it is unable to reproduce the binding energies of finite nuclei at Hartree-Fock level. Thus, the density dependence in the interaction and the spin-orbit terms are added to the core term of the Gogny force. The divergence of zero-range pairing is avoided and that enables to use Gogny interaction simultaneously in both mean-field and pairing channels. The Coulomb energy contribution is exactly calculated from the direct and exchange part of the Coulomb interaction.

The powerful and widely used tool for describing various aspects of many body problem is the mean-field theory [8, 46]. This approach provides an elegant and economic framework for calculation of nuclear system for a widely extrapolated region. The first attempt started with the re-normalized field theory of baryons and mesons, calibrated over the observed nuclear properties and characterized by finite number of coupling constants and masses [7, 8]. Then it is possible to extrapolate to high density and high temperature regions without any additional parameters. It is empirically proved that there exist a large scalar and vector fields in nucleon-nucleon interaction, which is comparable with the nucleon mass. So it is important and necessity to take the relativistic effects into account. Relativistic treatments have several advantages:

- The natural incorporation of the spin-orbit force [8].
- The shift of the saturation curve, so-called Coester band towards the empirical values [35].
- The successful description of finite nuclei on the β-stable and drip line regions including superheavy nuclei of the nuclear chart [46, 47, 48, 9, 10, 12].

Now a days, the properties of exotic nuclei with high isospin asymmetry are possible to measure by the new experimental facility like particle accelerators. Additionally, the more precise observations and measurements of properties of neutron stars and supernovae have been carried out. Which need a better description of isospin degree of freedom and can be possible by enhancing the relativistic Lagrangian corresponding to the isovector meson fields. The cross interactions between isovector and isoscalar fields are also important, which have been introduced [49] and used in this work.

The basic assumption of the relativistic-mean-field theory (RMFT) is the ladder of many-body state, which is an independent quasi-particle state from single-particle wave functions with four-component Dirac spinors. The interaction through meson fields is considered to be an effective one. The main concept behind RMFT are the interacting nucleons and mesons (self interaction and with other mesons) inside the nucleus, which is an effective interaction and introduced through Klein-Gordon equations for the meson fields. These field equations are solved self consistently by taking several approximations. One can use the density dependence of the coupling constants and make model as density dependence. More detailed information about mean-field framework will be given in *Chapter-2* of the this thesis work.

### 1.2.2 Beyond Mean-Field

The static mean-field approach is able to describe the bulk properties of many nuclei over nuclear chart. To achieve higher precision or to describe larger set of data, one has to consider additional correlations. Various attempt have been made in this direction and explained so many concepts related to these areas. For example, the generator coordinate method, which is closely related to multi-configurational Hartree-Fock method. These are used in atomic physics and similar application like Monte Carlo shell model in nuclear physics. There are other two different methods, first one is the path integral method, which deals with the large-amplitude collective motions that appear to be the most important correlation effect. And second one is diagrammatic method which is also useful for collective motion study.

The relations between the single-particle wave functions through symmetries is a characteristic feature of the many-body problem. But in case of self-consistent mean-field theory, wave functions are often constructed in a superposition manner. They break symmetries of nuclear Hamiltonian and these symmetries associated with zero excitation energy and large-amplitude motion have to be restored. The angular momentum projection is used [50] together with several additional approximations [51] satisfactorily describing properties of deformed nuclei. The last, but important restoration procedure is center-of-mass projection [52], induced by broken translational invariance following from localization of mean field in space. The relative contribution of center-of-mass correction to the total binding energy is largest for light nuclei since its value decreases with increasing nucleon number and vanishes for infinite nuclear matter.

The straight forward extension of static mean-field models is represented by the timedependent mean-field method. There are various approaches such as time-dependent density-functional theory [53], in the nuclear dynamics known as the time-dependent Hartree-Fock (TDHF), and the time-dependent Hartree-Fock-Bogoliubov (TDHFB) in the case of pairing. These methods are applicable to explain some features in nuclear and heavy-ion dynamics [54]. For example, the low-energy region of surface vibrations and fission is reached by adiabatic TDHF. As it is the first derivation with diagrammatic techniques [55], one can say that the TDHFB is a starting point for quasi-particle Random-Phase Approximation (QRPA). It is also a basic theory of nuclear excitations in the regime of giant resonances. There exists many different notations for the Random-Phase Approximation RPA equations and techniques for their solution.

### 1.3 Scope of this work

In this section, we briefly reported the contents of subsequent chapters. Basically, the whole effort devoted for the development of new ideas and explaining the structural properties of drip-line nuclei including superheavy. The thesis is organized as follows:

In **Chapter 2**, we introduced and develop the theoretical formalisms of the relativistic mean field (RMF) and Skryme-Hartree-Fock (SHF) approaches. We start with the basic concept of standard RMF & SHF, and outlined their importance over the nuclear structure study, which includes the comparison between different models. In case of RMF, the field equations are derived for different fields  $\psi$ ,  $\sigma$ ,  $\omega$ ,  $\rho$  and electromagnetic fields. For SHF, the density functionals are obtained from the effective interaction. The pairing correlation, which is important for the open shell nuclei also included in this section. A schematic diagram is given for reader to determine the importance of pairing in finite nuclei. The compilation of various observables for fitting of different forces for RMF & SHF along with other mean-field models are briefly presented in this chapter.

First of all, a microscopic nucleon-nucleon (NN) interaction potential is derived from the popular relativistic-mean-field Lagrangian. This NN potential is entitled as R3Y, which could replace the phenomenological M3Y NN-interaction for most of the calculations of nuclear observables. The R3Y is presented eloquently in terms of the well-known inbuilt RMF theory parameters. In other word, the potential can be expressed in terms of meson masses  $(m_{\sigma}, m_{\omega}, m_{\rho} \text{ and } m_{\delta})$  and their coupling constants  $(g_{\sigma}, g_{\omega}, g_{\rho} \text{ and } g_{\delta})$ for different fields. The results obtained from different force parameters are compared with M3Y potentials. Further, we used the microscopic origin NN-potential to the exotic cluster radioactive decays and  $\alpha + \alpha$  scattering to determined the applicability. The details of the derivation along with the results with suitable comparisons are given in **Chapter 3** of this thesis work.

In Chapter 4, we applied RMF and SHF formalisms to study the ground state properties of Z=115,117,120 and 122 isotopes. First of all, the potential energy surfaces (PES) is calculated by using both the RMF and SHF theories in a constrained calculation, i.e., instead of minimizing the  $H_0$ , we have minimized  $H = H_0 - \lambda Q_2$ , with  $\lambda$  as a Lagrange multiplier and  $Q_2$  is the quadrupole moment. From that curve, we found shape of the ground and intrinsic excited states of the nuclei for various force parameters. The gross properties, such as binding energy (BE), root mean square charge radius  $r_{ch}$ , proton radius  $r_p$ , neutron radius  $r_n$ , matter radius  $r_m$  and quadrupole deformation parameter  $\beta_2$  are calculated. From the calculated binding energy, we also estimated the two-neutron separation energy  $S_{2n}$  and the decay energy  $Q_{\alpha}$  values for the decay chains. The alpha decay properties such as half-life  $t_{1/2}^{\alpha}$  and mean-life  $\tau^{\alpha}$  for these atomic nucleus also studied. The results obtained from our calculations compared with other theoretical models and experimental data.

In Chapter 5, we have extended our calculation to the superheavy valley to find the next magic nuclei beyond Z = 82 and N = 126. According to the previous calculation (*Chapter-3*), we get a little shell structure at N=172, 182 or 184 in the isotopic chain of all atomic studied nuclei, which increase our curiosity to found a suitable combination of neutron and proton number at superheavy island with magic properties. For this we scanned a wide range of elements Z = 112-130 and their isotopes using spherical RMF and SHF models for various force parameters. Based on the calculated observables like

pairing gap  $\Delta$ , two neutron separation energy  $S_{2n}$ , single particle energy levels  $\epsilon_{n,p}$  (for neutron and proton) and the shell correction energy  $E_{shell}$ , we predict Z = 120 as the next proton magic and N=182/184 the subsequent neutron magic numbers. The highly discussed proton magic number Z = 114 in the recent past (last four decades) is found to be feebly magic in nature. It is well accepted that the sequence of the magic number for exotic system is much different from that of the normal nuclei, which is quite normal in superheavy region.

As we know, the clustering is a novel phenomenon from few decades in the light and intermediate mass region. In **Chapter 6**, we include such clustering structure (nuclear sub-structure) of Ba (in intermediate) and Mg (in light mass region) isotopes in an axially deformed cylindrical coordinate. The clustering configurations inside the nucleus determined from the total (neutrons-plus-protons) density distributions for both the ground and excited states. The important steps, carried out here for first time is the counting of number of protons and neutrons present in the clustering region(s). Presence of <sup>12</sup>C along with other lighter clusters such as <sup>2</sup>H, <sup>3</sup>H and nuclei in the neighborhood of N = Z are the constitute the clusters in prolate-deformed ground-states of <sup>112116</sup>Ba and oblate-deformed first excited states of <sup>118122</sup>Ba nuclei. Further, in light mass region, we have found the oxygen (<sup>16</sup>O) as a core and bubble like  $\alpha$  along with some excess neutron(s) in magnesium isotopes. All these results are of interest for the observed intermediate-mass-fragments and fusion-fission processes, and the so far unobserved evaporation residues from the decaying Ba compound nuclei formed in heavy ion reactions.

# Chapter 2

# **Theoretical Formalisms**

The effective interactions or effective energy-density functional are employed at the intermediate level of nuclear models. The self-consistent mean-field, is one of the approach belongs to the effective interaction, proved as a powerful and versatile tool for providing a microscopic quantum mechanical understanding of matter. The main objective of this approach to get a prejudice free, self-consistent determination of the nuclear ground state and low-energy collective dynamics. One can say, the self-consistent mean-field models are one big forward step towards the microscopic description of nuclei as compare to the macroscopic-microscopic (in short mic-mic) method. The genuine nuclear interaction induces huge short-range correlations that are not naturally included in this method, because of that we cannot be regarded these as an *ab initio* treatment. They produce the appropriate single-particle potential corresponding to the actual density distribution for a given nucleus [56, 26, 27].

There are three most prominent and quite successful mean-field approaches are as: (1) the Skyrme energy functional, traditionally called Skyrme-Hartree-Fock (SHF), (2) the finite range Gogny model, and (3) the relativistic mean field model (RMF) [for a recent review see Ref. [28]]. We have already mentioned that the self-consistent mean-field models lie between *ab initio* theories and the *mac-mic* method. It is worth mentioning that the relation between *ab initio* and mean-field is still under development [56, 28], which is not the case in connection between mean-field and the *mac-mic* approach [26, 27]. For example, the extended Thomas-Fermi Skyrme interaction scheme (ETFSI) starts from SHF and derives an effective *mac-mic* model by semi-classical expansion [29, 30]. On the other hand, there is an attempt to include more self-consistency by virtue of a Thomas-Fermi approach [31, 32], which turns out to be useful to gain more insight into the crucial constituents of models. The uncertainty in the phenomenological determination of the free parameters in the effective energy functional [36] is one of the burden in applying mean-field models. There are more than hundred forces (or sets of parameter) are already developed within few decades. Still, the main problem is not yet solved, i.e. one does not find the correspondence between individual parameter and link for the experimental informations. The method for determining the parameter are almost same for all fitting i.e. the parameter sets which would fit the experiment with a comparable degree of accuracy. One of the crucial tasks in the development of the meanfield models to converge the free parameters used in the interaction and reproduced the new data for exotic regions of the nuclear chart. The role of the mean-field models (relativistic mean field and Skryme-Hartree-Fock theory) in providing such input to finite nucleus properties and its implication is discussed in this work. In this chapter, we discussed the present status of the mean-field models mainly relativistic mean field (RMF) and Skryme-Hartree-Fock (SHF) and their application to finite nuclei throughout the nuclear landscape. This also included the adjustment of the force parameters and resultant observables.

### 2.1 Relativistic Mean Field Theory

The concept of relativistic description of nuclear system raised in early 1960, by Schiff [57], Teller and Dũrr [58, 59], which was forgotten for nearly twenty years till 1970's. The idea come to a glory, when Miller and Green and just after by Walecka [7] pointed out the power, the simplicity form of the interaction of nucleon through meson with few degrees of freedom [8]. Simple Walecka model is not able to describe the surface properties of a nucleus to a large extent or properly. The inclusion or acquaint of non-linear coupling

Туре	Spin	Orbital angular moment	Parity	Total angular moment
	S	L	Р	J
Pseudoscalar	0	0	_	0
Pseudovector	0	1	+	1
Vector	1	0	_	1
Scalar	1	1	+	0
Tensor	1	1	+	2

Table 2.1: The mesons are classifies into different groups according to their quantum number.

terms among the mesons by [60] and further development by other [61] in the effective Lagrangian break through the situation. This non-linear model is entitled by Relativistic Mean Field (RMF) theory. This model is developed within the framework of quantum hadrodynamics (QHD). The spin-orbit splitting and the nucleon-nucleon potential are initially there in the effective density, which is not the case in Skryme and Gogny types. In this context, one may say that the model is more reliable than the non-relativistic one in predicting yet unknown properties of nuclei far from stability line, which are important in astrophysical situations. The details of the model is discussed in the section below.

#### 2.1.1 Basic concepts of relativistic mean field theory

The microscopic description of ground state and excitation properties of finite nuclei has been attempted using relativistic field theory from past few years. It starts from an effective Lagrangian containing the nucleonic and mesonic degrees of freedom, is a phenomenological theory of the nuclear many-body problem. There are four basic assumptions behind this theory as:

- The nucleons are treated like point particles.
- Nucleons are the efficient degrees of freedom at low energy and they are included

as Dirac spinor  $\psi_i$ . Further, their compositeness retain at the *tree* level through the inclusion of non-renormalizable interaction terms.

- These particles obey strictly the rules of relativity and causality.
- The theory is fully Lorentz invariant.
- The particles move independently in mean fields which originate from nucleonnucleon interaction.
- The other degrees of freedom are non-Goldsten bosons or mesons such as  $\sigma$ ,  $\omega$ ,  $\rho$  and  $\delta$ . These are responsible for the intermediate range interactions and conveniently describe the non-vanishing expectation values of nuclear bilinears.
- Finally, the QHD constraints are imposed through symmetry i.e. all allowed (*non-redundant*) terms must be included.

The exchange of effective mesons, which couple to the nucleons at local vertices, obey the conditions of causality and Lorentz invariance. Based on these assumptions the nucleons are treated as Dirac particles described by Dirac spinor  $\psi_i$ . The point-like particles are called mesons,  $\phi_j$ , where j stands for  $\sigma$ ,  $\omega$ ,  $\rho$ ,  $\delta$  and photon fields. They are characterized by their quantum numbers such as spin (S), orbital angular momentum (L), total angular momentum (J), parity (P). Here we have listed different types of meson with their fundamental quantum number for their identity in Table (2.1). The mesons dynamics can be determined through the Lagrangian density  $\mathcal{L}(\phi, \partial_{\mu}\phi, t)$  and variational principle:

$$\delta \int dt L = \delta \int d^4 x \mathcal{L}(\phi, \partial_\mu \phi, t) = 0, \qquad (2.1)$$

in classical level, the Euler-Lagrange equations of motion:

$$\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi_j)} \right) - \frac{\partial \mathcal{L}}{\partial \phi_j} = 0.$$
(2.2)

The energy momentum tensor [8, 60] is given by

$$T^{\mu\nu} = -g^{\mu\nu}\mathcal{L} + \frac{\partial\mathcal{L}}{\partial(\partial_{\mu}\phi_j)}\partial^{\nu}\phi_j.$$
(2.3)

The Euler-Lagrange equation ensures that this quality is conserved and the continuity equation is given by

$$\partial_{\mu}T^{\mu\nu} = 0, \qquad (2.4)$$

if  $\mathcal{L}$  has no explicit space dependence then the four-momentum is defined by  $P^{\nu} = \int d^3 r T^{0\nu}$  and the  $0^{th}$  component of the four-momentum is expressed as  $P^0 = E = \int d^3 r \mathcal{H}(r)$ . Now the Hamiltonian density is given by

$$\mathcal{H}(r) = T^{00} = \frac{\partial \mathcal{L}}{\partial q_j} \phi_j - \mathcal{L}.$$
 (2.5)

From this Hamiltonian density, the binding energy of the nucleus can calculated by using the relation:

$$E = \int d^3 r \mathcal{H}(r) = \int T^{00} d^3 r.$$
(2.6)

The mesons are characterized by the quantum numbers spin (S), parity (P) and isospin (T), which are already listed in Table 2.1. But, in case of  $\pi$ -meson (Pseudoscalar in nature) with -ve parity, the corresponding mean-field breaks on Hartree level and its contribution is zero, which is not the case in real nuclei [8, 62]. In mean-field level, the parity is conserving to a very high degree of accuracy, i.e. assumed to be well defined parity. Therefore, the effects of  $\pi$ -mesons average essentially to zero in the description of bulk properties of nuclei [8, 62]. It is well known that, two or any even number of pions contributes positive parity, therefore one includes the phenomenological  $\sigma$ -meson (resonance states of two  $\pi$ -mesons), have treated beyond mean field. The exchange of  $\sigma$ -meson leads to attractive nuclear force among the nucleons and the corresponding field is scalar field  $\phi$  (r). The exchange of vector mesons generating the repulsive component

to the nuclear potential. The most important one is the  $\omega$ -meson ( $3\pi$ -resonance state), which is experimentally found. The field generated from this meson called as  $W(\mathbf{r})$ and the time-like component is responsible for repulsive force. The isospin dependence of nuclear force is taken care by the exchange of  $\rho$ -mesons. The  $\rho$ -field (R(r)) is the  $2\pi$ (p-state) and is taken care by phenomenological aspect. The electromagnetic field of photon is described by vector potential  $A^{\mu}$  (r) and its time-like component represents Coulomb repulsion. The  $\rho$ -mesons have the same quark composition as that of  $\pi$ , but the mass is about five and one half times the  $\pi$ -mesons, therefore,  $\rho$ -mesons are considered to be the excited state of  $\pi$ -mesons. There are other mesons, which play a little role in the quantitative description of bare nucleon-nucleon interaction by meson exchange [62]. For example  $\delta$ -meson leads to scalar nuclear potential slightly different for protons and neutrons. The contribution of this meson is small for finite nuclei and the effect of which can be achieved by a suitable adjustment of parameters in Lagrangian for the other mesons. Therefore, neglecting the other mesons; only  $\phi$  (r), W (r), R (r) and the photon  $A^{\mu}$  fields are considered. The masses of other mesons are more than the mass of nucleons, and the contribution of heavy mass mesons can be neglected to a good approximation. The assumption of naturalness and the observation shows that the mean fields and their derivatives are small compared to mass of the nucleon M upto moderate density. Which allows us to organize the Lagrangian in powers of the fields and their derivatives. This is one of the advantage to redefine the fields simplify the interaction terms between the nucleons and the non-Goldstone bosons, where the scalar and vector meson parts of the Lagrangian can contain powers of  $\partial^2$  in addition to the kinetic terms [63, 64]. It is important to note that, the key observation at normal nuclear matter density (or in the central part of a nucleus), the scalar  $g_s \phi$  and vector  $g_\omega W_0$  mean fields are  $\leq 0.25$ M and 0.4M, respectively.

#### 2.1.2 Relativistic mean field Lagrangian density

Based on the above discussion, the non-linear effective Lagrangian density here used to investigate the ground state properties of nuclei in the nuclear chart describing the contribution of all mesons and nucleon as:

$$\mathcal{L} = \mathcal{L}_{\mathcal{N}} + \mathcal{L}_{\mathcal{M}}.$$
(2.7)

Here  $\mathcal{L}_{\mathcal{N}}$  and  $\mathcal{L}_{\mathcal{M}}$  are the nucleonic and mesonic part of the effective Lagrangian, respectively. Each terms are truncated upto the order,  $\nu=4$ , which is sufficient for the finite nuclei and infinite nuclear matter calculation [63, 64]. The quantity  $\nu$  is an index, assign to each interaction terms and is defined as:

$$\nu = d + \frac{n}{2} + b, \tag{2.8}$$

where, 'd' is the number of derivatives, 'n' is the number of nucleon fields and 'b' is the number of non-Goldstone boson fields in the interactions. The term 'd' does not contain the derivatives on the nucleon fields because of the power of the nucleon mass, which lead to a higher values in the expansion parameters. Again the term 'b' arises due to non-Goldstone boson couples with two nucleon fields. The details of these terms are given in Ref. [65]. The first term of the effective Lagrangian involves nucleon with  $\nu = 4$ and is given by [63, 64]

$$\mathcal{L}_{\mathcal{N}} = \overline{\psi_{i}} \left[ i \gamma^{\mu} D_{\mu} + g_{A} \gamma^{\mu} \gamma_{5} a_{\mu} - M + g_{s} \phi \right] \psi_{i} - \frac{f_{\rho} g_{\rho}}{4M} \overline{\psi_{i}} \rho_{\mu\nu} \sigma^{\mu\nu} \psi_{i} - \frac{f_{\omega} g_{\omega}}{4M} \overline{\psi_{i}} V_{\mu\nu} \sigma^{\mu\nu} \psi_{i} - \frac{\kappa_{\pi}}{M} \overline{\psi_{i}} \omega_{\mu\nu} \sigma^{\mu\nu} \psi_{i} - \frac{e}{2M} F_{\mu\nu} \overline{\psi_{i}} \lambda \sigma^{\mu\nu} \psi_{i} - \frac{e}{2M^{2}} \overline{\psi_{i}} \gamma_{\mu} \left(\beta_{s} + \beta_{v} \tau_{3}\right) \psi_{i} \partial_{\nu} F_{\mu\nu},$$

$$(2.9)$$

where M is the mass of nucleon and  $\psi_i$  is Dirac spinor. The  $D_{\mu}$  is the covariant derivatives and is given by

$$D_{\mu} = \partial_{\mu} + i\omega_{\mu} + ig_{\rho}\rho_{\mu} + ig_{\omega}V_{\mu} + \frac{ieA_{\mu}(1+\tau_3)}{2}.$$
 (2.10)

The mesonic part (second term of Eqn. (2.7)) of the Lagrangian can also organized in terms of the fields and their derivatives, as:

$$\mathcal{L}_{\mathcal{M}} = \frac{1}{2} \left[ 1 + \alpha_1 \frac{g_s \phi}{M} \right] \partial_\mu \phi \partial^\mu \phi + \frac{f_\pi^2}{4} tr(\partial \mu U \partial^\mu U^\dagger) - \frac{1}{2} tr(\rho_{\mu\nu} \rho^{\mu\nu}) - \frac{1}{4} \left[ 1 + \alpha_2 \frac{g_s \phi}{M} \right] V_{\mu\nu} V^{\mu\nu} - g_{\rho\pi\pi} \frac{2f_\pi^2}{m_\rho^2} tr(\rho_{\mu\nu} \rho^{\mu\nu}) + \frac{1}{2} \left[ 1 + \eta_1 \frac{g_s \phi}{M} + \frac{\eta_2}{2} \frac{g_s^2 \phi^2}{M^2} \right] m_\omega^2 V_\mu V^\mu + \frac{1}{4!} \zeta_0 g_\omega^2 (V_\mu V^\mu)^2 + \left[ 1 + \eta_\rho \frac{g_s \phi}{M} \right] m_\rho^2 (\rho_\mu \rho^\mu) - m_s^2 \phi^2 \left[ 1 + \frac{\kappa_3}{3!} \frac{g_s \phi}{M} + \frac{\kappa_4}{4!} \frac{g_s^2 \phi^2}{M^2} \right] - 2e f_\pi^2 A^\mu tr(\omega_\mu \tau_3) - \frac{e}{2g_\gamma} F_{\mu\nu} \left[ tr(\tau_3 \rho^{\mu\nu}) + \frac{1}{3} V^{\mu\nu} \right], \qquad (2.11)$$

here, the coupling constants in the above equations,  $g_s$ ,  $g_{\omega}$ ,  $g_{\rho}$  and  $\frac{e}{4\pi} = \frac{1}{137}$  are for  $\sigma-$ ,  $\omega-$ ,  $\rho-$ mesons and photon, respectively. The Pauli isospin matrix  $\vec{\tau}$  ( $\vec{\tau}_3$ ) ( $\vec{\tau}_3$  is the third component of  $\tau$ ) for the nucleon spinor. The value of  $\tau_3$  is -1 and +1 for neutron and proton, respectively. The coupling constant  $\eta_1$ ,  $\eta_2$ ,  $\eta_{\rho}$  and  $\zeta_0$  are induced for the non-linear terms of meson fields. The field tensors  $V^{\mu\nu}$ ,  $\rho^{\mu\nu}$  and  $F^{\mu\nu}$  corresponding to the  $\omega$ -,  $\rho$ -mesons and the electromagnetic field. The  $\alpha_1$  and  $\alpha_2$  are the terms correspond to the derivatives of the meson field and with  $\nu=5$ . However, we have retain them because of the same contributions in magnitude to the surface energy as the quartic scalar term. The numerical factor 1/n! determines the important of the term in contribution in the energy.

#### 2.1.3 Relativistic mean field equation

The variational principle is used here to generate the equations of motion for the nucleons and mesons. Instead of quantize the fields, the mean field approximation is introduced, in which the meson field operators are replaced by their expectation values (classical fields) and hence removing the quantum fluctuations. The other approximation is the "no sea" approximation, in which the different densities and currents for the sources of meson fields are obtained by summing over all occupied states in Slater determinant of baryons. This means that the contribution of anti-particles is neglected. In other word, the negative energy solutions of Dirac equation is not included i.e. the vacuum polarization effects are not taken into account. However, one can not say that the vacuum polarization is neglected completely. It is taken care in a global way by the phenomenological adjustment of the parameters. The negative and positive energy states in Dirac equation (neglecting Dirac sea using "*no sea*" approximation) is shown in Fig. 2.1.

Figure 2.1: The qualitative structure of the scalar field S and vector field V in finite nuclei. Dirac positive energy (V+S) and negative energy (V-S) states are shown.

The nucleon spinor for the single particle contains spatial and time-like components. Here, the space-like components of the vector fields is neglected, i.e. we neglecting the nuclear magnetism [66]. We need the static state solutions of the equations to determine the ground state properties of the nuclei. The vector potential  $[W_0(\mathbf{r}), \mathbf{W}(\mathbf{r})]$ ,  $[R_0(\mathbf{r}),$   $\mathbf{R}(\mathbf{r})$ ] and the electromagnetic potential  $[A_0(\mathbf{r}), \mathbf{A}(\mathbf{r})]$  are four-vectors under Lorentz transformations. The component with subscript 0 stands for time-like components and the *bold front* for the space-like components of the vector fields, respectively. The single-particle wave function  $\psi_i$  is four-dimensional spinor. The subscript *i* denotes the quantum numbers that specify the single-particle state and  $E_i$  is the corresponding energy. In static case the time derivative of the meson fields vanish i.e.

$$\frac{\partial \phi}{\partial t} = \dot{\phi} = 0; \qquad \frac{\partial W}{\partial t} = \dot{\omega} = 0; \qquad \frac{\partial R}{\partial t} = \dot{\rho} = 0.$$
 (2.12)

The time-reversal symmetry is broken for a nucleus contains *odd* number of nucleon. But, it is well known that, the odd particle responsible for the polarization currents and *time-odd* components in the mean fields. The time-odd components are essential for the description of magnetic moments [67] and moments of inertia in rotating nuclei [68, 69]. Again, the bulk properties of a nucleus like binding energies and deformation  $\beta_2$ also effected with odd nucleons, however, is very small and can be neglected to a good approximation [66]. To take care of odd - odd and even - odd nuclei, one has to violate time-reversal symmetry in the mean field. To avoid such difficulty in our calculations of odd-nuclei we employ the well known Pauli blocking approximation, which restores the time-reversal symmetry. In this approach one pair of conjugate states  $\pm m$  is taken out of the pairing scheme. The *odd-nucleon* stays in one of these states and its corresponding conjugate state remains empty. In general, one has to block different states around Fermi level to find the one which gives the maximum binding energy of the nucleus. For odd - odd nuclei we block both neutron and proton [70]. In case of even - even system, the nucleus (Slater determinant) has time reversal symmetry. This means if the state i is occupied then its time reversed partner must there. In other words if an angular momentum state j (m) is occupied then its time reversed partner j(-m) is also occupied. This implies that there are no spatial currents in the nucleus. Therefore, the spatial vector components of the fields vanish and we are left with time-like components of Lorentz vector and corresponds to Coulomb field in electrodynamics and a scalar

potential, which contributes to effective mass  $M^*$  (r). The  $M^*$  (r) is the shift in the mass of nucleons M due to the strong scalar field [71], which is expected to be  $\frac{1}{2}M$  at center of the nucleus and rises back to M on the surface. Now the single-particle Dirac Hamiltonian for finite nuclei for Eqn. (2.7) can be written as [72],

$$h(r) = -i\alpha \cdot \nabla + W(r) + \frac{1}{2}\tau_3 R(r) + \beta (M - \phi(r)) + \frac{1 + \tau_3}{2} A(r) - i\beta\alpha 2M \left(\frac{1}{2}f_\rho \tau_3 \nabla R + f_v \nabla W\right) + \frac{1}{2M^2} (\beta_s + \beta_v \tau_3) \nabla^2 A - \frac{i}{2M} \lambda \beta \alpha \cdot \nabla A, \qquad (2.13)$$

where,  $W(r) = g_{\omega}V_0(r)$ ,  $\phi(r) = g_s\phi_0(r)$ ,  $R(r) = g_{\rho}\rho_0(r)$  and  $A(r) = eA_0(r)$  are the scaled mean-fields with coupling [48] and  $\beta = \gamma_0$  and  $\alpha = \gamma_0\gamma$  are the Dirac matrices. The terms with  $\lambda$ ,  $\beta_s$  and  $\beta_v$  takes care for the effect of electromagnetic structure of the nucleons. The constant  $\lambda$  needed to reproduce magnetic moments of the nucleons and it is given by,

$$\lambda = \frac{1}{2}\lambda_p(1+\tau_3) + \frac{1}{2}\lambda_n(1-\tau_3), \qquad (2.14)$$

here, the value of  $\lambda_p$  and  $\lambda_n$  are 1.793 and -1.913, the anomalous magnetic moments of the proton and neutron, respectively. The quantities  $\beta_s$  and  $\beta_v$  are important for the charge radii of the nucleon. The Dirac equation with the eigen values  $E_i$  and eigen function  $\Psi_i(r)$  are given by [8, 73],

$$h\Psi_i(r) = E_i\Psi_i(r), \qquad (2.15)$$

with the normalization condition,

$$\int d^3 r \Psi_i^{\dagger}(r) \Psi_i(r) = 1.$$
(2.16)

The eigen functions and its components (upper and lower) along with the single-particle potentials are given in **Appendix-A**. The equations of motions for various mesons and

photon fields are:

$$-\nabla^{2}\phi + m_{s}^{2}\phi = g_{s}^{2}\rho_{s}(r) - \left(\frac{\kappa_{3}}{2} + \frac{\kappa_{4}}{3!}\frac{\phi}{M}\right)\frac{m_{s}^{2}\phi^{2}}{M} + \frac{\eta_{\rho}}{2M}\frac{g_{s}^{2}}{g_{\rho}^{2}}m_{\rho}^{2}R^{2} + \frac{\alpha_{2}}{2M}\frac{g_{s}^{2}}{g_{v}^{2}}(\nabla W)^{2} + \frac{g_{s}^{2}}{2M}\left(\eta_{1} + \eta_{2}\frac{\phi}{M}\right)\frac{m_{v}^{2}}{g_{v}^{2}}W^{2} + \frac{\alpha_{1}}{2M}[(\nabla\phi)^{2} + 2\phi\nabla^{2}\phi], \qquad (2.17)$$

$$-\nabla^2 W + m_v^2 W = g_v^2 \left( \rho_s(r) + \frac{f_v}{2} \rho_T(r) \right) - \frac{\phi}{M} m_v^2 W \left( \eta_1 + \frac{\eta_2}{2} \frac{\phi}{M} \right) - \frac{1}{3!} \zeta_0 W^3 + \frac{\alpha_2}{M} \left( \nabla \phi \cdot \nabla W + \phi \nabla^2 W \right), \qquad (2.18)$$

$$-\nabla^2 R + m_{\rho}^2 R = \frac{1}{2} g_{\rho}^2 \left( \rho_3(r) + \frac{f_{\rho}}{2} \rho_{T,3}(r) \right) - \eta_{\rho} \frac{\phi}{M} m_{\rho}^2 R, \qquad (2.19)$$

$$-\nabla^2 A = e^2 \rho_p(r). \tag{2.20}$$

Here,  $\phi$ , W, R and A stands for the field of  $\sigma$ -,  $\omega$ -,  $\rho$ -meson and the electromagnetic field, respectively. The masses of the  $\sigma$ ,  $\omega$  and  $\rho$ -mesons are denoted as  $m_s$ ,  $m_{\omega}$  and  $m_{\rho}$ , respectively. The relativistic mean field equations are coupled equations of unknown fields (mesons and nucleons) and each field correspond to a density and are given below:

$$\rho_s(r) = \sum_{i=1}^{A} \overline{\psi}_i(r) \psi_i(r) = \sum_{i=1}^{A} \frac{2j_a + 1}{4\pi r^2} \left( G_a^2(r) - F_a^2(r) \right)$$
(2.21)

The  $\rho_s(r)$  is the scalar density contains difference of the squares of large and small components and is not normalized,

$$\rho_v(r) = \sum_{i=1}^A \psi_i^{\dagger}(r)\psi_i(r) = \sum_{i=1}^A \frac{2j_a+1}{4\pi r^2} \left(G_a^2(r) + F_a^2(r)\right), \qquad (2.22)$$

It is baryon density (vector density) the sum of squares of large and small components of Dirac spinor which are normalized to unity.

$$\rho_3(r) = \sum_{i=1}^A \psi_i^{\dagger}(r) \tau_3 \psi_i(r) = \sum_{i=1}^A \frac{2j_a + 1}{4\pi r^2} 2t_a \left( G_a^2(r) + F_a^2(r) \right), \qquad (2.23)$$

The  $\rho_3$  (r) is called as *isovector* density and the tensor densities are expressed as:

$$\rho_v^T(r) = \sum_{i=1}^A \psi_i^{\dagger}(r) i\beta \alpha \cdot \hat{r} \psi_i(r) = \sum_{i=1}^A \frac{2j_a + 1}{4\pi r^2} 2\left(G_a(r)F_a(r)\right), \qquad (2.24)$$

$$\rho_3^T(r) = \sum_{i=1}^A \psi_i^{\dagger}(r) i\tau_3 \beta \alpha \cdot \hat{r} \psi_i(r) = \sum_{i=1}^A \frac{2j_a + 1}{4\pi r^2} 2t_a \left( 2G_a(r) F_a(r) \right).$$
(2.25)

Now the proton density or the charge density can be expressed as

$$\rho_{ch}(r) = \sum_{i=1}^{A} \psi_i^{\dagger}(r) \frac{(1+\tau_3)}{2} \psi_i(r) = \frac{1}{2} \left( \rho_v(r) + \rho_3(r) \right).$$
(2.26)

The sum extends over the occupied shell model states of the positive energy (no sea approximation). The Eqns. (2.21-2.26) for densities serve as the sources in meson equations, which are ingredient to determine the meson fields. Finally, the meson-fields enters the Dirac equation and determine the motion of nucleons in a self-consistent way. The whole system of equations are solved iteratively. Since the nuclear force does not depend on the charge, so neutron and proton are considered to be separate manifestations of the same particle, the nucleon. The isotopic spin entitled as isospin ( $\tau$ ) is an additional quantum number to label neutron and proton. The values of the third component of isospin ( $\tau_3$ ) is +1 (-1) for proton (neutron). Finally, the energy density for finite nuclei can given by [64],

$$\begin{aligned} \mathcal{E}(\mathbf{r}) &= \sum_{\alpha} \varphi_{\alpha}^{\dagger} \Biggl\{ -i\alpha \cdot \nabla + \beta(M-\phi) + W + \frac{1}{2}\tau_{3}R + \frac{1+\tau_{3}}{2}A \\ &- \frac{i}{2M}\beta\alpha \cdot \left( f_{v}\nabla W + \frac{1}{2}f_{\rho}\tau_{3}\nabla R + \lambda\nabla A \right) + \frac{1}{2M^{2}}\left( \beta_{s} + \beta_{v}\tau_{3} \right)\Delta A \Biggr\} \varphi_{\alpha} \\ &+ \left( \frac{1}{2} + \frac{\kappa_{3}}{3!}\frac{\phi}{M} + \frac{\kappa_{4}}{4!}\frac{\phi^{2}}{M^{2}} \right) \frac{m_{s}^{2}}{g_{s}^{2}}\phi^{2} - \frac{\zeta_{0}}{4!}\frac{1}{g_{v}^{2}}W^{4} + \frac{1}{2g_{s}^{2}}\left( 1 + \alpha_{1}\frac{\phi}{M} \right) \left( \nabla \phi \right)^{2} \\ &- \frac{1}{2g_{v}^{2}}\left( 1 + \alpha_{2}\frac{\phi}{M} \right) \left( \nabla W \right)^{2} - \frac{1}{2}\left( 1 + \eta_{1}\frac{\phi}{M} + \frac{\eta_{2}}{2}\frac{\phi^{2}}{M^{2}} \right) \frac{m_{v}^{2}}{g_{v}^{2}}W^{2} \\ &- \frac{1}{2g_{\rho}^{2}}\left( \nabla R \right)^{2} - \frac{1}{2}\left( 1 + \eta_{\rho}\frac{\phi}{M} \right) \frac{m_{\rho}^{2}}{g_{\rho}^{2}}R^{2} - \frac{1}{2e^{2}}\left( \nabla A \right)^{2}. \end{aligned}$$
(2.27)

The center-of-mass (c.m.) correction to the nuclear binding energy can generated non-relativistically using the simple relation [74] as:

$$E_{c.m.} = \frac{\langle P_{c.m.}^2 \rangle}{2MA},\tag{2.28}$$

here, A is the mass number and A = Z + N for a given nucleus. And the momentum of the given system can be expressed as:

$$\langle P_{c.m.}^2 \rangle \equiv -\sum_{i=1}^A \langle \alpha | \nabla^2 | \alpha \rangle + \sum_{i,j=1}^A | \langle \alpha | \nabla^2 | \beta \rangle |^2, \qquad (2.29)$$

with

$$\langle \alpha | \hat{O} | \beta \rangle \equiv \int d^3 x \psi_i^{\dagger}(r) \hat{O} \psi_i(r).$$
(2.30)

Here, we used the same procedure to estimate the center-of-mass correction, which is an empirical method given by [75] :

$$E_{c.m.} = \frac{17.2}{A^{\frac{1}{5}}} MeV, \qquad (2.31)$$

which determines the expectation value of  $\langle P_{c.m.}^2 \rangle$  from Eqn. (2.29). The binding energy of a nucleus is given by,

$$\epsilon = A \cdot M - E + E_{c.m.},\tag{2.32}$$

where, A is the mass number of the nucleus and M is the mass of the nucleon. Here we have taken  $m_p = m_n = M$ , in case of  $m_n \neq m_p$ , one can use  $Z \cdot m_p + N \cdot m_n$  for  $A \cdot M$ . The *c.m.* correction for the root-mean-square charge radius is given by

$$\langle r^2 \rangle_{ch} = \langle r^2 \rangle - \frac{3}{8M \cdot AE_{c.m.}},\tag{2.33}$$

where

$$\langle r^2 \rangle = \frac{1}{Z} \int d^3x x^2 \rho_{ch}(r). \tag{2.34}$$

Now the above expressions are sufficient for the determination of the structural properties of finite nuclei.

### 2.2 The Skryme-Hartree-Fock Formalism

The central assumption of the Hartree-Fock approach is the force felt by each nucleon moving independently in an average potential (or mean field) [5]. And this mean field described by nucleon-nucleon force, which is generated from the interactions between all the constituent nucleons inside the nucleus. As we know, the nucleus is a many-body system (few number of fermions), it implies that the constituents must obey the Pauli exclusion principle and the wave-function of the collective state must be antisymmetric under the interchange of the coordinates of any two nucleons. Hence, the Hartree-Fock approximation for the ground-state trial wave-function of a nucleus with A particles can be written as a Slater determinant or an antisymmetrised product of occupied states. The Slater determinant is built from a complete orthonormal set of single-particle wavefunctions  $\phi_i$  ( $r_j$ ) (the Hartree-Fock basis). Here  $r_j$  stands for all coordinates (*spatial*, *spin* and *isospin*) of the  $j^{th}$  nucleon.

$$\Phi(r_1, ..., r_A) \longrightarrow \Phi_{HF}(r_1, ..., r_A) = \frac{1}{\sqrt{A!}} \begin{bmatrix} \phi_1(r_1) & \phi_2(r_1) & \phi_3(r_1) & \cdots & \phi_A(r_1) \\ \phi_1(r_2) & \phi_2(r_2) & \phi_3(r_2) & \cdots & \phi_A(r_2) \\ \phi_1(r_3) & \phi_2(r_3) & \phi_3(r_3) & \cdots & \phi_A(r_3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \phi_1(r_A) & \phi_2(r_A) & \phi_3(r_A) & \cdots & \phi_A(r_A) \end{bmatrix}$$
(2.35)

Initially, the exact spatial form of the single-particle wave-functions are unknown, they may be approximated by oscillator wave-functions [76, 77], with the total number of nucleons in the nucleus, unless pairing correlations are considered. Starting with the full many-body Hamiltonian, which can be written in terms of a one-body kinetic energy term and a two-body force for a system of A particles as:

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_{i}^{2}}{2m_{i}} + \frac{1}{2} \sum_{i \neq j}^{A} V(\mathbf{r}_{i}, \mathbf{r}_{j}), \qquad (2.36)$$

where  $V(\mathbf{r_i}, \mathbf{r_j})$  contains all parts of the nucleon-nucleon force, including the Coulomb interaction. The main aim of mean-field to simplify the two-body potential in terms of a one-body mean-field,  $U(r_i)$ , that incorporates as much of the physics of  $V(\mathbf{r_i}, \mathbf{r_j})$  as possible. In the Hartree-Fock approach the expectation value of the total Hamiltonian with respect to the Hartree-Fock wave-function gives the approximated ground-state energy, which can written as:

$$E_{HF}^{0} = \langle \Phi_{HF} | H | \Phi_{HF} \rangle$$

$$= -\frac{\hbar^{2}}{2m} \sum_{i \neq j}^{A} \int \phi_{i}^{*}(\mathbf{r}) \nabla^{2} \phi_{i}(\mathbf{r}) d\mathbf{r}$$

$$+ \frac{1}{2} \sum_{i \neq j}^{A} \int \int \phi_{i}^{*}(\mathbf{r}) \phi_{j}^{*}(\mathbf{r}') V(\mathbf{r_{i}}, \mathbf{r_{j}}) \phi_{i}(\mathbf{r}) \phi_{j}^{(\mathbf{r}')} d\mathbf{r} d\mathbf{r}'$$

$$- \frac{1}{2} \sum_{i \neq j}^{A} \int \int \phi_{i}^{*}(\mathbf{r}) \phi_{j}^{*}(\mathbf{r}') V(\mathbf{r_{i}}, \mathbf{r_{j}}) \phi_{i}(\mathbf{r}) \phi_{j}^{(\mathbf{r}')} d\mathbf{r} d\mathbf{r}', \qquad (2.37)$$

here the notation  $\int d\mathbf{r} = \sum_{i\neq j}^{A} d^3 r$  is used throughout the section. The final term in Eqn. (2.37) plays the role of industrialization under the interchange of any two particles. The ground-state of the system is one that minimizes the expectation value in Slater level i.e. the generation of lowest energy. Which requires the first derivative of the expectation value with respect to small changes in all of the single-particle wave-function must be zero by variational principle. This can be expressed in terms of Hartree-Fock ground

state energy  $E_{HF}^0$  and Lagrange multiplier  $\epsilon_i$ ,

$$\frac{\delta}{\delta\phi_a^*(\mathbf{r})} \left[ E_{HF}^0 - \sum_i^A \epsilon_i \int |\phi_i(\mathbf{r})|^2 d\mathbf{r} \right] = 0, \qquad (2.38)$$

with  $\frac{\delta}{\delta \phi_a^*(\mathbf{r})} \phi_a^*(\mathbf{r}) = \delta_{ia} \delta(\mathbf{r} - \mathbf{r}')$ . Here,  $\epsilon_i$  ensure the correct normalization of the wavefunctions throughout the variation and include the constraint for the conservation of particle number within the system. Now the normalization condition for a system of Aparticle can be given as:

$$\sum_{i=1}^{A} \int |\phi_i(\mathbf{r})|^2 d\mathbf{r} = A, \qquad (2.39)$$

which is nothing but the single-particle energies calculated from solution of the Schrodinger equation for the single-particle Hamiltonian, and is given by,

$$h|\phi_i(\mathbf{r})\rangle = \epsilon_i |\phi_i(\mathbf{r})\rangle. \tag{2.40}$$

This leads to a simplified form for the Hartree-Fock equation and is given as:

$$\epsilon_i = -\frac{\hbar^2}{2m} + U_H^{(i)}(\mathbf{r})\phi_i(\mathbf{r}) - \int U_F^{(i)}(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}')d\mathbf{r}', \qquad (2.41)$$

where,  $U_H^{(i)}$  and  $U_F^{(i)}$  are known as the direct or Hartree and exchange or Fock potential term, respectively. The detail expressions for Hartree-Fock equations as well as the direct and exchange potential are given in **Appendix-B**. This equation look like the regular one-body Schrödinger equation with extra non-local term. The solution of this equation yield a set of single-particle wave-functions that form the ground-state Slater determinant, which needs a self-consistent, or iterative solution [78, 79, 80]. In practical, the terms starting with the trial single-particle wave-functions, then using the chosen interaction to construct the potential, solving the Schrödinger equation. In the presence of this potential to calculate new values for the single-particle energies and corresponding wave-functions until convergence is reached according to the set criteria.

#### 2.2.1 The Skryme effective interaction

The basic idea of the Skyrme interaction for nuclear structure calculations to develop an energy functional, which could be expressed in terms of a zero-range expansion, leading to a simple derivation of the Hartree-Fock equations. The energy functional containing two parts such as the direct and exchange terms, having same mathematical structure. The Skyrme effective interaction that leads to a two-body density-dependent interaction that models the strong force in the particle-hole channel and contains central, spin-orbit and tensor contributions in coordinate space and called the standard analytical form, given by [78, 4],

$$v(\mathbf{r_1}, \mathbf{r_2}) = t_0(1 + x_0 \mathbf{P}_{\sigma})\delta(\mathbf{r}) + \frac{1}{2}t_1(1 + x_1 \mathbf{P}_{\sigma}) \left[\mathbf{P}^{\prime 2}\delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{P}^2\right] + t_2(1 + x_2 \mathbf{P}_{\sigma})\mathbf{P}^{\prime} \cdot \delta(\mathbf{r})\mathbf{P} + \frac{1}{6}t_3(1 + x_3 P_{\sigma}) \left[\rho(\mathbf{R})\right]^{\sigma}\delta(\mathbf{r}) + iW_0 \sigma \cdot \left[\mathbf{P}^{\prime} \times \delta(\mathbf{r})\mathbf{P}\right].$$
(2.42)

In the given effective interaction, the 1<sup>st</sup> term correspond to central part, 2<sup>nd</sup> & 3<sup>rd</sup> term are the non-local terms, 4<sup>th</sup> for density-dependent and *last* one for the spin-orbit interaction. Again,  $\mathbf{R} = \frac{1}{2}(\mathbf{r_1} + \mathbf{r_2})$  and  $\mathbf{r} = \frac{1}{2}(\mathbf{r_1} - \mathbf{r_2})$  are center-of-mass (*c.m.*) and relative co-ordinate respectively. The operators  $\mathbf{P}$  and  $\mathbf{P}'$  are acting on left with the expression,  $\mathbf{P} = \frac{1}{2i} (\nabla_1 - \nabla_2)$ . The *spin* operator  $\sigma = \sigma_1 + \sigma_2$  and the  $P_{\sigma} = \frac{(1+\sigma_1\cdot\sigma_2)}{2}$ . From this standard form of Eqn. (2.42), the total binding energy of a nucleus can be expressed as [78]:

$$\langle |H| \rangle = \int \mathcal{H}(\mathbf{r}) dr,$$
 (2.43)

here,  $\mathcal{H}$ , is the total Hamiltonian density functional, and is given by,

$$\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{eff} + \mathcal{H}_{fin} + \mathcal{H}_{so} + \mathcal{H}_{sg} + \mathcal{H}_{Coul}, \qquad (2.44)$$

where,  $\mathcal{K}$  is the kinetic term and is expressed as:

$$\mathcal{K} = \frac{\hbar^2}{2m}\tau = \frac{\hbar^2}{2m}(\tau_n + \tau_p), \qquad (2.45)$$

with  $\tau = \tau_n + \tau_p$ , called the total (sum of proton and neutron) kinetic energy density. The terms,  $\mathcal{H}_0$ ,  $\mathcal{H}_3$ ,  $\mathcal{H}_{eff}$ ,  $\mathcal{H}_{fin}$ ,  $\mathcal{H}_{so}$ ,  $\mathcal{H}_{sg}$  and  $\mathcal{H}_{Coul}$  are the density functional for zero-range, density-dependent, effective-mass, finite-range, spin-orbit, tensor-coupling and Coulomb correction, respectively. The corresponding expression for these terms are as follow:

$$\mathcal{H}_0 = \frac{1}{4} t_0 \left[ (2+x_0)\rho^2 - (2x_0+1)(\rho_p^2+\rho_n^2) \right],$$

$$\mathcal{H}_3 = \frac{1}{24} t_3 \rho^{\eta} \left[ (2+x_3)\rho^2 - (2x_3+1)(\rho_p^2+\rho_n^2) \right],$$

$$\mathcal{H}_{eff} = \frac{1}{8} \left[ t_1(2+x_1) + t_2(2+x_2) \right] \tau \rho + \frac{1}{8} \left[ t_2(2x_2+1) - t_1(2x_1+1) \right] (\tau_p \rho_p + \tau_n \rho_n).$$

$$\mathcal{H}_{fin} = \frac{1}{32} \left[ 3t_1(2+x_1) - t_2(2+x_2) \right] (\nabla \rho)^2 - \frac{1}{32} \left[ 3t_1(2x_1+1) + t_2(2x_2+1) \right] \times \left[ (\nabla \rho_{\mathbf{n}})^2 + (\nabla \rho_{\mathbf{p}})^2 \right]$$

$$\mathcal{H}_{so} = \frac{1}{2} W_0 \left[ \mathbf{J} \cdot \nabla \rho + \mathbf{J}_{\mathbf{p}} \cdot \nabla \rho_{\mathbf{p}} + \mathbf{J}_{\mathbf{n}} \cdot \nabla \rho_{\mathbf{n}} \right]$$

$$\mathcal{H}_{sg} = -\frac{1}{16} \left[ (t_1 x_1 + t_2 x_2) \mathbf{J}^2 - (t_1 - t_2) (\mathbf{J}_{\mathbf{p}}^2 + \mathbf{J}_{\mathbf{n}}^2) \right]$$
  
and

$$\mathcal{H}_{Coul} = \frac{1}{2} \int \frac{\rho_p(\mathbf{r_2})}{|\mathbf{r_1} - \mathbf{r_2}|} d^3 r_2 - \frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3}(\mathbf{r_1}).$$
(2.46)
The term  $\mathcal{H}_{Coul}$ , containing two parts correspond to direct and exchange at Slater level [78]. The total density  $\rho = \rho_p + \rho_n$ , kinetic density  $\tau = \tau_n + \tau_p$  and the spin density  $\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p$ . The corresponding expressions for these density are as follow:

$$\rho_q(\mathbf{r}) = \sum_{i=1}^{A_q} \sum_{\sigma} |\phi_i(\mathbf{r}, \sigma, q)|^2, \qquad (2.47)$$

$$\tau_q(\mathbf{r}) = \sum_{i=1}^{A_q} \sum_{\sigma} |\nabla \phi_i(\mathbf{r}, \sigma, q)|^2, \qquad (2.48)$$

and

$$J_q(\mathbf{r}) = i \sum_{i=1}^{A_q} \sum_{\sigma,\sigma'} \phi_i^*(\mathbf{r},\sigma,q) \left[ (\sigma)_{\sigma,\sigma'} \times \nabla \right] \phi_i(\mathbf{r},\sigma,q), \qquad (2.49)$$

where,  $\phi_i$  is the single-particle wave function with *orbital*, *spin* and *isospin* quantum numbers. The total binding energy (BE) of a nucleus is the integral of the energy density functional  $\mathcal{H}$ . At least more than one-hundred parameterizations of the Skyrme interaction are published since 2012 (see, e.g., [81]). This parameter sets are designed for considerations of proper experimental data for finite nuclei and saturation properties of infinite nuclear matter [78, 82, 83, 79, 84]. The details of the analytical expression and method of calculations are given in Refs. [78, 79, 84].

## 2.3 Pairing Correlations

The pairing effect plays an important role in the correct description of nuclear structure phenomena in open-shell and deformed nuclei. We know that the mean-field calculations are only taken care to the long-range part of the nucleon-nucleon interaction, the shortrange pairing correlations have to be incorporated in addition. It is an attractive force that occurs between identical nucleons in the same *j*-orbit. For examples the groundstate spin of all even-even nuclei is  $0\hbar$ , which implies that there is an induction of force that couples the nucleons pair such that their angular momenta cancel out. According to extreme particle model, the ground-state spin is determined by the spin of last nucleon, which plays for an important contribution to the ground state energy of that nucleus. In general, the masses of even-even nuclei are much larger than the neighboring even-oddor odd - odd mass nuclei which suggests that the binding energy is much larger when a nucleon is added to an odd-mass than to an even-mass nuclei. The pairing not only couples nucleons in states j to  $J^{\pi} = 0^+$  but also to  $J'^{\pi} = 0^+$  composed from two nucleons in different states j and j'. The nucleons of an orbit scatter to another orbit by the effect of pairing. This phenomenon is not the case for the nucleons far below the Fermi surface but near the Fermi surface, there is some probability that orbits are not fully occupied, may cause this scattering to take place, which causes the smearing of Fermi surface. The smearing of the surface leads to the concept of quasi-particles which can be considered as the linear combination of hole and particle wave functions.

The Lagrangian density of the RMF and the effective interaction in the SHF used here, does not contain any term to include pairing correlations to the interaction. The pairing correlations can only be described in a generalized single-particle theory by field operators  $\psi^{\dagger}\psi^{\dagger}$  or  $\psi\psi$  and two-body interaction of the type  $\psi^{\dagger}\psi^{\dagger}\psi\psi$  on the classical level, which do not conserve the particle number. Therefore, the pairing correlations are often included in a phenomenological way with the simple BCS [85] approximation. It is worth mentioning that the BCS approach provides a reasonably good description of the pairing properties for known nuclei, close to or not too far from the stability line. However, for the nuclei in the vicinity of the drip-lines or to the super-heavy region the coupling to the continuum becomes important. It has been shown that the self-consistent treatment of the BCS approximation breaks down when coupling between bound states and states in the continuum takes place [86]. The derivation of these correlations on quantum level would be possible by deducing the nucleon-nucleon interaction resulting after the quantization of meson fields from exchange of mesons. However, we are not taking that aspect here and adopted a simpler approach incorporating the effects in a constant gap approximation in the above mentioned scheme introducing occupation

numbers  $(n_i)$ . The occupation number  $(n_i)$  for pure Hartree approximation is:

$$n_i = \begin{cases} 1 & \text{for occupied levels} \\ 0 & \text{for non-occupied levels.} \end{cases}$$
(2.50)

We have already mentioned that the smearing of the Fermi surface is due to the unoccupied (not completely occupied) orbit near to the Fermi and causes scattering. In case of without pairing, the orbits would simply be filled sequentially in accordance with the Pauli principle until all A nucleons had been placed in the lowest orbits, giving sharply defined surface, which clearly reflect in the schematic diagram (Fig. 2.2). The effect of pairing causes the smearing of Fermi surface which leads to the concept of quasi-particle, and can be considered as a linear combination of particle and hole wave functions. The occupation probability of  $i^{th}$  state can expressed in terms of a particle  $v_i^2$  and a hole  $u_i^2$  (see Eqns. 2.53-2.54). One can say, the RMF and SHF approaches without pairing interaction can be applied to doubly magic nuclei and the nuclei at very large angular momenta where the pairing is considerably quenched. The variation with the occupation number  $v_i^2$  gives the BCS-equations:

$$2\epsilon_i u_i v_i - \Delta (u_i^2 - v_i^2) = 0 \tag{2.51}$$

with

$$\Delta = G \sum_{i=1}^{N} u_i v_i, \tag{2.52}$$

here, G and  $\Delta$  are the pairing strength and constant pairing gap parameter, respectively. The  $\Delta$  is basically of the order of spacing between single-particle energies in the neighborhood of Fermi energy. This equation has well known solution  $v_i^2$ , the occupation and  $u_i^2$  ( $v_i^2 + u_i^2 = 1$ ), the non-occupation probabilities are given by [87, 88],

$$v_i^2 = \frac{1}{2} \left\{ 1 - \frac{\epsilon_i - \lambda}{\sqrt{(\epsilon_i - \lambda)^2 + \Delta^2}} \right\}$$
(2.53)

Figure 2.2: The schematic diagram for the smearing of the Fermi surface due to the pairing interaction, which is understood in terms of the scattering of pairs of particles in a time reversed orbit, j to another, j'.

and

$$u_i^2 = \frac{1}{2} \{ 1 + \frac{\epsilon_i - \lambda}{\sqrt{(\epsilon_i - \lambda)^2 + \Delta^2}} \}, \qquad (2.54)$$

where  $\epsilon_i$  is the single particle energy of  $i^{th}$  nucleon,  $\lambda$  is the chemical potential. The pairing gap for protons and neutrons, as given in Ref. [87, 88], which is valid for the nuclei on or away from the  $\beta$ -stability line and are as follows:

$$\Delta_p = RB_s e^{sI - tI^2} / Z^{1/3}$$
 and (2.55)

$$\Delta_n = RB_s e^{-sI - tI^2} / A^{1/3}, \tag{2.56}$$

with R = 5.72, s = 0.118, t = 8.12,  $B_s = 1$ , and I = (N - Z)/(N + Z). The pairing force constant G is not calculated explicitly in solving the RMF equations. Using the above gap parameter, we calculate directly the occupation probability. The chemical potentials  $\lambda_n$  and  $\lambda_p$  are determined by the particle numbers for protons and neutrons. Using these above equations, the pairing energy is:

$$E_{pair} = -\Delta \sum_{i=1}^{A} u_i v_i. \tag{2.57}$$

The above prescription for pairing effects, both in relativistic mean field and Skryme-Hartree-Fock, has already been used by us and many other authors [70, 89, 90]. For this pairing approach, it is shown [70, 89, 66, 91] that the results for binding energies and quadruple deformations are almost identical with the predictions of relativistic Hartree-Bogoliubov (RHB) approach.

### 2.3.1 Pauli Blocking

The bulk properties of odd-even, even-odd or odd-odd nuclei in mean-field approach is not conventional, because of the violation in the time reversal symmetry. To deal such nuclei, one needs to include some additional time-odd term, as is done in the SHF Hamiltonian [4], or has to include empirically the pairing force in order to take care the effect of odd-nor odd-p [92]. In case of RMF, the space component of the vector fields, which are odd under time reversal and parity, are neglected. These are important in the determination of magnetic moments [67], but have a very small effect on bulk properties like binding energies or quadrupole deformations, and can be neglected [66] in the present context. Here, for the odd-A calculations, we employ the blocking approximation, which restores the time-reversal symmetry.

In this approach one pair of conjugate states,  $\pm m$ , is taken out from the pairing scheme. The odd particle stays in one of these states and its corresponding conjugate state remains empty. In principle, one has to block in turn different states around the Fermi level to find the one which gives the lowest energy configuration of the odd nucleus. For *odd-odd* nuclei, one needed to block both the *odd-n* and *odd-p*. Similar procedure is carried for *odd-A* calculations in the SHF formalism. For details we refer the readers to see Ref. [70].

## 2.4 Parametrizations

Based on the bulk properties of finite nuclei and key features of nuclear matter at saturation density are used as a phenomenological input for adjustment of the effective forces. The most paramount one is the total binging energy of nucleus which can be obtained by numerical solutions of the mean-field equations, corrected also for spurious motion. The nuclear charge density also provides some structure information like nuclear shape and is determined by elastic electron scattering. It is important to take separately the density for proton and neutron in a nucleus to determine the intrinsic electromagnetic structure of the nucleons. The diffraction radius, root-mean-square radius and surface thickness are the responsible against for the determination of the charge form factor at low momentum. For this region, the calculation of charge radius from full charge form factor is difficult, approximations are often used for simplification [93]. Again, the isotopic shift of charge mean-square radii also an observable can directly accessible from experiments. In case of charge radius, the most useful information comes from proton distribution than that of a neutron, since some information also related to neutron distribution.

The effective interactions are also widely characterized by infinite nuclear matter properties at saturation density. The most important and common features are energy per particle (often called energy density) with its minimum value at saturation density. The symmetry energy and compressibility of nuclear matter corresponding to the curvature around saturation point and related to, e.g., giant monopole resonance. Isovector curvature at saturation point determines the symmetry energy, and due to quasi-particle nature of mean-field models, an important quantity is also nucleon effective mass. The

Table 2.2: The nuclear matter properties at saturation density for different force parameters. Here,  $\rho_0$  is the saturation density,  $e(\rho)$  stands for binding energy per particle,  $E_{sym}$  is the symmetry energy,  $K_0$  is the incompressibility and the nucleon effective mass  $m^*/m$ , all at saturation density  $\rho_0$ .

Force	Ref.	$ ho_0$	$e(\rho)$	$E_{sym}$	$K_0$
		$(fm^{-3})$	MeV)	(MeV)	(MeV)
Simple effective Interaction					
SEI-I	[95]	0.157	-16.0	34.0	245.0
SEI-II	[95]	0.161	-15.9	33.0	247.0
SEI-III	[95]	0.161	-15.8	32.0	242.0
Gogny effective interaction					
D1	[43]	1.35	-16.02	29.04	228.0
D1S	[96]	0.35	-16.32	27.39	209.0
D1M	[92]	0.165	-16.03	28.55	225.0
Skryme effective interaction					
SIII	[97]	0.145	-15.85	28.16	355.4
SkI4	[44]	0.160	-15.95	29.50	247.9
SkMP	[98]	0.157	-15.56	29.89	230.9
SLy4	[79]	0.160	-15.97	32.0	229.9
Relativistiv mean field					
NL-Z2	[53]	0.151	-16.07	30.03	172.0
NL-BA	[100]	0.150	-16.19	34.73	248.0
NL3	[101]	0.148	-16.24	37.40	272.0
NL3*	[99]	0.150	-16.31	38.68	258.3
G2	[70]	0.153	-16.07	36.40	215.0

Table 2.3: The compilation of various observables considered for different forces, taken from Ref. [3]. Here, E = binding energy,  $r_{ch} =$  charge radius,  $R_{ch} =$  charge diffraction radius,  $\sigma_{ch} =$  charge surface thickness,  $\delta r_{ch}^2 =$  isotopic shift in charge radius,  $r_n =$  neutron root-mean-square radius and  $W_0$  for spin-orbit strength parameter for finite nuclei and the quantity such as  $e(\rho) =$  binding energy per particle,  $E_{sym} =$  symmetry energy,  $K_0$ = incompressibility moduli  $m^*/m$  = nucleon effective mass for infinite nuclear matter at saturation density  $\rho_0$ .

Simple effective Interaction (SEI-I-III [95])	
E	$^{16}O,  {}^{40}Ca,  {}^{208}Pb$
$r_{ch}$	$^{16}$ O, $^{40}$ Ca, $^{208}$ Pb
$W_0$	<sup>16</sup> O (1 $p_{3/2}$ ; 1 $p_{1/2}$ )
Pairing	even - odd energy in Sn isotopes
INM	$e(\rho), E_{sym}, m^*/m, K_0$
Gogny effective interaction $(D1 \text{ and } D1S [43, 96])$	
E	$^{16}$ O, $^{40}$ Ca, $^{90}$ Zr
$r_{ch}$	$^{16}$ O, $^{40}$ Ca, $^{90}$ Zr
$W_0$	<sup>16</sup> O (1 $p_{3/2}$ ; 1 $p_{1/2}$ )
Pairing	even - odd energy in Sn isotopes
INM	$e(\rho), E_{sym}, m^*/m, K_0$
Skryme effective interaction $(SkI1-5 [44])$	
E	$^{16}\mathrm{O},^{40,48}\mathrm{Ca},^{56,78}\mathrm{Ni},^{132}\mathrm{Sn},^{208}\mathrm{Pb}$
$r_{ch}$	$^{16}\mathrm{O},~^{40,48}\mathrm{Ca},~^{56}\mathrm{Ni},~^{208}\mathrm{Pb}$
$W_0$	<sup>208</sup> Pb $(3p_{3/2}; 3p_{1/2})$
INM	$e(\rho), E_{sym}, m^*/m, K_0, EOS_{ns}$
Relativistic mean field ( $NL3 & NL3^*$ [101, 99])	
E	<sup>16</sup> O, <sup>40,48</sup> Ca, more <sup>208</sup> Pb, <sup>214</sup> Pb
$r_{ch}$	$^{16}\mathrm{O},^{40,48}\mathrm{Ca},\mathrm{more}^{208}\mathrm{Pb},^{214}\mathrm{Pb}$
$r_n$	$^{40,48}\mathrm{Ca},^{58}\mathrm{Ni},^{116}\mathrm{Sn},^{208}\mathrm{Pb}$
INM	$e(\rho), E_{sym}, m^*/m, K_0$

nucleon effective mass is the key quantity for determining the splitting of level in finite nuclear properties. For more detailed information and definition of these quantities see Refs.[3, 81]. The actual values these infinite nuclear matter observables saturation density for different forces are listed in Table. 2.2 [43, 79, 92, 94, 95, 96, 97, 98, 99, 100, 101].

In relativistic mean-field and Skryme-Hartree-Fock, the extension have been made to study of surface properties (key observables) like asymmetry coefficients and the surface thickness, in case of semi-infinite nuclear matter. A special attention or effort has been paid to deal open shell nuclei i.e. the the pairing gap and odd-even staggering of masses. The most general thing is that, in case a unpaired nucleon, the contribution is not half of a full pair, and it also break the intrinsic time-reversal invariance. Which cause, all other nucleons to rearrange themselves, that adds a contribution from the mean-field to odd-even staggering [94]. Which cause bail one out situation to deal both mean-field and pairing contributions at one. So, inclusion of pairing correlations give significant corrections to several observables which can be used to determine the parameters of more complicated pairing interactions. There are many possibilities or different way for a choice of phenomenological input for an effective force. Some of the popular and mostly used parametrizations with these inputs are listed in Tables. 2.2-2-3 [43, 79, 92, 94, 95, 96, 97, 98, 99, 100, 101]. One can find, there are some differences between relativistic and non-relativistic models in their kinematics such as the energy per baryon, saturation density, effective mass ratio and also incompressibility modulus. Still, the Gogny force, the Skyrme energy functional as well as the relativistic meanfield parametrizations are able to describe nuclear bulk properties of nuclear matter and finite nuclei very satisfactorily. Addition to these, the excitation properties such as fission, vibrational states, rotations and giant resonances also be very well accommodated. However, some problems arise in these models in some observables for extrapolate region or exotic regions. For more detailed information about weaknesses and open problems in description of finite nuclei and nuclear matter for these effective model, see the review of Ref. [3].

# Chapter 3

# Microscopic origin of NN- Potential

## 3.1 Introduction

In the preceding half century, the work had been devoted to the nucleon-nucleon (NN) interaction problem than to any other question in nuclear physics [102]. This field of research is born since 1932, the discovery of neutron by Chadwick as the heart of nucleus. In fact, during the first few decades, the term "Nuclear Force" was usually used as synonymous for the force as a whole. At that time, the exact form of inter-nucleon force is not known as explicitly than that of the Coulomb force. In its simplest form the nucleon-nucleon (NN) potential is considered as central and to have square-well, Gaussian or Yukawa potential form. Usually a finite sum of Yukawa potentials of various ranges and strengths are able to obtain agreement with the observed phase shifts in elastic-scattering processes for the NN potential. Still, this form of the potential is one obtained by fitting to the experimental data. The traditional goal of nuclear physics is to understand properties of atomic nuclei in terms of the 'bare' interaction between pairs of nucleons. Though substantial progress has taken place to understand it in a number of theoretical (and experimental) attempts, it still remains an open problem. A large number of interactions have been constructed via studying NN scattering, but extensive modifications in the scattering behaviour due to the presence of many other nucleons inside the nucleus. The phenomenological effective effective or averaged interactions

having appropriate form to use, which typically depend on the local density of nuclear matter.

In the intermediate stage, H. Yukawa suggested that the interaction between two nucleons is affected by the exchange of a particle, like the interaction between the electric charges by the exchange of a photon. As the nucleon interactions is short-range in nature, this implies the intermediate particle must be finite mass. From quantum uncertainty principle, one can correlate the range and mass roughly as  $r \sim \frac{1}{m}$ , therefore, the mass of one unit (quanta) exchanged is about  $fm^{-1}$ , which is around 200 MeV. Almost after 20 years, the particle was identified as  $\pi$ -meson (and mass 140 MeV). This is one of the most significant aspect of the Yukawa theory is generalizing the relation between particles and forces. The existence of strong interactions implies the existence of a new particle, was considered a novel and radical idea at that time. The modern theory of NN potential through particle exchanges is made possible by the development of quantum field theory. However, at low-energy, one can assume that the interactions is instantaneous and therefore the concept of interaction potential becomes useful. The derivation of a potential through particle exchange, is important to understand the nuclear force as well as structural properties. For example, the effective NN interaction is remarkably related to the nucleus-nucleus optical potential [103] for the study of radioactivity. The present chapter is organized as follows. Section II includes the details of derivation of NN-potential through meson exchange from linear and non-liner relativistic mean field Lagrangian. The obtained results and their application in nuclear radioactivity are discussed in section III. A summary of the results obtained, together with concluding remarks, is given in Section IV.

## **3.2** Mathematical formulation

### 3.2.1 Linear case

The present study is motivated toward the derivation of the microscopic origin of nucleonnucleon interaction from the relativistic mean field (RMF) Lagrangian density [104, 105]. In the earlier discussion (see Chapter 2), the nucleons fields in RMF are given by the wave-function of the nucleons, several mesons and electromagnetic fields. Here, the nucleons are not interact to each other directly, but the interaction only possible via meson fields. Hence, the linear relativistic mean field (L-RMF) Lagrangian density for a nucleon-meson many-body system [104, 105], is given as:

$$L = \overline{\psi_i} \{ i\gamma^{\mu} \partial_{\mu} - M \} \psi_i + \frac{1}{2} \partial^{\mu} \sigma \partial_{\mu} \sigma - \frac{1}{2} m_{\sigma}^2 \sigma^2 - g_{\sigma} \overline{\psi_i} \psi_i \sigma - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_w^2 V^{\mu} V_{\mu} - g_w \overline{\psi_i} \gamma^{\mu} \psi_i V_{\mu} - \frac{1}{4} \vec{B}^{\mu\nu} . \vec{B}_{\mu\nu} + \frac{1}{2} m_{\rho}^2 \vec{R}^{\mu} . \vec{R}_{\mu} - g_{\rho} \overline{\psi_i} \gamma^{\mu} \vec{\tau} \psi_i . \vec{R}_{\mu} - \frac{1}{2} m_{\delta}^2 \delta^2 + g_{\delta} \overline{\psi_i} \delta \vec{\tau} \psi_i,$$
(3.1)

where, the field for  $\sigma$  meson is denoted by  $\sigma$ , for  $\omega$  meson by  $V_{\mu}$ , and for the iso-vector  $\rho$ and  $\delta$  mesons by  $\vec{R}_{\mu}$  and  $\delta$ , respectively. The  $\psi_i$  are the Dirac spinors for the nucleons. The iso-spin and the third component of the iso-spin are denoted by  $\tau$  and  $\tau_3$ , respectively. Here  $g_{\sigma}$ ,  $g_{\omega}$ ,  $g_{\rho}$  and  $g_{\delta}$  are the coupling constants for  $\sigma$ ,  $\omega$ ,  $\rho$  and  $\delta$  mesons, respectively. The masses of nucleons,  $\sigma$ ,  $\omega$ ,  $\rho$  and  $\delta$  mesons are denoted by M,  $m_{\sigma}$ ,  $m_{\omega}$ ,  $m_{\rho}$  and  $m_{\delta}$ , respectively.  $\Omega^{\mu\nu}$  and  $\vec{B}_{\mu\nu}$  are the field tensors for the  $V^{\mu}$  and  $\vec{R}_{\mu}$ , respectively. If, we neglect the  $\rho$ - and  $\delta$  meson, it correspond to Walecka model in its original form [7, 8]. From the above relativistic Lagrangian, we obtain the field equations for the nucleons and mesons as,

$$\left(-i\alpha. \nabla + \beta(M + g_{\sigma}\sigma) + g_{\omega}\omega + g_{\rho}\tau_{3}\rho_{3} + g_{\delta}\delta\tau\right)\psi_{i} = \epsilon_{i}\psi_{i}, \qquad (3.2)$$

$$(-\nabla^2 + m_{\sigma}^2)\sigma(r) = -g_{\sigma}\rho_s(r), \qquad (3.3)$$

$$(-\nabla^2 + m_{\omega}^2)V(r) = g_{\omega}\rho(r), \qquad (3.4)$$

$$(-\nabla^2 + m_{\rho}^2)\rho(r) = g_{\rho}\rho_3(r),$$
 (3.5)

$$(-\nabla^2 + m_\delta^2)\delta(r) = -g_\delta\rho_3(r), \qquad (3.6)$$

for Dirac nucleons,  $\sigma$ ,  $\omega$ ,  $\rho$ ,  $\delta$  mesons, respectively. In the limit of one-meson exchange, for a heavy and static baryonic medium, the solution of single nucleon-nucleon potential for scalar ( $\sigma$ ,  $\delta$ ) and vector ( $\omega$ ,  $\rho$ ) fields are given by,

$$V_{\sigma}(r) = -\frac{g_{\sigma}^{2}}{4\pi} \frac{e^{-m_{\sigma}r}}{r}, \quad V_{\delta}(r) = -\frac{g_{\delta}^{2}}{4\pi} \frac{e^{-m_{\delta}r}}{r}$$
  
and  
$$V_{\omega}(r) = +\frac{g_{\omega}^{2}}{4\pi} \frac{e^{-m_{\omega}r}}{r}, \quad V_{\rho}(r) = +\frac{g_{\rho}^{2}}{4\pi} \frac{e^{-m_{\rho}r}}{r}.$$
(3.7)

The total effective nucleon-nucleon potential is obtained from the scalar and vector parts of the meson fields. This can be expressed as [104],

$$v_{eff}(r) = V_{\omega} + V_{\rho} + V_{\sigma} + V_{\delta} = \frac{g_{\omega}^2}{4\pi} \frac{e^{-m_{\omega}r}}{r} + \frac{g_{\rho}^2}{4\pi} \frac{e^{-m_{\rho}r}}{r} - \frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r} - \frac{g_{\delta}^2}{4\pi} \frac{e^{-m_{\delta}r}}{r}.$$
 (3.8)

For a normal nuclear medium, the contribution of  $\delta$ -meson to the potential ,  $V_{\delta}$  can be neglected, compared to the magnitudes of both  $V_{\omega}$  and  $V_{\sigma}$ . It is important to include the contribution of single-nucleon exchange effects to the effective interaction [103]. Hence, Eqn. (3.8) becomes

$$v_{eff}(r) = \frac{g_{\omega}^2}{4\pi} \frac{e^{-m_{\omega}r}}{r} + \frac{g_{\rho}^2}{4\pi} \frac{e^{-m_{\rho}r}}{r} - \frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r} + J_{00}(E)\delta(s),$$
(3.9)

with  $J_{00}(E)\delta(s) = -276(1 - 0.005E/A_{c(\alpha)})MeVfm^3$  as the zero-range pseudo-potential representing the exchange contribution.

### 3.2.2 Non-linear case

The Lagrangian density in the above Eqn. (3.1) contains only linear coupling terms, which is able to give a qualitative description of the nuclei [7, 8]. The essential nuclear matter properties like incompressibility and the surface properties of the finite nuclei cannot be reproduced quantitatively within this Lagrangian density. Again the interaction between a pair of nucleons when they are embedded in a heavy nucleus is less than when they are in empty space. This suppression of the two-body interactions within a nucleus in favour of the interaction of each nucleon with the average nucleon density, means that the non-linearity acts as a smoothing mechanism and hence leads in the direction of the one-body potential and shell structure [60, 57]. The replacement of mass term  $\frac{1}{2}m_{\sigma}^2$  of  $\sigma$ field by  $U(\sigma)$ , which is nothing but the non-linear self coupling amongst the  $\sigma$  mesons and the form as [60, 57]:

$$U(\sigma) = \frac{1}{2}m_{\sigma}^{2} + \frac{1}{3}g_{2}\sigma^{3} + \frac{1}{4}g_{3}\sigma^{4}.$$
 (3.10)

Here, the non-linear parameter  $g_2$  and  $g_3$  are adjusted to the surface properties of finite nuclei. The most successful fits yield, the +ve and -ve signs for  $g_2$  and  $g_3$ , respectively. The negative value of  $g_3$  is a serious problem in quantum field theory. As, we are dealing within the mean field level and with normal nuclear matter density, the corresponding  $\sigma$  field is very small and the -ve value of  $g_3$  is still allowed [57]. Now the field equation for for  $\sigma$ - field (in Eqn. (3.2)) is modified with the form,

$$(-\nabla^2 + m_{\sigma}^2)\sigma(r) = -g_{\sigma}\rho_s(r) - g_2\sigma^2(r) - g_3\sigma^3(r).$$
(3.11)

Because of the great difficulty in solving the above nonlinear differential equations, it is essential to have a variation principle available for the estimation of the energies associated with various source distributions. In the static case, the negative sign of the third term in the Lagrangian is computed with the correct source function and an arbitrary trial wave function. The limit on the energy has a stationary value equal to the correct energy when the trial function is in the infinitesimal neighborhood of the correct wave function. Now, the solution for the modified  $\sigma$  field is given as [57]

$$V_{\sigma} = -\frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r} + \frac{g_2^2}{4\pi} \frac{e^{-2m_{\sigma}r}}{r^2} + \frac{g_3^2}{4\pi} \frac{e^{-3m_{\sigma}r}}{r^3},$$
(3.12)

Table 3.1: The values of  $m_{\sigma}$ ,  $m_{\omega}$ ,  $m_{\rho}$  (in MeV) and  $g_{\sigma}$ ,  $g_{\omega}$ ,  $g_{\rho}$  for different RMF forces, along with  $\frac{g_{\sigma}^2}{\pi}$ ,  $\frac{g_{\omega}^2}{\pi}$ ,  $\frac{g_{\rho}^2}{\pi}$  (in MeV) [104, 105]. The values for the non-linear self-coupling constant for RMF (NL3) such as  $g_2$  and  $g_3$  are not listed.

Set	$m_{\sigma}$	$m_{\omega}$	$m_{ ho}$	$g_{\sigma}$	$g_\omega$	$g_ ho$	$\frac{g_{\sigma}^2}{\pi}$	$rac{g_\omega^2}{\pi}$	$\frac{g_{ ho}^2}{\pi}$
HS	520	783	770	10.47	13.80	08.08	6882.64	11956.94	4099.06
Z	551.31	780	763	11.19	13.83	10.89	7861.80	12008.98	7445.91
W	550	783	_	09.57	11.67	_	5750.24	8550.74	_
L1	550	783	_	10.30	12.60	_	6660.95	9967.88	_
NL3	508.194	782.5	763.0	08.31	13.18	6.37	6554.34	10395.78	1257.92

The new NN-interaction analogous to M3Y form and is able to improve the incompressibility and deformation of the finite nuclei results [42]. In addition to this, the non-linear self coupling of the  $\sigma$ -meson helps to generate the repulsive part of the NN potential at long distance to satisfy the saturation properties (Coester-band problem) [35]. The modified effective nucleon-nucleon interaction is defined as [104, 105]:

$$v_{eff}(r) = V_{\omega} + V_{\rho} + V_{\sigma} + V_{\delta}$$
  
=  $\frac{g_{\omega}^2}{4\pi} \frac{e^{-m_{\omega}r}}{r} + \frac{g_{\rho}^2}{4\pi} \frac{e^{-m_{\rho}r}}{r} - \frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r}$   
+  $\frac{g_2^2}{4\pi} \frac{e^{-2m_{\sigma}r}}{r^2} + \frac{g_3^2}{4\pi} \frac{e^{-3m_{\sigma}r}}{r^3} - \frac{g_{\delta}^2}{4\pi} \frac{e^{-m_{\delta}r}}{r}.$  (3.13)

Neglecting the contribution  $V_{\delta}$  of  $\delta$ -meson and the introduction of the single-nucleon exchange effects [103], becomes

$$v_{eff}(r) = \frac{g_{\omega}^2}{4\pi} \frac{e^{-m_{\omega}r}}{r} + \frac{g_{\rho}^2}{4\pi} \frac{e^{-m_{\rho}r}}{r} - \frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r} + \frac{g_{2}^2}{4\pi} \frac{e^{-2m_{\sigma}r}}{r^2} + \frac{g_{3}^2}{4\pi} \frac{e^{-3m_{\sigma}r}}{r^3} + J_{00}(E)\delta(s).$$
(3.14)

## 3.3 Results and Discussion

From the above expression in Eqns. (3.9, 3.14), the effective nucleon-nucleon potential entitled as R3Y is presented eloquently in terms of the well known inbuilt RMF theory parameters of  $\sigma$ ,  $\omega$  and  $\rho$  meson fields, i.e., their masses  $(m_{\sigma}, m_{\omega}, m_{\rho})$  and coupling constants  $(g_{\sigma}, g_{\omega}, g_{\rho})$ . The values of these constants are different from each other for various forces of RMFT. Here we have taken few forces and their constants, the estimate values of  $\frac{g_{\omega}^2}{\pi}$ ,  $\frac{g_{\rho}^2}{\pi}$  and  $\frac{g_{\sigma}^2}{\pi}$  are also listed in Table 3.1 [104, 105]. For the W and L1 sets, only  $\frac{g_{\omega}^2}{\pi}$  and  $\frac{g_{\sigma}^2}{\pi}$  are given since the contribution of  $\rho$  meson is ignored for these two parameter sets. Except, *NL3* force in the table, all other are applicable to linear Lagrangian density. As an illustrative case, the  $v_{eff}(r)$  for HS parameter (see Table 3.1) by using in Eqn. (3.9) is given as:

$$v_{eff}(r) = 11957 \frac{e^{-3.97r}}{4r} + 4099 \frac{e^{-3.90r}}{4r} - 6883 \frac{e^{-2.64r}}{4r},$$
 (3.15)

and for the L1 parameters, Eqn. (3.1) becomes

$$v_{eff}(r) = 9968 \frac{e^{-3.97r}}{4r} - 6661 \frac{e^{-2.79r}}{4r}.$$
(3.16)

The corresponding effective NN-interaction potentials, denoted by L-R3Y (HS) and L-R3Y(L1), etc. with L at the initial of R3Y stands for linear case. Similarly for non-linear case using NL3 parameter, Eqn. (3.14) becomes,

$$v_{eff}(r) = 10395 \frac{e^{-3.97r}}{4r} + 1257 \frac{e^{-3.87r}}{4r} - 6554 \frac{e^{-2.58r}}{4r} + 6830 \frac{e^{-5.15r}}{4r^2} + 52384 \frac{e^{-7.73r}}{4r^3} + J_{00}(E)\delta(s).$$
(3.17)

The corresponding NN-interaction denoted by N-R3Y (NL3) with N at the initial of R3Y stands for non-linear case. The well known effective NN-interaction potentials, like M3Y [Eqn. (3.18) below] and other R3Y's based on Eqn. (3.15-3.17). The M3Y effective

interaction, obtained from a fit of the G - matrix elements based on Reid-Elliott softcore NN interaction [103], in an oscillator basis, is the sum of three Yukawa's with ranges 0.25 fm for a medium-range attractive part, 0.4 fm for a short-range repulsive part and 1.414 fm to ensure a long-range tail of the one-pion exchange potential (OPEP). The widely used M3Y effective interaction  $v_{eff}(r)$  without the OPEP term is given by

$$v_{eff}(r) = 7999 \frac{e^{-4r}}{4r} - 2134 \frac{e^{-2.5r}}{2.5r},$$
(3.18)

where ranges are in fm and the strength is in MeV. Note that Eqns. (3.9,3.18) represents the spin- and isospin-independent parts of the central component of the effective NN interaction, and that the OPEP contribution is absent here. The results obtained for the NN-potential from Eqns. (3.9) and (3.14) for these forces (see. Table 3.1) are shown in Fig. 3.1 along with the M3Y-interaction. Comparing Eqns.(3.9) and (3.14) with (3.18), we find very good similarity in behaviour of the NN-interactions, which makes us believe that Eqns. (3.9, 3.14) can be used to obtain the nucleus-nucleus optical potential. Using the NN-potentials so obtained, the optical potential for the study of cluster radioactivity is demonstrated in the next sub-section. Which is the one of the best applications of Eqns. (3.9) and (3.14).

### **3.3.1** *R3Y* on cluster radioactivity

The optical potential  $V_n(R)$  between the cluster (c) and daughter (d) nuclei is determined from the well known double folding and by single folding procedure [103] with the respective RMF density of the nuclei  $\rho_c$  and  $\rho_d$ . If the cluster is a nucleon, then double folding gives the form of single folding. The form of the potential are given as [104, 105]:

$$V_{n}(\vec{R}) = \int \rho_{c}(\vec{r}_{c})\rho_{d}(\vec{r}_{d})v_{eff}(|\vec{r}_{c} - \vec{r}_{d} + \vec{R}| \equiv r)d^{3}r_{c}d^{3}r_{d}$$
  
or  

$$V_{n}(\vec{R}) = \int \rho_{d}(\vec{r})v(|\vec{r} - \vec{R}|)d^{3}r.$$
(3.19)

Figure 3.1: The L-R3Y (for HS, Z, W and L1), N-R3Y for NL3 parameter set (see Table 3.1) and the M3Y effective NN interaction potentials as a function of r [104, 105].

Adding Coulomb potential  $V_C(R)$  (= $Z_d Z_c e^2/R$ ) results in cluster-daughter scattering potential V(R) [=  $V_n(R) + V_C(R)$ ], used in the following for calculating the WKB penetrability P, representing the relative motion R. The decay constant  $\lambda$  or half-life time  $T_{1/2}$  in the preformed cluster model (PCM) is defined as

$$\lambda_{PCM} = \frac{\ln 2}{T_{1/2}} = \nu_0 P_0 P, \qquad (3.20)$$

with the 'assault frequency'  $\nu_0$ , i.e., the frequency with which the cluster hits the barrier, given by

$$\nu_0 = \frac{velocity}{R_0} = \frac{(2E_c/\mu)^{1/2}}{R_0}.$$
(3.21)

Here  $R_0$  is the radius of parent nucleus and  $E_c$  is the kinetic energy of the emitted cluster. The impinging frequency  $\nu_0$  is nearly constant ~  $10^{21}$  s<sup>-1</sup> for all the observed clusterdecays [106]. Since both the emitted cluster and daughter nuclei are produced in ground state, the entire positive Q-value of decay is the total kinetic energy ( $Q = E_d + E_c$ ), available for the decay process, which is shared between the two fragments, such that for the emitted cluster  $E_c = A_d Q/A$ , and  $E_d (=Q - E_c)$  is the recoil energy of the daughter nucleus. The WKB penetration probability P is determined from the cluster tunneling through the interaction potential V(R), as shown in Fig. 3.2, having energy equal to the Q-value of the decay. Fig. 3.2 illustrates the total interaction potentials V(R) for <sup>14</sup>C decay of <sup>222</sup>Ra, obtained for both the M3Y+EX and R3Y+EX NN-interactions using RMF-HS densities. The penetration path with an energy equal to the Q-value of decay is also shown here (marked P, with an arrow). This is given by the WKB integral

$$P = exp[-\frac{2}{\hbar} \int_{R_a}^{R_b} \{2\mu[V(R) - Q]\}^{1/2} dR], \qquad (3.22)$$

with  $R_a$  and  $R_b$  as the first and second turning points, satisfying  $V(R_a) = V(R_b) = Q$ . The kinetic energy  $Q = BE_p - (BE_d + BE_c)$ , where  $BE_p$ ,  $BE_c$  and  $BE_d$  are the experimental ground-state (g.s.) binding energies of the parent, cluster and daughter nuclei, taken from Audi and Wapstra [107]. The reduced mass of the system is given as  $\mu = A_d A_c / (A_d + A_c)$ . From the figure, one can notice that the two potentials (M3Y and R3Y) are very different, particularly in the inner part. Compared to the M3Y NNinteraction, the barrier for the R3Y case is a bit lowered (shown more clearly in the inset of Fig. 3.2) and hence P is increased by a few orders of magnitude, as is shown in Table 2 for some decays. Another point is to note that cluster decay probes only the potential near the surface, and it will be an interesting study to explore the inner part of potential through, say, the alpha-alpha ( $\alpha - \alpha$ ) potential in future. In this connection, however, we remind the following two works: (i) Kelkar and Castaneda [108] have shown that, within the WKB approximation, the contribution of inner part of the potential between  $R \to 0$  and  $R_a$  is nearly same as the 'assault frequency'  $\nu_0$  in both alpha and cluster radioactive decay studies, obtaining  $\nu_0 \sim 10^{21} \text{ s}^{-1}$  for alpha decays. (ii) In another study [109], the S-matrix approach, which should depend on the entire potential, give alpha decay widths that compare very closely with the WKB result. In other words, the inner part of the potential for  $\alpha$  decays does not seem to play much significant role in S-Matrix calculations, and play the role of  $\nu_0$  in WKB calculations.

Figure 3.2: The total nucleus-nucleus optical potential V(R) and the individual contributions [the nuclear  $V_n(R)(M3Y + EX)$  and  $V_n(R)(R3Y + EX)$  for the HS parameter set, and the Coulomb  $V_C(R)$  potential] as a function of radial separation R. The inset shows the barrier height and position on a magnified scale. In the main figure as well as the inset, P simply denotes the penetration path between the two turning points  $R_a$ and  $R_b$  of the integral for calculating the WKB penetration probability P.

From the calculated  $\nu_0 P$ , an empirical estimate of the preformation factor  $P_0$  can be

Figure 3.3: The  $P_0^{c(emp)}$  for the cluster-decays, respectively, from various parents evaluated with the use of R3Y+EX and M3Y+EX effective NN interaction compared with the phenomenological model of Blendowske and Walliser [112].

obtained from the experimental  $\lambda_{Expt}$  values [106] by defining [104, 105, 106]

$$P_0^{emp} = \frac{\lambda_{Expt}}{\nu_0 P}.$$
(3.23)

It is relevant to mention here that some authors [110, 111], working within the mean field based folding procedure using the Skyrme or M3Y force, assumes the preformation factor  $P_0=1$ , whereas we show in the following (Table 3.2) that empirical value,  $P_0^{emp}$ , is much smaller,  $\sim 10^{-8} - 10^{-23}$ , for cluster decays. The values of  $P_0^{emp}$  for cluster decays,  $P_0^{c(emp)}$ , are deduced by using the optical potentials based on the R3Y and M3Y NNinteractions, supplemented by the zero-range pseudo-potential  $J_{00}(E)\delta(s)$  representing

Table 3.2: P and  $P_0^{c(emp)}$  for cluster-decays of some parents with <sup>208</sup>Pb as the daughter nucleus, calculated for the R3Y+EX and compared with the M3Y+EX NN interaction potential, for RMF-HS densities. The experimental data on cluster-decay constant  $\lambda_{Expt}^c$ are from [106], and the Q-values are calculated by using the experimental ground-state binding energies [107].

Parent	Cluster	Q	F	)	$\lambda_{Expt}^{c}$	$P_0^{\ c(emp)}$			
		(MeV)	(M3Y + EX)	(R3Y + EX)	$(s^{-1})$	(M3Y + EX)	(R3Y + EX)		
<sup>222</sup> Ra	$^{14}\mathrm{C}$	33.050	$1.728 \times 10^{-25}$	$2.277 \times 10^{-24}$	$6.749 \times 10^{-12}$	$1.044 \times 10^{-08}$	$7.921 \times 10^{-10}$		
<sup>230</sup> U	<sup>22</sup> Ne	61.388	$1.378\times10^{-29}$	$7.615 \times 10^{-27}$	$4.243 \times 10^{-19}$	$7.664 \times 10^{-12}$	$1.387 \times 10^{-14}$		
<sup>231</sup> Pa	$^{23}\mathrm{F}$	51.844	$6.613\times10^{-33}$	$1.593 \times 10^{-30}$	$1.682 \times 10^{-25}$	$7.062 \times 10^{-15}$	$2.932 \times 10^{-17}$		
<sup>232</sup> U	<sup>24</sup> Ne	62.311	$1.047\times10^{-28}$	$1.753 \times 10^{-26}$	$2.720 \times 10^{-21}$	$6.731 \times 10^{-15}$	$4.019 \times 10^{-17}$		
<sup>236</sup> Pu	$^{28}Mg$	79.670	$5.710 \times 10^{-27}$	$3.815 \times 10^{-23}$	$1.469 \times 10^{-22}$	$6.401 \times 10^{-18}$	$9.580 \times 10^{-22}$		
<sup>238</sup> Pu	<sup>30</sup> Mg	76.824	$1.873 \times 10^{-30}$	$1.185 \times 10^{-25}$	$1.412 \times 10^{-26}$	$1.984 \times 10^{-18}$	$3.136 \times 10^{-23}$		

the single-nucleon exchange (EX) effects, which defined in above subsection [106, 104, 105].

Calculations are made for a few exotic cluster radioactive (CR) decays in the translead region having doubly magic <sup>208</sup>Pb as daughters, using the HS parameter set based spherical relativistic mean field (RMF-HS) densities. As a consequence of the above result for P, the deduced  $P_0^{c(emp)}(R3Y + EX)$  are also affected. However, interestingly, in Fig. 3.3, we find that the values of  $P_0^{c(emp)}(R3Y + EX)$  are closer to the well accepted phenomenological formula of Blendowske and Walliser (BW) [112] whereas the same for  $P_0^{c(emp)}(M3Y + EX)$  are within two to three orders of magnitude with the BW results. Evidently, the effective NN-interaction obtained from the RMF Lagrangian, the R3Y, is applicable to study the exotic cluster radioactive decays within a satisfactory precision.

Further, we have shown the applicability of L - R3Y and N - R3Y (linear and non-linear) on proton radioactivity. The region of nuclides just above  ${}^{100}Sn$  is of special interest for such studies since it includes the heaviest  $Z \cong N$  known nuclei, stable to the proton emission, and offers an unexpected richness and diversity of nuclear structures and new decay modes [105]. Nevertheless our present formalism with the inclusion of

Table 3.3: The calculated half-lives of proton emitters are presented using M3Y+EX and N-R3Y+EX NN interactions. The results of the present calculations have been compared with the experimental values. The asterisk symbol ( $\star$ ) denotes the isomeric state. [105]

Nuclei	Q	L	Expt.	(M3Y + EX)	(LR3Y + EX)	(M3Y + EX)	(NR3Y + EX)
	•		-	HS	HS	NL3 (	NL3
nuclei	(MeV)		$log_{10}T$	$log_{10}T$	$log_{10}T$	$log_{10}T$	$log_{10}T(s)$
105Sb	0 491	2	2.049	3.07	2 436	3.1	1 113
$^{109}I$	$0.491 \\ 0.819$	$\tilde{0}$	-3.987	-5.627	-5.897	-5.593	-6.941
$^{112}Cs$	0.814	$\overline{2}$	-3.301	-2.857	-3.555	-2.835	-4.705
$^{113}Cs$	0.973	2	-4.777	-5.236	-5.803	-5.204	-7.017
$^{117}$ La	0.803	2	-1.628	-1.943	-2.504	-1.922	-3.878
$^{117}\text{La}^*$	0.954	5	-2.0	2.794	1.203	_	-1.241
$^{131}\mathrm{Eu}$	0.940	2	-1.749	-2.097	-2.764	-2.085	-4.256
$^{140}\mathrm{Ho}$	1.094	3	-2.221	-1.374	-2.132	-1.376	-4.007
$^{141}\mathrm{Ho}$	1.177	3	-2.387	-2.487	-3.298	-2.468	-5.038
$^{141}\mathrm{Ho}^*$	1.256	0	-5.180	-6.374	-6.846	-6.366	-8.047
$^{145}\mathrm{Tm}$	1.753	5	-5.409	-3.415	-4.698	-3.278	-6.962
$^{146}\mathrm{Tm}$	1.127	5	-1.096	3.384	1.945	3.51	-0.547
$^{146}{\rm Tm^{*}}$	1.307	5	-0.698	0.919	-0.484	1.043	-2.870

R3Y (for linear (NL-HS) and non-linear (NL3)) in predictions of half-life of proton emitter shows a good agreement with the experimental. The results are listed in Table 3.3. From table, one can find that, in many cases the N - R3Y + EX is more closure to experimental value and in few of the cases the L - R3Y + EX gives the Superior results. This implies the cluster decay property is little sensitive to the non-linear complying in the Lagrangian density. Also, perhaps this value is indifferent to the detail nuclear structure inherit by the density while calculating the cluster decay property (mostly a surface phenomena). However, if one apply these folding potential to some other nuclear phenomena where structural property of the nuclei is important in that case the N - R3Y + EX may work better. This is because of the high quality predictive power of NL3 over NL-HS through out the periodic table [105]. We also study the sensitivity of half-lives to the orbital angular momentum L in Table 3.3 [105]. It is seen that L - R3Y + EX NN and N - R3Y + EX interaction gives remarkable good result with the experiment, in fact the Q-value is very compatible with the half-life.

## **3.4** Summary and Conclusion

In this work, we have shown the microscopic origin effective NN interaction, denoted here as R3Y, could be derived from the simple RMF Lagrangian. This could replace the phenomenological M3Y NN-interaction for most of the calculations of nuclear observables like cluster (proton) radioactivity etc. The R3Y is presented eloquently in terms of the well known inbuilt RMF theory parameters of  $\sigma$ ,  $\omega$  and  $\rho$  meson fields, i.e., their masses  $(m_{\sigma}, m_{\omega}, m_{\rho})$  and coupling constants  $(g_{\sigma}, g_{\omega}, g_{\rho})$ . It is worth mentioning that the R3Y, basically depend on the mass and coupling constant for a particular force of RMFT, which varies for different parameter sets. Furthermore, in terms of the nucleusnucleus (nucleon-nucleus) folding optical potential, we have generated a bridge between the R3Y and M3Y which can be considered as a unification of the RMF model to predict the nuclear cluster (proton) decay property, i.e., we can explain the cluster (proton) decay properties of the cluster (proton) decaying nuclei by using the RMF-derived R3Ypotential instead of the phenomenological M3Y potential. The improvement of the R3Yinteraction is also derived from the most successful non-linear RMF. The obtained results for linear and non-linear cases are compared with M3Y potential. Also, the present work could be considered as the motivation for other similar models for the generation of different types of NN-interactions, as well as an additional feather to the RMF theory for its being considered as a unified formalism for studying a number of nuclear phenomena or, at least one step forward in our understanding the NN interaction within a well established theoretical formalism.

# Chapter 4

# Structure of Superheavy Elements

## 4.1 Introduction

There are about 300 nuclei occur in nature, representing isotopes of elements starting from Z = 1 to at most 94. Around 3000 additional nuclei have been made artificially during last seven decades. To make or synthesize heavier nuclei, it becomes increase in difficulty because of the disruptive electrostatic forces between the positively charged protons grow faster than the cohesive nuclear forces that hold the nucleons (protons and neutrons) together. This cause the superheavy nuclei to decay rapidly by the emission of alpha  $(\alpha)$  particles (Helium nucleus) and by spontaneous fission. Nuclei with increased stability beyond the  $\beta$ - stable region of the nuclear chart can exist because of the closing proton and neutron shells. One can say that the necessary balance between the nuclear and Coulomb force through shell stabilization effects can survive the nuclei beyond the macroscopic limit, far away from the trans-uranium region [113, 114, 115, 116]. For more detail information, one can see the historical review on theoretical predictions and new experimental possibilities is available in Ref. [117]. The half-lives of nuclei near the shell closures must be long enough and possible to synthesize in laboratory is predicted by Myers and Swiatecki [118]. In other words, nuclei without shell effects would not be stable and would decay immediately, as was predicted by macroscopic liquid drop models for Z > 100 includes. Recently, the microscopic studies of the nuclei beyond Z = 100 is possible [119], and the heaviest nucleus studied so far in this series of experiments [120] is  ${}^{254}$ No (Z = 102 and N = 152). Similarly, the electronic configurations for nuclei with Z < 112 are well studied due to their relatively longer lifetimes (> 1s) [121].

Experimentally, till now, the quest for superheavy nuclei has been dramatically rejuvenated in recent years owing to the emergence of hot and cold fusion reactions. In cold fusion reactions involving a doubly magic spherical target and a deformed projectile were used at GSI [122, 123, 124, 125, 126] to produce heavy elements up to Z = 110-112. In hot fusion evaporation reactions with a deformed trans-uranium target and a doubly magic spherical projectile were used in the synthesis of superheavy nuclei Z = 112-118 at Dubna [127, 128, 129, 130, 131, 132, 133]. The half-lives of these newly synthesized nuclei ranging from a few minutes to about a millisecond. However, the data for these nuclei are scarce since the production cross-sections decrease rapidly with increasing proton number, down to 1pb for Z=112 [125, 126]. This is a major challenge for experimental investigations of new nuclei to isotopes that are richer in protons than the expected most stable superheavy elements. More detailed spectroscopic studies are becoming promising around the trans-fermium region towards the island of stability [119, 134].

The emergence of a region of long-lived elements beyond the actinides has been predicted since the earliest nuclear models [31, 116]. It is well verified that the nuclei with Z > 104 should not exist, without the shell effects and large spin-orbit splitting of single-particle levels at magic numbers. These effects overcome to the long-range Coulomb repulsion between protons and stabilize the nuclei from induced fission. To determine and well understanding of these special characteristic or features of a closed shell nuclei is also a considerable challenges from theoretical perspective. Generally, the forces (parameters) from different models are capabled to reproduce the bulk properties of the established superheavy elements, indicating that their features could be an essential ingredient to describe the distribution of levels of these superheavy nuclei [135]. It is well known that, the single-particle level density is large for the superheavy nuclei. Which need an accuracy of describing the single-particle energies and the spin-orbit interactions. In other word, the position of the shell gaps is quite sensitive to the single-particle energies and the spin-orbit interaction. For example, the small shifts in the position of the single-particle levels will lead to gaps at different particle numbers. This is one of the cause for the discrepancies between the different parameterisations of self-consistent mean-field models. Hence, it is important to see these superheavy region with newly developed advance forces of different formalism such as the non-linear relativistic mean field, Gogny and modified Skyrme-Hartree-Fock. Again, the progress in experimental techniques has drawn our attention and opened up the field once again for further theoretical investigations in structure physics of nuclei in the superheavy mass region. Based on the present experimental status and theoretical predictions, we have considered few atomic nucleus such as Z = 115, 117, 120 and 122 and their isotopic chain in this present study. The schematic chart for these nuclei and the experimental findings are given in Fig. 4.1.

The chapter is organized as follows. Section II includes the details of the calculations and results. Some special properties like effects of pairing for open shell nuclei, the ground and excited state configuration and the shape co-existence are included in this section. The decay properties of these sperheavy nuclei are discussed in section III. A summary of the results obtained, together with concluding remarks, is given in Section IV.

## 4.2 Method of calculation and results

There exist a number of parameter sets for solving the standard SHF Hamiltonians and RMF Lagrangians. In many of our previous works, the ground state properties, like the binding energies (*BE*), quadrupole deformation parameters  $\beta_2$ , root mean square charge radii ( $r_{ch}$ ), and other bulk properties, are evaluated by using the various non-relativistic and relativistic parameter sets. It is found that, most of the recent parameter sets reproduce well the ground state properties not only of stable normal nuclei but also of exotic nuclei that far away from the valley of  $\beta$ - stability. This means that if one uses a reasonably acceptable parameter set, the predictions of the model will remain nearly

Figure 4.1: The schematic diagram for the experimentally synthesized superheavy nuclei. The shaded box with corresponding mass number are denoted as experimental findings.

force independent. In case of RMF, the mean-field equations are solved self-consistently by taking different inputs of the initial deformation  $\beta_0$ . For a normal ground state (g.s.) solution, in the considered mass region, the number of major shells for boson and Fermions needed are  $N_B = N_F = 12$  to reproduce a reasonable converge solution. However, in the present paper, we deal with a rather large deformed state with deformed harmonic oscillator basis with  $N_B = N_F = 20$  shells. The number of mesh points for Gauss-Hermite and Gauss-Lagueree integration are 20 and 24, respectively. On the other hand, the starting point for a numerical solution of the Hartree-Fock equations is a single-particle wave-functions. The trial states are assumed to be a set of harmonic oscillator wave-functions within a cartesian grid [136] with user-specified parameters that determine the shape and depth of the potential in all coordinates. The ground-state for a certain nucleus is calculated for a given set of input data including the proton and neutron number, pairing and spatial discrimination options using a damped gradient iteration scheme and Gram-Schmidt orthonormalisation [137, 138] to calculate the new wave-functions until convergence is reached. There is no mixing between proton and neutron states, although the single-particle wave-functions are a mixture of spin up and spin down solutions. The derivatives of the densities in the energy functional are calculated by the seven point method for first derivatives and nine points for second-order derivatives. The effects of pairing interaction in *odd-even* and *odd-odd* nuclei are taken in the present investigation by using BCS formalism with constant pairing strength, this contributes a little to the total binding. The results remain unchanged unless the pairing gap is varied considerably. This type of prescription has already been adopted in the past [139, 32, 29]. The axially deformed relativistic mean field (RMF) method and Skryme-Hartree-Fock (SHF) methods are used for considered complete isotopic chain from proton to neutron drip line of these atomic nucleus (Z = 115, 117, 120, 122). These isotopes carry a special place due to its unknown chemistry, because of their shorter life times. Thus, a thorough analysis of these isotopes with suitable models are quite instructive for the chemistry of the superheavy elements.

### 4.2.1 The potential energy surface

In this calculation, we employed the most successful NL3, NL3<sup>\*</sup> forces in RMF and SLy4 and SkI4 in SHF [9, 10, 12, 13, 17]. The existence of a superheavy nuclei is governed from the magnitude of shell correction energy, which play a crucial role in their half-life. Further, the energy favours some deformed (may be super-deformed or hyper-deformed) shapes along with spherical structure in the isotopic chain in this region, which contrary to the situation for the lighter Z elements [9]. In fact, the deformed shell effects play an important role in the description of these super-heavy elements. Practically, the deformed gap near the Fermi surface gives rise to a local minimum in the potential energy surface (PES). Hence, it is fundamental need to see the behaviour of PES curves with respect to deformation (different solution at different deformation).

Figure 4.2: The potential energy surfaces for <sup>292</sup>122 nucleus as a function of quadrupole deformation parameter. The squares with solid-line is for SHF using SkI4 parameter set, and the circles with solid-line is for RMF calculations using NL3 parameter set.

In constrained method [9, 11], instead of minimizing the  $H_0$ , we have minimized  $H' = H_0 - \lambda Q_2$  to perform the calculation of the potential energy surfaces in both the RMF and SHF theories. Here,  $\lambda$  as a Lagrange multiplier and  $Q_2$  the quadrupole moment. Thus, we calculated the binding energy corresponding to the solution at a given quadrupole deformation  $\beta_2$ . Here,  $H_0$  is the Dirac mean field Hamiltonian in Refs. [9, 11]) for RMF model and it is a Schrödinger mean field Hamiltonian for SHF model. In other words, we get the constrained binding energy from  $E_c = \sum_{ij} \frac{\langle \psi_i | H_0 - \lambda Q_2 | \psi_j \rangle}{\langle \psi_i | \psi_j \rangle}$  and

the 'free energy' from  $BE = \sum_{ij} \frac{\langle \psi_i | H_0 | \psi_j \rangle}{\langle \psi_i | \psi_j \rangle}$ . In our calculations, the free energy solution does not depend on the initial guess value of the basis deformation  $\beta_0$  as long as it is nearer to the minimum in PES. However it converges to some other local minimum when  $\beta_0$  is drastically different, and in this way we evaluate a different isomeric state for a given nucleus. The PES, i.e., the potential energy as a function of quadrupole deformation parameter  $\beta_2$ , for the superheavy nucleus <sup>292</sup>122, are shown in Fig. 4.2. Both the RMF and SHF results are given for comparisons. The calculated PES is shown for a wide range of oblate to prolate deformations. We notice from this figure that in RMF, minima appear at around  $\beta_2 = -0.436$ , -0.032 and 0.523. The energy differences between the ground and the isomeric states are found to be 0.48 and 1.84 MeV for the nearest consecutive minimas. For SHF, the minima appear at around  $\beta_2 = -0.459$ ,-0.159 and 0.511 with the intrinsic excited state energy differences are 1.30 and 0.48 MeV. From the figure it is clear that the minima and the maxima in both the RMF and SHF are qualitatively similar.

Further, we have extended the calculation to see the PES with and without reflectional symmetry. Because, the work of Ref. [140], claimed that the super-deformed or hyper-deformed state of a superheavy nuclei washed away by introducing reflectional asymmetric in account. To verify this fact, we have done the calculation with and without reflectional symmetry for <sup>292</sup>120 and <sup>292</sup>118 with SLy4 and SkI4 forces. To our surprise, we do not get any significant change in the PES diagram, confirming the existence of super-deformed states of these SHE similar to the prediction of Z. Ren and H. Toki [141, 142] for <sup>287</sup>114 and <sup>292</sup>118 nuclei. The obtained curve for the potential energy surface is shown in Fig. 4.3. From, the figure, one can notice that there are three minima in the energy surfaces of both the nucleus <sup>292</sup>120 and <sup>288</sup>118, at around  $\beta_2 =$ -0.125, +0.125, +0.56. Further getting a minima beyond  $\beta_2 \sim 1.0$ , which shows the fission path of these nuclei. Therefore, we can say that there is a super-deformed solution or a shape co-existence with  $\beta_2 \sim 0.0$ . The PES is an important scheme to determine the shape of the nuclei in their ground state as well as in intrinsic excited states. This is also reflected in the binding energy calculations of this nucleus in an isotopic chain, which

Figure 4.3: The potential energy surfaces for the nucleus  $^{292}120$  and  $^{288}118$  obtained by constrained non-relativistic SHF(SkI4 and SLy4) calculations with symmetric and asymmetric conditions.

will be discussed in the following subsection.

### 4.2.2 Nuclear binding energy

Nuclear binding energy is the most fundamental and precise measured observable in the laboratory. The efficiency of a theoretical model is determined from its accuracy in producing the experimental binding energy. The calculated bulk properties obtained in both the SHF (SkI4 and SLy4) and RMF (NL3 and NL3<sup>\*</sup>) formalisms for *even – even* (Z=120 and 122) [11, 9] and *odd – odd* (Z=115 and 117) [12, 10] nuclei.

Table 4.1: The RMF(NL3<sup>\*</sup>), RMF(NL3), SHF (SkI4) and SHF (SLy4) results for binding energy BE, the quadrupole deformation parameter  $\beta_2$ , two-neutron separation energy  $S_{2n}$  and the binding energy difference  $\Delta E$  between the ground- and first-exited state, compared with the corresponding Finite Range Droplet Model (FRDM) results [29, 11] for the isotopic chain of Z=120. The energy is in MeV.

Nucleus	Formalism	BE	$\beta_2$	$S_{2n}$	$\Delta E$
288	RMF (NL3)	2031.75	$0.5\tilde{6}0$	16.28	0.929
	RMF (NL3∗́)	2029.97	0.562	16.19	
	SHF (SkI4)	2014.83	0.523	16.48	0.408
	SHF(SLv4)	1996.23	0.122	16.51	0.593
290	RMF (NĽ3)	2047.50	0.551	15.75	0.301
	RMF (NL3 <sup>*</sup> )	2045.56	0.556	15.59	
	SHF (SkI4)	2031.31	0.119	16.37	0.135
	SHF(SLv4)	2012.74	0.115	15.98	1.310
	FRDM	2039.49			
292	RMF (NL3)	2064.11	0.540	16.61	0.730
	RMF (NL3∗́)	2060.87	0.547	15.31	
	SHF (SkI4)	2047.68	0.113	15.53	0.591
	SHF(SLy4)	2028.71	0.107	15.38	1.966
	FRDM	2055.19	-0.130	15.70	
294	RMF (NL3)	2078.43	0.536	14.61	0.916
	RMF (NL3*)	2075.85	0.541	14.98	
	SHF (SkI4)	2063.21	0.110	14.75	0.688
	SHF (SLy4)	2044.09	0.097	14.69	2.528
	FRDM	2070.87	0.081	15.68	
296	RMF (NL3)	2093.19	0.542	14.76	2.394
	$RMF (NL3^*)$	2090.29	0.545	14.44	
	SHF (SkI4)	2077.96	0.087	14.59	0.529
	SHF ( $SLy4$ )	2058.78	0.088	14.03	2.887
	FRDM	2085.32	-0.096	14.45	
298	RMF (NL3)	2107.35	0.551	14.16	0.058
	$RMF (NL3^*)$	2104.30	0.554	14.01	
	SHF (SkI4)	2092.55	0.066	14.38	0.583
	SHF(SLy4)	2072.81	0.060	13.86	3.026
200	FRDM	2099.73	-0.079	14.41	2 2 2 2
300	RMF(NL3)	2120.92	0.561	13.57	3.292
	$RMF(NL3^*)$	2117.63	0.564	13.33	1
	SHF (Sk14)	2106.94	0.045	14.16	1.026
	SHF (SLy4)	2086.68	0.040	13.19	3.446
202	FRDM	2113.39	-0.008	13.66	0.001
302	$\operatorname{KMF}(\operatorname{NL3})$	2133.86	0.579	12.94	3.691
	$\operatorname{KMF}(\operatorname{NL3}^{*})$	2130.28	0.586	12.65	1 011
	SHF (Sk14)	2121.09	0.024	13.86	1.611
	SHF (SLy4)	2099.87	0.019	12.5	3.791
	FRDM	2126.05	0.000	12.66	

Figure 4.4: The binding energy for the nucleus Z=120 and 122 obtained from SHF(SkI4 and SLy4) and RMF (NL3 and NL3<sup>\*</sup>) calculations. The FRDM predictions are given for comparison [9, 11].

#### Even-even nuclei

#### For Z=120 isotopic chain

The obtained results for binding energy BE and binding energy per particle BE/A for Z=120 from RMF(NL3<sup>\*</sup>), RMF(NL3), SHF (SkI4) and SHF (SLy4) are shown in Fig. 4.4(a) and Table. 4.1 along with the FRDM results [11]. From the figure and table it is clear that, the binding energy obtained in both the RMF and SHF models are qualitatively similar. We notice that the binding energy, obtained with NL3 and NL3<sup>\*</sup> parameter sets are almost equal within lower mass region but, towards higher

Table 4.2: The SHF(SkI4) and the RMF(NL3) results for binding energy BE, twoneutron separation energy  $S_{2n}$  and the quadrupole deformation parameter  $\beta_2$ , compared with the Finite Range Droplet Model (FRDM) data for the isotopic chain of Z=122 [9]. The energy is in MeV.

	SHF(SkI4 parameter set)			RMF(NL3 parameter set)			FRDM results		
Nucleus	BE	$S_{2n}$	$\beta_2$	BE	$S_{2n}$	$\beta_2$	BE	$S_{2n}$	$\beta_2$
294	2045.52	16.29	0.534	2062.49	16.71	0.530	2053.16		-0.155
296	2061.74	15.94	0.529	2078.46	16.21	0.527	2068.99	15.84	-0.130
298	2077.44	15.34	0.526	2093.81	15.70	0.536	2084.26	15.26	-0.096
300	2092.62	14.81	0.526	2108.67	15.18	0.548	2099.64	15.38	0.009
302	2107.30	14.34	0.529	2123.01	14.68	0.562	2113.98	14.34	0.418
304	2121.47	13.82	0.545	2136.83	14.17	0.603	2126.87	12.89	0.000
306	2132.71	13.20	0.556	2150.03	13.76	0.608	2139.43	12.56	0.000
308	2148.31	12.45	0.560	2162.49	13.08	0.618	2150.84	11.41	0.001
310	2160.66	12.00	0.571	2174.49	12.35	0.641	2162.05	11.22	0.003
312	2172.58	12.62	0.584	2187.10	11.92	0.742	2173.42	11.36	0.005
314	2184.17	12.02	0.594	2199.12	11.59	0.739	2184.67	11.25	0.006
316	2295.39	11.37	0.595	2210.49	11.22	0.736	2195.74	11.07	0.007
318	2206.30	10.65	0.588	2221.02	10.91	0.722	2214.11	18.37	0.541
320	2216.96	10.21	0.575	2231.23	10.67	0.728	2224.88	10.76	0.543

mass region, the binding energy using NL3\* parameter set, is gradually getting lower values than NL3 set, which are over-estimated to both the SHF (SkI4) and SHF (SLy4) results by a constant factor. In an isotopic chain, we notice that the macro-microscopic FRDM calculation lies in between RMF and SHF. But, the difference decreases gradually towards the higher mass region in case of SHF (SkI4). The binding energy per particle (BE/A) for the isotopic chain is also plotted in Fig 4.4 (b). Qualitatively, all the curves show a similar behavior. Again a detail inspection shows that the BE/A value starts increasing with the increase of mass number, reaching a peak value at A ~ 302-304 for RMF, SHF and FRDM models. This means that  $^{302,304}120$  is the most stable element, which is situated at N=182-184. Interestingly, this neutron number N = 184 is the next predicted magic number [17]. It is worthy to mention that the results obtained in the present calculation are almost consistent to the prediction by earlier calculations [11] using some different force parameters. Hence, we may note that the results for binding energy and related observables like magic numbers are independent of force parameters.

#### For Z=122 isotopic chain

Table 4.2 and Fig. 4.4 (c) shows the calculated binding energy obtained from SHF (SkI4) and RMF (NL3) formalisms [9]. Similar to Fig. 4.2, the binding energy obtained in the RMF model also over-estimates the SHF result by a constant factor. In other words similar to the chain of Z=120, here also the multiplication by a constant factor will make the two curves overlap with one another. This means that a slight modification of the parameter set of one formalism can predict the binding energy similar to that of the other. Table 4.2 shows a comparison of the calculated binding energies with the FRDM predictions of Ref. [32, 29], wherever possible. The binding energy per particle for the isotopic chain is also plotted in Fig. 4.4 (d). We notice that here again the SHF and RMF curves differ from one another through a constant scaling factor, and the FRDM calculation lie in between these two calculations. This means qualitatively, all the three curves show a similar behavior. However, unlike the BE/A curve for SHF or RMF, the FRDM results do not show the regular behaviour. In general, the BE/A start increasing with the increase of mass number A, reaching a peak value at A=302 for all the three formalisms. This means that <sup>302</sup>122 is the most stable element from binding energy point of view. Interestingly, <sup>302</sup>122 is situated towards the neutron deficient side of the isotopic series of Z=122, and could be taken as a suggestion to synthesize this superheavy nucleus experimentally.

#### Odd-odd Nuclei

The calculations for odd-even and odd-odd nuclei in an axially deformed basis is a tough task in the mean-field model. To take care of the lone odd nucleon, one has to violate the time-reversal symmetry in the mean field (already mention in *Chapter 2*). So, we use Pauli blocking approach to deal such open shell nuclei. The effects of pairing interaction in *odd-even* and *odd-odd* nuclei are expected to be considerably decreased [143]. Therefore, in the present investigation we have chosen to use a BCS formalism with a small constant pairing strength, which contributes little to the total binding energy. This type of prescription has already been adopted in the past [139, 32, 29].
Figure 4.5: The binding energy for the nucleus Z=115 and 117 obtained from RMF (NL3) calculations along with FRDM predictions [10, 12]

#### For Z=115 isotopic chain

The total binding energy (BE) for whole isotopic chain for Z = 115 is plotted in Fig. 4.5 (a) and also listed in Table 4.3. From the figure and table, we notice that the microscopic RMF (NL3) BE over-estimated than that of FRDM at N = 156 - 167, after that the difference in binding energy decreasing towards the higher mass region (around A=287). And beyond to this mass number the two curves again showing a similar behaviour. The binding energy per nucleon (BE/A) for the isotopic chain is plotted in Fig. 4.5 (b). This value starts reaching a peak value at A = 282 for RMF (NL3) and at A = 286 for

Table 4.3: The RMF (NL3) results for binding energy BE, two-neutron separation energy  $S_{2n}$ , pairing energy  $E_{pair}$ , the binding energy difference  $\Delta E$  between the ground- and first-excited state solutions, and the quadrupole deformation parameter  $\beta_2$ , compared with the corresponding Finite Range Droplet Model (FRDM) results [12]. The energy is in MeV.

		(NL3) R	FRDM Result					
Nucleus	BE	$S_{2n}$	$E_{pair}$	$\Delta E$	$\beta_2$	BE	$S_{2n}$	$\beta_2$
272	1944.3	16.7	17.3	6.51	0.255	1932.8		0.182
274	1961.0	16.6	16.9	6.20	0.244	1950.3	17.5	0.192
276	1977.2	16.3	16.3	5.87	0.232	1967.4	17.1	0.202
278	1992.8	15.6	15.8	5.30	0.218	1983.9	16.5	0.202
280	2008.0	15.1	15.4	4.77	0.196	2000.3	16.4	0.053
282	2022.8	14.7	14.7	4.15	0.182	2015.8	15.5	0.053
284	2036.7	13.9	14.3	3.18	0.173	2030.8	15.0	0.062
286	2049.8	13.1	14.0	2.06	0.165	2045.2	14.4	0.071
288	2062.5	12.7	13.7	1.23	0.152	2059.1	13.8	-0.087
290	2074.5	11.9	13.6	0.15	0.103	2072.6	13.5	-0.079
292	2086.5	11.9	13.5	0.02	0.060	2085.7	13.1	-0.061

FRDM [12]. It means <sup>282</sup>115 is the most stable isotope from the RMF (NL3) and <sup>286</sup>115 from the FRDM results [32, 29]. Hence, the predicted shell closure from FRDM in the isotopic chain of Z=115 is  $N \sim 172$ , which is not appear in case of RMF (NL3).

#### For Z=117 isotopic chain

The obtained results for binding energy per nucleon BE/A and the binding energy BE from the RMF(NL3) formalism are compared with FRDM results [10] in Figs. 4.5 (c) and in Table 4.4. Similar to the *even – even* nuclei, the results of RMF(NL3) over-estimates the FRDM result. In general, the BE/A value starts increasing with the increase of mass number A, reaching a peak value at A=288 for RMF(NL3) and at A=290 for the FRDM formalism. This means to say that <sup>288</sup>117 is the most stable isotope from the RMF(NL3) model results and <sup>290</sup>117 from the FRDM predictions. Interestingly, <sup>288</sup>117 (with N=171) and <sup>290</sup>117 (with N=173) are both closure to the predicted shell closure at N=172 than at N=184. Note that the isotopes <sup>300,302</sup>117, next to the magic number N=184, are also included in this study. For the total binding energy BE in the isotopic

Table 4.4: The RMF(NL3) results for binding energy BE, two-neutron separation energy  $S_{2n}$ , pairing energy  $E_{pair}$ , the binding energy difference  $\triangle E$  between the ground- and first-exited state solutions, and the quadrupole deformation parameter  $\beta_2$ , compared with the corresponding Finite Range Droplet Model (FRDM) results [10]. The energy is in MeV.

		FRDM Result						
Nucleus	BE	$S_{2n}$	$E_{pair}$	$\Delta E$	$\beta_2$	BE	$S_{2n}$	$\beta_2$
288	2052.58	14.836	14.698	0.333	0.018	2047.09	15.16	0.080
290	2066.13	13.552	14.274	0.360	0.017	2061.65	14.56	0.080
292	2079.80	13.664	14.109	0.096	-0.017	2075.72	14.07	0.072
294	2092.46	12.775	13.653	0.031	0.041	2089.22	13.50	-0.087
296	2104.80	12.335	13.583	0.104	0.028	2102.66	13.45	-0.035
298	2116.59	11.691	13.274	0.389	0.015	2114.79	12.13	-0.008
300	2128.17	11.576	12.841	0.970	0.005	2126.14	11.34	0.000
302	2138.66	10.488	12.623	0.596	0.004	2136.25	10.11	0.000
304	2148.29	9.634	12.695	0.012	0.002	2145.71	9.46	0.000
306	2157.72	9.430	12.348	0.004	0.030	2154.84	9.13	0.000
308	2167.32	9.601	11.912	0.304	0.047	2163.93	9.09	0.001
310	2176.65	9.329	11.538	0.512	0.051	2172.61	8.68	0.000

chain from microscopic RMF agree well with the macro-microscopic FRDM calculations, their differences decreasing gradually towards the higher mass region (around A=298), and then beyond this mass number the two curves again show a similar behavior.

# 4.2.3 The pairing energy

Pairing is a crucial quantity for open shell nuclei in determining the nuclear gross properties like binding energy, deformation, nucleonic density distribution and single particle energy level etc. To deal such open shell nuclei in the present study, we have adopted the constant gap BCS-pairing scheme to care the pairing correlation. This prescribed BCS approach is valid for nuclei in the valley of  $\beta$ - stability line. However, this method breaks down when the coupling of the continuum becomes important. The detail description and the corresponding expression for pairing energy  $E_{pair}$  are given in the Chapter 2. Here, we deal with nuclei on or near the valley of stability line since the superheavy

Figure 4.6: The pairing energy  $E_{pair}$ , for the isotopic chain of Z= 115, 117, 120 and 122 from RMF(NL3). Here, the g.s. and e.s. in the lebel of the figure stands for ground and first intrinsic excited state respectively [9, 10, 11, 12].

elements, though very exotic in nature, lie on the  $\beta$ -stability line. These nuclei are unstable because of the repulsive Coulomb force, but the attractive nuclear shell effects come to their rescue, making the superheavy element possible to be synthesized, particularly when a combination of magic proton and neutron number happens to occur (largest shell correction). Certainly, for a given nucleus, the magnitude of the pairing contribution depends marginally on the quadrupole deformation  $\beta_2$ . This means to say that for differing  $\beta_2$ -values in a nucleus, the pairing energy  $E_{pair}$  changes only marginally (~5-6%). On the other hand, even if the  $\beta_2$  values for two nuclei are same, the  $E_{pair}$  values are different from one another depending on the filling of the nucleons. The obtained results for even - even Z=120,122 and odd - odd Z = 115, 117 are shown in Fig. 4.6 for the RMF(NL3) calculation [9, 10, 11, 12]. The pairing energy  $E_{pair}$  in the isotopic chain of Z=120,122 for both the ground-state (g.s.) and the first excited state (e.s.), referring to different  $\beta_2$ -values. It is clear from Fig. 4.6 that the  $E_{pair}$  decreases with increase in mass number A, i.e., even if the  $\beta_2$  values for two nuclei are the same, the pairing energies are different from one another. This variation of  $E_{pair}$  is ~25% in an isotopic chain of a particular Z-value. This change may cause due to their different configurations (different  $\beta_2$  values) and the splitting of the single particle levels of nucleons inside a nucleus.

Figure 4.7: The shape co-existence  $\Delta E$ , for the isotopic chain of Z= 115, 117, 120 and 122 from RMF and SHF for various parameter sets [9, 10, 11, 12].

#### 4.2.4 Shape co-existence

Shape coexistence is a phenomenon exhibited by atomic nucleus, where configurations possessing remarkably different shapes with almost similar binding energies. In other word, the collective motion of the nucleons inside a nucleus for certain proton (Z) and neutron (N) can drive a system into dramatically different coexisting nuclear shapes with very small difference in binding energy. The measure of the energy difference between the ground and the first intrinsic excited state is given as [9, 10, 11, 12]:

$$\Delta E(N,Z) = \left[BE(N,Z)\right]_{q.s.} - \left[BE(N,Z)\right]_{e.s.}.$$
(4.1)

Here, we have also calculated the "free solutions" for the whole isotopic chain for all the atomic nuclei (i.e. Z=115,117,120 and 122), both in prolate and oblate deformed configurations. In many cases, we find low lying excited states [9, 10, 11, 12]. As measure from the binding energy difference  $\Delta E$  between two solutions from RMF and SHF for Z=115, 117, 120 and 120 are shown in Fig (4.7) and listed in Table 4.1-4.4 [9, 10, 11, 12]. The maximum binding energy solution refers to the ground state and all other solutions to the intrinsic excited state(s). The energy difference  $\Delta E$  is small for neutron-deficient isotopes, but it increases with the increase of mass number A in the isotopic series. This small difference in the binding energy for neutron-deficient isotopes is an indication of shape co-existence. In other words, the two solutions in these nuclei are almost degenerate and might have large shape fluctuations. Further, a deep inspection shows that all the atomic nucleus follows a low laying excited correspond to their ground state around the mass number  $\sim$  286 - 296. On the other hand, in SHF formalism,  $\triangle E$  value remains small throughout the isotopic chain. For example, in <sup>308</sup>122 the two solutions for  $\beta_2 = 0.56$  and  $\beta_2 = 0.008$  are completely degenerate with binding energies 2148.31 and 2148.12 MeV. Similar case one can see for the isotopic chain of Z=115, 117 and 120. This later result means to suggest that the ground state can be changed to the excited state and vice-versa by a small change in the input, like the pairing strength, etc., in the calculations. In any case, such a phenomenon is known to exist in many

other regions [139] of the periodic table.

Figure 4.8: The quadrupole deformation parameter  $\beta_2$ , for the isotopic chain of Z= 115, 117, 120 and 122 from RMF and SHF for various forces [9, 10, 11, 12].

# 4.2.5 Quadrupole deformation parameter

The quadrupole deformation parameter  $\beta_2$  is evaluated from the resulting proton and neutron quadrupole moments [9, 10, 11, 12] as:

$$Q = Q_n + Q_p = \sqrt{\frac{16\pi}{5}} \left(\frac{3}{4\pi} A R^2 \beta_2\right),$$
 (4.2)

where,  $Q_n$  and  $Q_p$  are the proton and neutron quadrupole moments, respectively. The shape of a nuclei for a given state can be determined from this observables. The quadrupole deformation parameter  $\beta_2$ , for both the ground and first excited states, are calculated within these two formalisms for isotopic chain of Z=115, 117, 120 and 122. The obtained results from our calculation are compared with the FRDM results are shown in Fig. (4.8) and listed in Table (4.1-4.4) [9, 10, 11, 12]. In some of the earlier RMF and SHF calculations, it was shown that the quadrupole moment obtained from these theories reproduce the experimental data pretty well [70, 78, 83, 8, 85, 101, 9, 79]. The calculated value of  $\beta_2$  in the ground and intrinsic excited states for SHF and RMF results agree well with each other (the excited solution are not included in the figure). From the figure, it is clearly identified that (g.s.) quadrupole parameter  $\beta_2$  for SHF and RMF, differ strongly from FRDM results [32, 29] for Z=120, 122. For example, in case of Z=122, both SHF and RMF with highly deformed oblates configuration for isotopes near the low mass region. Then, with increase of mass number there is a shape change from highly oblate to highly prolate but which is not the case for FRDM. The interesting point is that, most of the isotopes are super-deformed or / and hyper-deformed in their q.s. configurations for Z=120 and 122, but are spherical solution for Z=115 and 117.

#### 4.2.6 Two-nucleon separation energy

The two-nucleon separation energy is a crucial observable to predict the most stable nuclei in an isotopic chain and also important to determine the magic properties of a nucleus. The two-neutron separation energy  $S_{2n}$  (N, Z)can be calculated from the binding energies using the expression:

$$S_{2n}(N,Z) = BE(N,Z) - BE(N-2,Z),$$
(4.3)

here, N and Z are the neutron and proton number of a nucleus, respectively. The estimated  $S_{2n}$  energy from microscopic binding energies for Z=115, 117, 120 and 122 isotopic chains are displayed in Fig. 4.9 (also listed in Table 4.1-4.4) along with the



macro-microscopic FRDM prediction. From the figure and table, it is clear that  $S_{2n}$  values agree well with the FRDM calculations. The comparison of  $S_{2n}$  for the SHF and RMF with the FRDM result are further shown in Fig. 4.9, which shows clearly that the two  $S_{2n}$  values coincide remarkably well, except at mass A=316 and A=318 of Z=120 and Z=122, respectively, which seems spurious due to some error somewhere in FRDM data. Apparently, the  $S_{2n}$  decreases gradually with increase of neutron number, except for the noticeable kinks at  $N \sim 172$  and  $N \sim 188 - 190$  in RMF, and at  $N \sim 182$  and  $N \sim 186$  in FRDM. Interestingly, these neutron numbers are close to either N=172 or 184 magic numbers. However, the SHF results are almost smooth for whole isotopic

chain.

Figure 4.10: The root-mean-square charge  $r_{ch}$ , neutron  $r_p$  and matter  $r_m$  for the isotopic chain of Z= 122 from RMF (NL3) and SHF (SkI4) [9].

## 4.2.7 Nuclear radius

The root mean square (rms) matter radius is defined as

$$\langle r_m^2 \rangle = \frac{1}{A} \int \rho(r_\perp, z) r^2 d\tau, \qquad (4.4)$$

where A is the mass number and  $\rho(r_{\perp}, z)$  is the deformed density. Here, the rms radii for neutron and proton are calculated separately by taking the normalization to their number. The rms charge radius estimated from the simple expression,

$$r_{ch} = \sqrt{r_p^2 + 0.64},\tag{4.5}$$

taking into account the finite size of the proton radius as 0.8fm and  $r_p$  is the rms radius of the proton distribution in the nucleus. The rms radius for charge  $(r_{ch})$ , neutron  $(r_n)$ and matter distribution  $(r_m)$  from SHF and RMF formalisms are shown in Fig. 4.10 for Z=122 as a representative case. The upper panel (of Fig. 4.10) is for the RMF and the lower one (Fig. 4.10) for the SHF calculations. As expected, the neutron and matter distribution radius increases with increase of the neutron number. Although, the proton number (Z=122) is constant in the isotopic series, still the value of  $r_{ch}$  also increase as shown in the figure. This trend is similar in both the RMF and SHF formalisms. A detailed inspection of the figure shows that, in RMF calculation, the radii show a jump at A=312 (N=190) after the monotonic increase of radii till A=310. Note that a similar trend was observed in RMF calculations for  $S_{2n}$  for Z=122 (see, Fig. 3.9), which indicate some special attention for detail study of this nuclei.

# 4.3 The $\alpha$ decay properties of superheavy nuclei

The synthesis of superheavy nuclei has been dramatically rejuvenated in recent years owing to the emergence of hot and cold fusion reactions [122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133]. With these advent of modern accelerators and suitable detectors technique, it is possible to synthesize superheavy nuclei such as Z = 110-118[122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133]. At present, it is important and crucial to see the mode of decay and the stability of these newly synthesized nuclei. The sustainability of these superheavy nuclei are controlled mainly by the spontaneous fission and alpha decay processes. The decay of superheavy nuclei is possible if the shell effect supplies the extra binding energy and increases the barrier height of fission [144, 145, 20, 21]. The situation in spontaneous fission is very complex as compared to the  $\alpha$  decay. There is another possible decay mode called  $\beta$ -decay. Still, the  $\beta$ - decay proceeds via a weak interaction and is very slow and less favored compared to spontaneous fission and alpha decay. Here, we have studied the  $\alpha$ -decay properties of newly synthesized Z=115, 117 and to be synthesized Z=120, 122 using RMF and SHF formalisms.

Figure 4.11: The  $\alpha$ - decay energy  $Q_{\alpha}$  obtained from RMF and SHF for the isotopic chain of Z= 115, 117, 120 and 122 are compared with other theoretical prediction as well as experimental data, whereever available [9, 10, 11, 12].

#### 4.3.1 The $\alpha$ -decay energy

The alpha decay energy  $Q_{\alpha}$  is obtained from the relation [9, 10, 11, 12]:

$$Q_{\alpha}(N,Z) = BE(N,Z) - BE(N-2,Z-2) - BE(2,2).$$
(4.6)

Here, BE(2,2) is the binding energy of the  $\alpha$ -particle (<sup>4</sup>He), i.e., 28.296 MeV, and BE(N-2, Z-2) is the binding energy of the daughter nucleus after the emission of an  $\alpha$ - particle. The binding energy of the parent and daughter are obtained from the microscopic RMF and SHF formalisms for some selected force parameters. Using these binding energies, the  $Q_{\alpha}$  is estimated from the above relation in Eqn. (4.6). Here, we have calculated the  $Q_{\alpha}$  for the  $\alpha$ - decay chain of <sup>287,288</sup>115, <sup>293,294</sup>117, <sup>292,304</sup>120 and <sup>292</sup>122. The obtained  $Q_{\alpha}$ -values are compared with FRDM [32, 29], other theoretical predictions [146, 147, 148, 149] and experimental data [129, 130, 131, 132], whereever available [9, 10, 11, 12]. From the Fig. 4.11, one can notice that the calculated values the  $Q_{\alpha}$  agree well with the known experimental data as well as with the other calculations [146, 147, 148, 149, 150, 151], but slightly over-estimated with respect to the FRDM predictions. Furthermore, the possible shell structure effects in  $Q_{\alpha}$  is noticeable for the neutron number N=172 and 182/184 for both the RMF predictions and experimental data.

## 4.3.2 The $\alpha$ -decay half-life

The  $\alpha$ - decay half-life time  $T^{\alpha}_{1/2}$  can estimated by using the phenomenological formula of Viola and Seaborg [152]:

$$\log_{10}T^{\alpha}_{1/2}(s) = \frac{aZ - b}{\sqrt{Q_{\alpha}}} - (cZ + d) + h_{log}, \qquad (4.7)$$

with Z as the atomic number of the parent nucleus. For the constants a, b, c and d, instead of using the original set of constants from Viola and Seaborg [152], we use here the more recent values suggested by Sobiczewski *et al.* [153]. The value of these constants are a=1.66175, b=8.5166, c=0.20228, and d=33.9069. The quantity  $h_{log}$  accounts for the hindrances associated with the odd nucleon number. The value of  $h_{log}$  as given by Viola and Seaborg [152], is:

$$h_{log} = 0, Z \text{ and } N \text{ even}$$

Figure 4.12: The  $\alpha$ - decay-half life  $T^{\alpha}_{1/2}$  of Z= 115, 117, 120 and 122 from RMF and SHF are compared with other theoretical prediction as well as experimental data, whereever available [9, 10, 11, 12].

= 0.772, Z odd and N even
= 1.066, Z even and N odd
= 1.114, Z and N odd.

Moreover, here we have also included the recent phenomenological formula of Ref. [154] to estimate the  $\alpha$ - decay half-life time  $T^{\alpha}_{1/2}$ :

$$log_{10}T^{ph}_{\alpha}(Z,N) = aZ[Q_{\alpha}(Z,N) - \overline{E_i}]^{-1/2} + bZ + c.$$
(4.8)

Where the parameters a = 1.5372, b = -0.1607, c = -36.573 and the parameter  $\overline{E_i}$  (average excitation energy of the daughter nucleus) is,

 $\overline{E_i} = 0 \quad \text{for } Z \text{ even} - N \text{ even}$  $= 0.113 \quad \text{for } Z \text{ odd} - N \text{ even}$  $= 0.171 \quad \text{for } Z \text{ even} - N \text{ odd}$  $= 0.284 \quad \text{for } Z \text{ odd} - N \text{ odd.}$ 

Here, in the above equation of  $T_{1/2}^{\alpha}$ ,  $Q_{\alpha}(Z, N)$  is the crucial variable and is estimated from RMF and SHF formalism. From these  $Q_{\alpha}(Z, N)$  values, the  $\alpha$ -decay half-life  $T_{1/2}^{\alpha}$ are calculated by using Eqn. (4.7) and Eqn. (4.8) for <sup>293,294</sup>117, <sup>292,304</sup>120, <sup>292</sup>122 and <sup>287,288</sup>115, respectively. The calculation of  $T_{1/2}^{\alpha}$  from Ref. [154] is carried out to see the effect of that formula to the Eqn. (4.7). Note that the Eqn. (4.8) for  $T_{1/2}^{\alpha}$  is only applied to the  $\alpha$ - decay chain of <sup>287,288</sup>115. From Fig. 4.12, we found almost similar results as for all the  $\alpha$ - decay series. Specifically, the RMF and SHF results for  $T_{1/2}^{\alpha}$  agree well with the experimental data, as well as the calculations of other authors [146, 147, 148, 149, 150, 151], but slightly over-estimate to the FRDM results [32, 29]. Similar to the  $Q_{\alpha}$ , some possible shell structure also appear at N=172, 182/184, which need a careful inspection.

# 4.4 Summary and Conclusion

We have calculated the binding energy, the rms charge, neutron and matter radii, and quadrupole deformation parameter for the isotopic chain of recently synthesized Z=115, 117 and predicted to be synthesized Z=120, 122 superheavy element for both the groundas well as intrinsic first-excited states using the RMF and SHF formalism with various forces. From the calculated binding energy, we have estimated the two-neutron separation energy and the energy difference between ground- and first-excited state for studying the shape co-existence. Also, we have estimated the pairing energy for the ground-state solution in the whole isotopic chain for all atomic nucleus. We found a shape change from a prolate to an oblate deformation with increase of isotopic mass number are noticed. Most of the ground-state structures are with spherical solutions for Z=115, 117 and are super-deformed or/ and hyper-deformed solution in case of Z=120, 122. The obtained results are almost similar to other theoretical calculations and experimental data except few cases. From the binding energy analysis, we found that the most stable isotope in the isotopic series of all Z-values is close to predicted magic number at N=172 or 184. Our predicted  $\alpha$ -decay energy  $Q_{\alpha}$  and half-life  $T_{1/2}^{\alpha}$  matches nicely with the available theoretical prediction as well as experimental data. Again, similar to the binding energy, some shell structure is also observed at N=172 and/ or 184 from the  $Q_{\alpha}$  and  $T_{1/2}^{\alpha}$  for both RMF and SHF calculations.

# Chapter 5

# Island of stability at superheavy valley

# 5.1 Introduction

The search of new elements is an important issue in nuclear science, after the discovery of artificial transmutation of elements by Sir Ernest Rutherford in 1919 [155]. The existence of Neptunium (Np), Plutonium (Pt) and other 14 elements (entitled as transuranium element) beyond the last heaviest naturally occurring <sup>238</sup>U, give a new form (a separate block) to the Mendeleev's periodic table, which was landmark in the Nuclear Chemistry. Further, the study of super-heavy nuclei explores the borderline of the nuclear chart. The production of super-heavy elements (SHE) turned out to be most tedious task in the field of exotic nuclei. The fundamental questions in the study of superheavy elements is the prediction and/ or production (synthesis) of the doubly magic nucleus, next to Z=82, N=126 (<sup>208</sup>Pb). A number of theoretical calculations [113, 118, 32] have been predicted that the next magic nucleus could be <sup>298</sup>114, later which is supported by other calculations [32, 29, 156]. At present, Z=114 nucleus is already synthesized but for only a lighter isotope <sup>289</sup>114 [127]. The  $\alpha$ -decay properties is also observed and the  $\alpha$ -decay energies or  $Q_{\alpha}$  values are explained on RMF calculation [157]. Recent experiments [158, 127, 128, 129, 130, 131, 132, 122, 123, 124, 125, 126] give some signature for nuclei even closure to the expected island of stability in superheavy valley. With the development of heavy ion beam it could be possible to make some progress in the super-heavy region. Recent theoretical calculations for super-heavy elements have generated quite an excitement where new magic numbers are predicted for both protons and neutrons. This excitement cover questions in our mind:

- Whether there is a limited number of elements that can exist either in nature or can be produced from artificial synthesis by using modern technique ?
- What is the maximum number of protons and neutrons of that of a nucleus ?
- What is the next double shell closure nucleus beyond <sup>208</sup>Pb ?

To answer these questions, first we have to understand the agent which is responsible to rescue the nucleus against Coulomb repulsion. The obvious reply is the shell energy, which stabilizes the nucleus against Coulomb disintegration [144]. Many theoretical models, like the macroscopic—microscopic (MM) calculations involves to explain some prior knowledge of densities, single-particle potentials and other bulk properties which may accumulate serious error in the largely extrapolated mass region of interest. They predict the magic shells at Z=114 and N=184 [145, 156, 159, 116, 160] which could have surprisingly long life time even of the order of a million years [113, 114, 115, 116, 161]. Some other such predictions of shell-closure for the superheavy region within the relativistic and non-relativistic theories also have some impact in this directions [53, 94].

Experimentally, till now, the quest for superheavy nuclei has been dramatically rejuvenated in recent years owing to the emergence of hot and cold fusion reactions. In cold fusion reactions involving a doubly magic spherical target and a deformed projectile were used by GSI [122, 123, 124, 125] to produce heavy elements up to Z = 110-112. In hot fusion evaporation reactions with a deformed trans-uranium target and a doubly magic spherical projectile were used in the synthesis of superheavy nuclei Z = 112-118at Dubna [127, 128, 129, 130, 131, 132, 133]. At the production time of Z = 112 nucleus at GSI the fusion cross section was extremely small (1pb), which led to the conclusion that reaching still heavier elements will be very difficult or/ and impossible. At present, the emergence of hot fusion reactions using  ${}^{48}Ca$  projectiles at Dubna has drastically changed the situation and nuclei with Z = 114-118 were synthesized and also observed their  $\alpha$ -decay as well as terminating spontaneous fission events. It is observed that Z =115–117 nuclei have a long  $\alpha$ -decay chains contrast to the short chains of Z = 114-118. Moreover, the life times of the superheavy nuclei with Z = 110-112 are in milliseconds and microseconds whereas the life time of Z = 114-118 up to 30 s. This pronounced increase in life times for these heavier nuclei has provided great encouragement to search the magic number somewhere beyond Z = 114. Moreover, it is also an interesting and important question for the recent experimental discovery [162, 163, 164, 9] say chemical method of Z = 122 from the natural <sup>211,213,217,218</sup> Th which have long lived super-deformed (SD) and/ or hyper-deformed (HD) isomeric states 16 to 22 orders of magnitude longer than their corresponding ground-state (half-life of  $^{292}122$  is  $t_{1/2} \ge 10^8$  years). Hence, it is an inbuilt motivation for all nuclear theorist as well as experimentalist to see the Island of Stability in superheavy valley. Here, we have scanned this region using recent developed and successful microscopic models to find some signature of shell closures for proton and neutron.

The *Chapter* is organized as as follows: The details of the calculations and results are given in Section II. A summary of the results together with a concluding remarks are given in Section III.

# 5.2 Result and Discussion

A number of force parameters are convenient to solving the standard SHF Hamiltonians and RMF Lagrangians. The ground state properties, like the binding energies (BE), quadrupole deformation parameters  $\beta_2$ , charge radii ( $r_c$ ), and other bulk properties are evaluated by using the various non-relativistic and relativistic parameter sets in some of our previous works and by other authors [70, 85, 101, 82, 165]. From these results, one can find that, more or less, most of the recent parameter sets reproduce well the

Figure 5.1: The proton (neutron) average pairing gap  $\Delta_p$  ( $\Delta_n$ ) for Z=78-82 with N=120-140 [17].

ground state properties, not only of stable normal nuclei but also of exotic nuclei which are far away from the valley of  $\beta$ -stability. This means that if one uses a reasonably acceptable parameter set, the predictions of the model will remain nearly force independent. Here, we have used two well-defined but distinct approaches (i) non-relativistic Skryme-Hartree-Fock (SHF) with FITZ, SIII, SkMP and SLy4 interactions [78, 79, 80, 4] (ii) Relativistic Mean Field (RMF) formalism [8, 46, 49, 63, 64, 85] with NL3, G1, G2 and NL-Z2 parameter sets. The constant strength scheme is adopted to take care of pairing correlation [70] and evaluated the pairing gaps  $\Delta_n$  and  $\Delta_p$  for neutron and proton respectively from the celebrity BCS equations [101]. This types of prescription for

Figure 5.2: The two neutron separation energy  $S_{2n}$  for Z=78-82 and N=120-140 in the framework of SHF and RMF theory [17].

pairing correlation both in RMF and SHF have been used by us and many other authors [85, 70, 139]. Within this pairing approach, it is shown that the results for binding energy are almost identical with the predictions of the Relativistic Hartree-Bogoliubov (RHB) approach [85, 66]. Here, our calculation has appeared as a powerful tool to study the shapes and collective properties of nuclei, which mainly connected with the stability of a nucleus. In order to get magic numbers for proton and neutron in the valley of super-heavy, we first established the basic magic properties. It is well understood and settled that the properties of a magic number for a nuclear system have following characteristics:

• The average pairing gap for proton  $\Delta_p$  and neutron  $\Delta_n$  at the magic number is

minimum.

- The binding energy per particle is maximum compared to the neighboring one, i.e. there must be a sudden decrease (jump) in two neutron (or two proton) separation energy  $S_{2n}$  just after the magic number in an isotopic or isotonic chain.
- At the magic number, the shell correction energy  $E_{shell}$  is maximum negative.
- A pronounced energy gap in the single-particle levels  $\epsilon_{n,p}$  appears at the magic number.

Here, we focus on the shell closure properties in the superheavy nuclei based on the above four important observables and identified the magic proton and neutron numbers. Before going to that region, first of all we have tested these observable for a well known and experimentally verified double closed Pb isotopes. For this representative case, we have taken the region Z=78-82 with N=120-140 and calculated the average pairing gap (for proton  $\Delta_p$  and neutron  $\Delta_n$ ), and two neutron separation energy  $S_{2n}$ . These are shown in Figs. 5.1 and 5.2 respectively [17]. The experimental values are given for comparisons. From Figures, it is clear that the  $\Delta_p$  gives the minimum value (almost zero) for Z=82 and  $\Delta_n$  is minimum at N=126 in the isotopic chain of all these atomic nuclei. The results also consistent to the  $S_{2n}$  energy calculation. The experimental datas are also showing same behaviour in both the case. It is worthy to mention that the above defined magic properties are clearly observed from figures (Fig 5.1 and 5.2 [17]) for Z=82 with N=126. To find the next magic nuclei beyond <sup>208</sup>Pb for that, we have to looked the above defined magic properties in the superheavy region.

#### 5.2.1 Average pairing gap

The average pairing gap is defined by [9, 10, 17],

$$\Delta_q = G_q \sum_{\alpha_q} \left[ n_{\alpha_q} \left( 1 - n_{\alpha_q} \right) \right]^{-1/2}.$$
(5.1)

Figure 5.3: The proton average pairing gap  $\Delta_p$  for Z=112-126 with N=162-220 and Z=112-130 with N=162-260 [17].

Here, q = Neutron or Proton,  $n_{\alpha_q}$  is the occupation probability of a state with quantum numbers  $\alpha_q = nljm$ . The quantity  $G_q$  stands for pairing strength and the sum is restricted to +ve values of m. This simple approach is used here to calculate the average pairing gap for proton  $(\Delta_p)$  and neutron  $(\Delta_n)$ . A wide range of nuclei starting from the proton-rich to the neutron-rich region is scanned in the superheavy valley (Z=112 to Z=130). The curves for  $\Delta_p$  are displayed in Fig. 5.1 obtained by SHF and RMF with FITZ, SIII, SLy4, SkMP and NL3,NL-Z2, G1, G2 force parametrizations. Analyzing the figure carefully, it is clear that the value of  $\Delta_p$  almost zero for the whole Z=120 isotopic chain in both the theoretical approaches. For example,  $\Delta_p \sim 0.0001$  for all isotopes of

Figure 5.4: Same as Fig. 5.1 but for neutron average pairing gap  $\Delta_n$  [17].

Z=120 and ~ 0.5 for all other case. Here, a similar  $\Delta_p$  is also observed for few isotopes of Z=114 and Z=124 in RMF (G2).

To predict the corresponding neutron shell closure of the magic Z=120, we have estimated the neutron pairing gap  $\Delta_n$  for all elements Z=112-130 with their corresponding isotopic chain. As a result, the calculated  $\Delta_n$  for the whole isotopic chains are displayed in Fig. 5.2. We obtained an arc like structure (similar to Fig. 5.1) with vanishing  $\Delta_n$ at N=182, 208 and N=172, 184, 258 respectively for SHF and RMF of the considered parameter sets. Further, the neutron pairing gap is found to be minimum among the isotopic chains pointing towards the magic nature of Z=120. Therefore, all of these force parameters are directing Z=120 as the next magic number after Z=82.

Figure 5.5: The two neutron separation energy  $S_{2n}$  for Z=112-126 and N=162-220 in the framework of SHF theory [17].

# 5.2.2 Two neutron separation energy

The two nucleon separation energy of a nucleus is defined as:

$$S_{2q}|_{q=n,p} = BE(N_q) - BE(N_q - 2), \tag{5.2}$$

where,  $N_q$  is the number of neutron (proton) for a given nucleus. A sharp fall in the  $S_{2q}$  value means that a very small amount of energy required to remove two nucleons as compared to its magic neighbor. Thus, the nucleus is significantly stable as compare to the daughter, which is a most basic characteristics of magic number. In other word, the

binding energy per particle (BE/A) is maximum for double closed nucleus (<sup>4</sup>He, <sup>16</sup>O, <sup>40</sup>Ca, <sup>48</sup>Ca, ... and <sup>208</sup>Pb) compared to the neighboring one. For example, the BE/A with SHF (FITZ set) for <sup>300,302,304</sup>120 are 7.046, 7.048 and 7.044 MeV corresponding to N=180, 182 and 184 respectively. Similarly with SLy4 these values are 6.950, 6.952 and 6.933 MeV. This is reflected in the sudden jump of  $S_{2n}$  from a higher value to a lower one at the magic number in an isotopic chain. This lowering in two neutron separation energy is an acid test for shell closure investigation. Fig. 5.3 shows the  $S_{2n}$  as a function of neutron number for all the isotopic chain of the considered elements for SHF formalisms [17]. In spite of the complexity about single-particle and collective properties of the nuclear interaction some simple phenomenological facts emerge from the bulk properties of the low-lying states in the even-even atomic nuclei. The  $S_{2n}$  energy is sensitive to this collective/ single-particle inter play and provides sufficient information about the nuclear structure effects. From Fig 5.3, we notice such effect, i.e., jump in two neutron separation energy at N=182 with SHF. However, we find similar results  $S_{2n}$  and  $E_{shell}$ energies for RMF calculation at neutron numbers 172 and 184.

## 5.2.3 The shell correction energy

According to Strutinsky energy theorem in liquid drop model [166, 167], the total quantal energy can be divided into two parts:

$$E_{tot} = E_{avq} + E_{shell},\tag{5.3}$$

here,  $E_{tot}$ ,  $E_{avg}$ , and  $E_{shell}$  are the total, average and shell correction energy, respectively. The addition of shell correction contribution to the total energy, the whole scenario of liquid properties converted to shell structure which could explain the magic shell even in the frame-work of liquid-drop model. The average part of the ground state energy of a shell model potential can be obtained by replacing the Hartree-Fock occupation number  $n_{\alpha}$  (see previous subsection 5.2.1) by average occupation number  $\overline{n}_{\alpha}$ . The values of  $n_{\alpha}$  is 1 and 0 for occupied and empty state, respectively. This implies that the shell correction

Figure 5.6: The shell correction energy  $E_{shell}$  for Z=112-126 and N=162-220 in the framework of SHF theory [17].

energy is the difference between the exact and average energy and is given by,

$$E_{shell} = \sum_{\alpha} \left( n_{\alpha} - \overline{n}_{\alpha} \right) \varepsilon_{\alpha}, \tag{5.4}$$

with  $\varepsilon_{\alpha}$  is the energy eigen values of the nuclear potential. The smoothed  $\overline{n}_{\alpha}$  are normalized separately for neutron and proton number for a given nucleus. Recently, it is reported by Satpathy *et al.* [144] that the shell effect is not only responsible for the stability of the superheavy nuclei but also balance the Coulomb repulsion. Hence, the shell correction energy  $E_{shell}$  is a key quantity to determine the shell closure of nucleon. The magnitude of total (proton plus neutron)  $E_{shell}$  energy is dictated by the level density around the Fermi level. A positive  $E_{shell}$  reduces the binding energy and a negative shell correction energy increases the stability of the nucleus. As a representative case, we have depicted our SHF result of  $E_{shell}$  in Fig 5.4. It is clear from the figure, the extra stability of <sup>302,328</sup>120. However, we find similar results for  $E_{shell}$  energies for RMF calculation at neutron numbers 172, 184.

Figure 5.7: The single-particle levels for neutron  $\epsilon_n$  and proton  $\epsilon_p$  nearer to the Fermi level for  $^{302}120$  in SHF(SLy4 and FITZ) and  $^{304}120$  in RMF (NL3 and G2). The energy is in MeV [17].

#### 5.2.4 Single-particle energy levels

From the above subsections 5.2.1-5.2.4, we have already found some signatures of magic properties for Z=120 at N=182 for SHF and N=184 for RMF formalisms. As a further confirmatory test, the single-particle energy levels for neutrons and protons  $\epsilon_{n,p}$  are analyzed. The calculated  $\epsilon_{n,p}$  nearer to the Fermi levels are shown in Fig. 5.5 for <sup>302</sup>120 (N=182) SHF (SLy4 and FITZ) and for <sup>304</sup>120 (N=184) RMF (NL3 and G2). From the figure, one can estimate the energy gaps  $\Delta \epsilon_{n,p}$  for neutron and proton orbits. For example, in <sup>302</sup>120 (FITZ), the gap  $\Delta \epsilon_n = \epsilon_n (3d_{3/2}) - \epsilon_n (4s_{1/2})$  at N=182 is 1.977 MeV and  $\Delta \epsilon_p = \epsilon_p (2f_{5/2}) - \epsilon_p (3p_{3/2}) = 1.340$  MeV at Z=120, which is considerably large value. Almost identical behaviour is noticed with RMF (at N=184) calculations, irrespective of parameter used, confirming Z=120 as a clear magic number. It is well accepted that the sequence of the magic number for exotic system is much different from that of the normal nuclei [168, 82, 157]. This phenomenon is quite normal in superheavy region. Hence, from these observables, one can conclude Z=120 is the next magic proton with corresponding neutron (s) N=172, 182/184 in the superheavy valley.

It is well known that, the double magic nuclei, <sup>4</sup>He, <sup>16</sup>O, <sup>40</sup>Ca, <sup>48</sup>Ca, <sup>56</sup>Ni, <sup>90</sup>Zr, <sup>132</sup>Sn and <sup>208</sup>Pb are spherical in their ground state. Here we are enthusiastic to know the shape of these predicted magic nuclei <sup>292,304</sup>120 in their ground state. For this we have calculated the quadupole deformation parameter  $\beta_2$  using axially deformed RMF and SHF formalisms for these force parameters. The results obtained from these calculations are quite interesting, because the ground state solution appear at  $\beta_2 \sim 0.0$ , which is also spherical in nature.

# 5.3 Summary and Conclusion

In summary, we have analyzed the pairing gap  $\Delta_p$  and  $\Delta_n$ , two-neutron separation energy  $S_{2n}$ , shell correction energy  $E_{shell}$  and single-particle energy  $\epsilon_{p,n}$  for the whole Z = 112-130 region covering the proton-rich to neutron-rich isotopes. To our knowledge, this is one of the first such extensive and rigorous calculation in both SHF and RMF models using a large number of parameter sets. The recently developed effective field theory motivated relativistic mean field forces G1 and G2 are also involved. Although the results depend slightly on the forces used, the general set of magic numbers beyond <sup>208</sup>Pb are Z=120 and N=172, 182/184. The highly discussed proton magic number Z = 114 in the past (last four decades) is found to be feebly magic in nature.

# Chapter 6

# **Evolution of clustering in Nuclei**

# 6.1 Introduction

Becquerel, first observed the natural radioactivity in 1896; the first experimental observation of  $\alpha$  – decay from nucleus was found in 1908 by Rutherford [169, 170]. The successful explanation of  $\alpha$  – radioactivity is carried out through quantum-tunneling effect by Gamow [171] and Gurney and Condon [172] in 1928. At the beginning of that time, the decay supposed to be one the possible way for a unstable nucleus to stabilized. But, the theoretical prediction of the new possible mode of decay called cluster decay (i.e. cluster radioactivity) was pointed in 1980, which is one of the land mark in nuclear physics [173]. In this decay, one or more small nuclei, heavier than  $\alpha$ - particle are emitted from the core of the parent nucleus. The experimental research on cluster radioactivity is started in 1984 [169, 174] and subsequently grew up reaching a steady state in the period 1990-2000. The consequent excitement led several experiments at Berkeley, Dubna, Orsay and Milano to develop experimental techniques to investigate such peculiar and extremely rare decay mode of nuclei. However, these are not only motivation of an intense experimental investigation in the course of twenty years but also this allowed to measure the decay properties of thousands of cases corresponding to different combinations of parent nuclei, emitted clusters and the Q-value for such radioactive decay. At present the clusters  $^{20}$ O,  $^{23}$ F,  $^{2426}$ Ne,  $^{28,30}$ Mg and  $^{32,34}$ Si are continuously found

in Fr, Ra, Ac, Th, Pa, U, Pu, and Cm nuclei in trans-lead region.

After the confirmation of clustering, few questions raised in our mind: (1) are they initially formed inside the parent nuclei; (2) how they look like i.e. what is the internal configuration of these sub-atomic nuclei; (3) what are the constituent of these cluster i.e. to count the nucleons for a cluster. Hence, it is important to see the preformed cluster(s) inside the parent nucleus and estimate their life time. Theoretically, the *shell model*, *cluster model* and *fission model* are used to describe the cluster radioactivity [175]. These models are based on two assumptions, such as pre- and post- formation of clusters in a nucleus. For example, in case of unified fission model (UFM), the basic concept is that the nucleus continuously deforms as it penetrates the barrier and reaches scission configuration. But, in case the preformation cluster model (PCM), the plenty of nucleons in the ground state of parent nuclei are considered to be cooled and reassigned and the cluster preformation is existed in the parent before penetrate the barrier.

Moreover, the relativistic mean field (RMF) calculations are very much successful in determining the clusters inside the parent nuclei from its intrinsic density distribution. For example, the  $\alpha - \alpha$  clustering in <sup>8</sup>Be, the  $3\alpha$ -equilateral triangle (co-existing with spherical shape) in <sup>12</sup>C, 4 $\alpha$ -tetrahedron (kite-like shape) in <sup>16</sup>O and the 3 $\alpha$  and 4 $\alpha$ linear chains for their excited state are some interesting results from RMF [176, 177]. Furthermore, <sup>56</sup>Ni shows [177] a preferred N=Z,  $\alpha$ -nucleus clustering for states with deformations up to hyper-deformation ( $\beta \leq 2.45$ ). Similarly, for heavy actinides (<sup>222</sup>Ra, <sup>232</sup>U, <sup>236</sup>Pu and <sup>242</sup>Cm), the RMF gives [178] not only the N $\approx$  Z,  $\alpha$ -like clustering in the g.s. but also the exotic  $N \neq Z$  clustering in excited states. Signatures of clustering structure in RMF calculations of super-heavy Z=114 and 120, N=172-184 nuclei [178, 179] are also obtained in terms of exotic  $N \neq Z$  clusters at the center of their super-deformed g.s. or the clustering in to two large and some small pieces is universal for all super-deformed ground states in Z=120 nuclei. The super-superheavy  $^{238}U+^{238}U\rightarrow^{476}184^*$  nucleus also supports the clustering phenomenon, with a kind of triple fission of an exotic cluster in the neck region of two equal fragments of N=Z matter [180]. From the calculated neutron and proton densities, only the N/Z  $(=\rho_n/\rho_p)$  ratios of the clusters were obtained

Table 6.1: The RMF(NL3) results of BE,  $\beta_2$ , and the root-mean-square radii of charge  $r_c$  and matter  $r_m$  for the <sup>112-122</sup>Ba nuclei in their ground-state (g.s.) and 1st, 2nd, etc., excited states (e.s.) are compared with FRDM, Hartree-Fock-BCS (HFBCS) and experimental data, whereeever available. The extrapolated binding energies marked with star (\*).

Nucl.	BE		$r_{rms}$ : RMF		$\beta_2$		BE	$r_c$	$\beta_2$
	RMF	Expt.	$r_m$	$r_c$	RMF	Expt.	FRDM	HFBCS	FRDM
<sup>112</sup> Ba	895.4		4.62	4.74	0.24		894.9	4.72	0.21
	893.3		4.80	4.99	-0.39				
	882.4		5.35	5.48	1.24				
<sup>114</sup> Ba	920.1	922.3	4.65	4.75	0.24		921.3	4.74	0.24
	918.1		4.78	4.90	-0.39				
	909.3		5.33	5.45	1.21				
<sup>116</sup> Ba	947.6	$947.0^{*}$	4.70	4.78	0.30		946.9	4.78	0.28
	943.7		4.80	4.90	-0.39				
	934.2		5.36	5.46	1.20				
<sup>118</sup> Ba	971.4	$971.0^{*}$	4.75	4.82	0.33		970.8	4.80	0.29
	969.2		4.71	4.81	-0.24				
<sup>120</sup> Ba	993.9	993.6	4.78	4.83	0.32		993.44	4.8	0.28
	991.6		4.75	4.81	-0.23				
<sup>122</sup> Ba	1015.5	1015.5	4.80	4.84	0.32	0.354	1015.2	4.81	0.27
	1013.5		4.77	4.82	-0.23				

[178, 180], which were indeterminate up to  $\sim 20\%$  since only the average densities could be used. However, the actual internal or sub-structure of the clusters was not determined in these calculations, which is one of the aims of the present study. The important step, carried out here for the first time is the counting of number of protons and neutrons present in the clustering region(s), which determines the sub-atomic nuclei in the cluster region.

The present chapter is organized as follows. In section Section II, the details of the calculations and the results are outlined. The evolution of clustering inside the parent nucleus and the counting of the nucleons inside the cluster are also included in this section. A summary of the results together with concluding the remarks are given in Section III.

# 6.2 Method of Calculation and result discussion

The mean-field equations are solved self-consistently taking different inputs of the initial deformation  $\beta_0$ . For a normal ground state solution in the considered mass region, the number of major shells for Fermions and bosons are used here  $N_F = N_B = 10$ . To test the convergence of the solutions, few calculations are done with  $N_F = N_B = 12$ also. The variation of these two solutions are  $\leq 0.02\%$  on binding energy and 0.01%on nuclear radii for drip-line nuclei. This implies that the used model space is good enough for the considered nuclei. However, in the present paper, we deal with a rather large deformed state. To get a self-consistently converged solution for such cases (large deformation), one may need a large model space for both the Fermions and bosons oscillator shells. For this reason, we have used an axially deformed harmonic oscillator basis with  $N_F = N_B = 20$  shells for these special cases. The number of mesh points for Gauss-Hermite and Gauss-Laguerre integration are 20 and 24, respectively. For a given nucleus, the maximum binding energy corresponds to the ground state and other solutions are obtained at various excited intrinsic states. In our calculations, we obtained different nucleonic potentials, densities, single-particle energy levels, root-mean-square (rms) radii, deformations and binding energies for different states. These observables explain the structure and sub-structure for a nucleus in a given state.

## 6.2.1 Potential Energy Surface

The potential energy surface (PES) is calculated by using the RMF formalism in a constrained method [181, 9, 10, 182, 183], i.e., instead of minimizing the  $H_0$ , we have minimized  $H' = H_0 - \lambda Q_2$ , with  $\lambda$  as a Lagrange multiplier and  $Q_2$ , the quadrupole moment. The details procedure for this calculations are already given in subsection 2.1. The term  $H_0$  is the Dirac mean field Hamiltonian for RMF model (the notations are standard and its form can be seen in Refs.[85, 183]). The converged free energy solution does not depend on the initial guess value of the basis deformation  $\beta_0$  as long as it is nearer to the minimum in PES. However, it converges to some other local minimum

Figure 6.1: The potential energy surfaces for <sup>112</sup>Ba and <sup>122</sup>Ba nuclei, i.e, constrained binding energy as a function of quadrupole deformation parameter in RMF (NL3) calculations [13].

when  $\beta_0$  is drastically different, and in this way we evaluate a different intrinsic isomeric state for a given nucleus.

The PES for the representative <sup>112</sup>Ba and <sup>122</sup>Ba nuclei are shown in Fig. 6.1 for a wide range of  $\beta_2$  starting from oblate to prolate deformation [13]. The upper panel is for <sup>112</sup>Ba and the lower one for <sup>122</sup>Ba. For <sup>112</sup>Ba, we notice the minima are around  $\beta_2$ =-0.39, -0.20, 0.24, 1.02 and 1.20, corresponding to binding energy  $BE_c$ = 890.6, 894.2, 896.7, 884.2 and 882.7 MeV, respectively, and their energy differences between the nearest consecutive minima are 3.60, 2.50, 12.93 and 1.52 MeV. However, in case of <sup>122</sup>Ba, only two minima exist around  $\beta_2$  = -0.23 and 0.26 at  $BE_c$  = 1012.4 and 1013.7 MeV. The

intrinsic energy difference between these two configurations is 1.3 MeV. From this figure, it is clear that there exists two identical major minima at  $\beta_2 \sim -0.23$  and 0.24 in both the <sup>112</sup>Ba and <sup>122</sup>Ba nuclei. A further investigation of the PES for other isotopes shows that actually the multi-minima structure of <sup>112</sup>Ba disappears gradually with the increase of mass number in the isotopic chain of Ba, and reaches to only two minima configuration, one oblate and another prolate, at mass number A=122. In other word, there is no solution exist at high deformation (super/hyper-deformation) for higher mass of the *Ba*.

## 6.2.2 Nuclear Bulk properties

The binding energies (BE) and quadrupole deformation parameters  $\beta_2$  for <sup>112–122</sup>Ba isotopes are evaluated for the ground as well as intrinsic excited states (e.s.). The obtained results are tabulated in Table 6.1, together with the experimental data[107, 184] and the extrapolated values (marked with star (\*)), wherever available. The finite range droplet model (FRDM) binding energies and  $\beta_2$ -values are also listed in the table for comparison [13]. Since no experimental data are available for  $r_{ch}$ , the tabulated values are the theoretical results from Hartree-Fock-BCS (HFBCS) method [13]. The first row in each nucleus corresponds to the ground state (g.s.) binding energy and all other energies are the first and second excited state BE's, respectively. The experimental value of g.s.  $\beta_2$  is available for <sup>122</sup>Ba only, since the neutron -deficient <sup>112–120</sup>Ba isotopes lie near the proton drip-line, and hence their deformation parameters are not yet known. Table 6.1 shows the binding energies, charge radii  $r_c$  and  $\beta_2$  values agree well with the available experimental data and with other theoretical calculations for both ground and excited states [13].

In Table 6.1, as discussed above, all the Ba isotopes are shown to have several intrinsic minima, where each minimum corresponds to a deformation and a binding energy. For example, the ground state deformation  $\beta_2=0.24$  for <sup>112</sup>Ba. Similarly the g.s. deformations for <sup>114</sup>Ba, <sup>116</sup>Ba, <sup>118</sup>Ba, <sup>120</sup>Ba and <sup>122</sup>Ba are 0.24, 0.30, 0.33, 0.32 and 0.32, respectively. All other intrinsic excited state deformations, with corresponding binding energies, are also listed in Table 6.1 [13]. For <sup>112,114,116</sup>Ba nuclei we get a solution at
a highly deformed configuration of  $\beta_2 \sim 1.2$ , whereas this hyper-deformed minimum is washed out with increase of mass number in the Ba isotopic chain. This means there is no hyper-deformed solutions for <sup>118–122</sup>Ba (see also, Fig. 4 where such highly deformed configurations are shown only for <sup>112,114,116</sup>Ba). The root mean square (rms) radii of matter and charge distribution are also calculated for various quadrupole deformations from oblate to prolate and hyper-deformed states. The matter rms radius  $r_m$  and charge distribution rms radius  $r_c$  are listed in Table 6.1 for different  $\beta_2$  values. From the table, it is observed that the  $r_m$  increases with increase of quadrupole deformation.

Figure 6.2: The internal sub-structure of  $^{24}$ Mg with and without pairing in the ground state configuration [14].

#### 6.2.3 Relativistic mean-field and clustering

It is well known that the RMF formalism reproduce the cluster structure of nuclei [185, 186, 13, 14] which are already predicted by several cluster models [187, 188, 189]. However, the mean field concept itself goes against the finding of clustering. In case of present RMF formalism, the mean-field approximation is taken for different meson fields considering as classical number. And the nucleons are treated as point particle, which oscillates in the mean field meson medium and gives the way for an independent constraint, results the clustering inside the nucleus. On the other hand, one can say that the fluctuation in the central density of the nucleons are due to the shell effect, which may caused by the pairing correlation of nucleons around the Fermi surface. If this is the case, then it would have hard to find the shell gaps and other magic properties in the RMF formalism. Further, to show the quantitative explanation, we have calculated the gross properties including the density profile for the well known nuclei such as <sup>24</sup>Mg with and without pairing correlations. The contour plot of the density profiles are shown in Fig. 6.2. From the figure, one can find almost identical structures in both the cases even the deformation also almost same for both the approximations. For example, the deformations with and without pairing correlations are 0.45 and 0.44, respectively (see Fig. 6.2) and the ground state solution for both the cases correspond to almost same binding energy (see Ref. [14]). This confirms the power of RMF theory for cluster prediction.

### 6.2.4 The Clustering and Sub-atomic Nuclei

The internal structure of a nucleus depends on the density distributions of protons and neutrons for a given state. Here, the densities are obtained from RMF (NL3) in the positive quadrant of the plane parallel to the symmetry z-axis. These are evaluated in the  $\rho z$  plane, where  $\rho = x = y = r_{\perp}$ . It is to be noted that, both the axes z and  $\rho$  are conserved in our formalism under the space reflection symmetry. Now we can obtain the complete picture of a nucleus in the  $\rho z$  plane by reflecting the first quadrant to other quadrants. Figs. 6.3-6.5 show the density plots for all the possible solutions,

Table 6.2: The number of protons  $Z_{clus.}$  and neutrons  $N_{clus.}$ , and mass  $A_{clus.}$ , in clusters inside the <sup>112–122</sup>Ba nuclei for different solutions from the RMF(NL3) formalism. The clusters are listed as the ground state (g.s.) and the first excited state (e.s. I) and the second excited state (e.s. II) solutions. The ranges of integration in Eq. (2), i.e.,  $r_1, r_2; z_1, z_2$  (in fm), for each cluster are also given.

Nucleus	State	$\beta_2$	Cluster	$Z_{clus.}$	$N_{clus.}$	$A_{clus.}$	Cluster
			range $(r_1, r_2; z_1, z_2)$				
<sup>112</sup> Ba	g.s.	0.24	(-1.5, 1.5; 1.9, 4.5)	17.7	18.3	36.0	<sup>36</sup> Ar
			(1.3, 2.45; -1.3, 1.3)	5.8	6.2	13.0	$^{12}\mathrm{C}$
			(2.9, 3.8; -2.0, 2.0)	7.1	7.4	14.5	$^{14}\mathrm{N}$
	e.s.I	-0.39	(-3.45, 3.45; -1.7, 1.7)	50.4	52.9	103.3	$^{103}\mathrm{Sn}$
	e.s.II	1.24	(-1.0, 1.0; -6.4, 6.4)	46.5	48.8	95.3	$^{95}\mathrm{Pd}$
$^{114}\text{Ba}$	g.s.	0.24	(-1.5, 1.5; 2.1, 4.6)	16.9	17.9	34.7	$^{35}\mathrm{Cl}$
			(1.25, 2.5; -1.1, 1.1)	5.8	6.2	12.0	$^{12}\mathrm{C}$
			(3.3,  3.7;  0.7,  2.0)	1.1	1.2	2.3	$^{2}\mathrm{H}$
	e.s.I	-0.39	(-3.35, 3.35; -1.5, 1.5)	49.9	54.7	104.6	$^{105}\mathrm{Sn}$
	e.s.II	1.21	(-1.0, 1.0; -6.5, 6.5)	46.2	49.6	95.8	$^{96}\mathrm{Pd}$
$^{116}Ba$	g.s.	0.30	(-1.5, 1.5; 2.2, 4.6)	16.8	17.9	34.7	$^{35}\mathrm{Cl}$
			(1.25, 2.25; -1.1, 1.1)	5.8	6.5	12.3	$^{12}\mathrm{C}$
			(3.3, 3.76; 0.6, 2.0)	1.1	2.3	3.4	$^{3}\mathrm{H}$
	e.s.I	-0.39	(-3.3, 3.3; -1.5, 1.5)	48.8	54.9	103.7	$^{104}$ In
	e.s.II	1.20	(-1.0, 1.0; -6.7, 6.7)	47.8	52.5	103.3	$^{103}\mathrm{Cd}$
$^{118}\mathrm{Ba}$	g.s.	0.33	(-1.6, 1.6; 2.5, 5.5)	19.9	22.2	42.0	$^{42}Ca$
			(3.3,  3.6;  0.7,  2.0)	0.8	0.9	1.7	$^{2}\mathrm{H}$
			(1.6, 2.1; -0.4, 0.4)	0.7	0.8	1.6	$^{2}\mathrm{H}$
	e.s.I	-0.24	(-1.1, 1.1; -0.6, 0.6)	5.6	6.4	12.0	$^{12}\mathrm{C}$
$^{120}Ba$	g.s.	0.32	(-1.7, 1.7; 2.6, 5.3)	19.3	23.2	42.5	$^{43}Ca$
			(3.4, 3.6; 0.8, 1.75)	0.7	1.2	1.9	$^{2}\mathrm{H}$
	e.s.I	-0.23	(-1.1, 1.1; -0.6, 0.6)	5.9	6.3	12.2	$^{12}\mathrm{C}$
$^{122}\text{Ba}$	g.s.	0.32	(-1.7, 1.7; 2.5, 5.3)	19.7	22.8	42.6	$^{43}Ca$
			(3.4, 3.7; 0.8, 2.0)	0.7	1.8	2.5	$^{3}\mathrm{H}$
	e.s.I	-0.23	(-1.1, 1.1; -0.55, 0.55)	5.6	6.4	12.0	$^{12}\mathrm{C}$

starting from oblate to prolate deformation of the Ba isotopic chain (see Table 6.1). The density profiles for the ground state of  $^{112-122}$ Ba follow the prolate ground state solution around  $\beta_2 \sim 0.25$  are shown Fig. 6.3. The oblate-deformed and hyper-deformed prolate solutions obtained for  $^{112-122}$ Ba isotopes around  $\beta_2 \sim -0.35$  and 1.1 are shown in Figs. 6.4-6.5, respectively. From these graphs, the clustering structures in Ba nuclei are quite evident. Considering the color code, starting from deep *violet* with maximum density distribution to *olive* bearing the minimum density, one can Analise the distribution of nucleons inside the various isotopes at various shapes. (In black and white figures, the color code is read as deep *black* with maximum density to light *qray* as minimum density distribution). In Fig. 6.4, the minimum density for the oblate-state starts from 0.001  $fm^{-3}$  and goes up to a maximum of 0.16  $fm^{-3}$ , but in case of the prolate-states in Figs. 6.3 and 6.5 it starts from  $0.001 \text{ fm}^{-3}$  and goes up to  $0.18 \text{ fm}^{-3}$ , which means that the size of cluster nucleus in the oblate-state is larger than that of the prolate-state. A careful inspection of the density distributions in different regions of the nucleus clearly shows the formation of various clusters inside the nuclei, which are listed in Table 6.2 as groundstate (g.s.) and excited state (e.s.) I or II cluster states, together with their deformations  $\beta_2$ . A prominent observation is that there is no configuration of deformation  $\beta_2 \sim 1.2$ , i.e., e.s.II, in cases of <sup>118–122</sup>Ba, similar to what is shown in Fig. 6.5 for lighter mass <sup>112–116</sup>Ba isotopes.

Basically, we predicted the clustering regions inside a nucleus on the basis of the total density distribution. A widely varying (total) density of the region inside the nucleus with respect to that of its surrounding region is called as the clustering region, which have very high preformation and the decaying probability. This region having the average density ranging from 0.150 to 0.171 fm<sup>-3</sup> for prolate and from 0.160 to 0.158<sup>-3</sup> for oblate states. Such regions are decorated with deep violet and red (in colored figures) and deep black and black (in B/W figures) for prolate and oblate solutions, respectively. Finally, if we concentrate on the cluster configuration of each of the nucleus in  $^{112-122}$ Ba chain, it is clear from the figures that there is a near gradual change in the prolate configuration inside the nucleus, i.e., the clusters inside the nucleus for different  $\beta_2$  values are distinct

from each other, but the same for oblate configuration is rather sudden in going from a heavy cluster to a small cluster. For example, the ground-state solution of <sup>112</sup>Ba contains three clusters ( $^{36}$ Ar,  $^{12}$ C and  $^{14}$ N), which is not the same for other cases of  $^{114-122}$ Ba. The same result holds good for intrinsic exited states also. Only <sup>12</sup>C cluster is consistently seen for <sup>112-116</sup>Ba and <sup>118-122</sup>Ba, respectively, for prolate ground-state and first excited states.

Figure 6.3: The cluster configurations of  $^{112-122}$ Ba for the prolate ground states in RMF(NL3) calculations [13].

Figure 6.4: The cluster configurations of  $^{112-122}$ Ba for the oblate intrinsic 1st excited states (e.s.I) in RMF(NL3) calculations [13].

### 6.2.5 Counting of nucleons inside the clusters

In this subsection, we count the number of nucleons in different clusters formed inside the <sup>112-122</sup>Ba isotopic chain, listed in the Table 6.2. The density distributions of these clusters obtained from the RMF(NL3) formalism for different solutions of deformation parameters  $\beta_2$  from oblate to prolate configurations are already shown in Figs. 6.3 to 6.5. From these density distribution plots of oblate or prolate configuration, we find the number of nucleons by using the general formula in Eqn. (6.1) (given below) for both the protons and neutrons (using individual density distributions) which together with

Figure 6.5: The cluster configurations of  $^{112-116}$ Ba for the intrinsic excited hyperdeformed states in RMF(NL3) calculations [13].

the total number of nucleons are listed in the Table 6.2. To perform this calculation, we need the ranges of the integral i.e. the dimension, which defines the lower and upper limit of the integral in Eqn. (6.1)  $[r_{\perp} (r_1, r_2) \text{ and } z (z_1, z_2)]$ . The values of the ranges for different clusters for some of the <sup>112-122</sup>Ba isotopes are listed in Table 6.2. The formula used to identify the ingredient (nucleons) of the cluster is given by [13]:

$$n = \int_{z_1}^{z_2} \int_{r_1}^{r_2} \rho(z, r_\perp) d\tau, \qquad (6.1)$$

where, n is the number of neutrons N or protons Z or mass A and z  $(z_1, z_2)$ ,  $r_{\perp}$   $(r_1, r_2)$  are the ranges. From the estimated proton and neutron numbers, we determine the mass of the cluster inside the nucleus. It is worth mentioning here that the ranges are guided by the graphical technique to some extent. As a result, the counting of nucleons inside a cluster may be undetermined to the extent of one unit each. In other words, the obtained  $Z_{clus.} + N_{clus.} = A_{clus.}$  may read as  $A_{clus.} \pm 1$ . With the ranges of a cluster for both the axes at hand, we solve the integral in Eqn. (6.1) within these limits, i.e., obtain a sum of all the densities of this region for each point corresponding to their individual density values over the nucleus, which gives the number of nucleons (proton or neutron). From this proton and neutron numbers, we determine the mass number of the cluster present inside the nucleus.

First of all, we notice from Table 6.2 that the ground-states (g.s.) of  $^{112-116}$ Ba nuclei, and the first excited oblate states (e.s.I) of  $^{118-122}$ Ba, show the presence of  $^{12}$ C cluster configuration. Note that <sup>12</sup>C cluster refers to <sup>100</sup>Sn daughter, and its existence inside the Ba nuclei has been of interest both from experimental and theoretical points of views. The g.s. of <sup>112–116</sup>Ba also show the presence of other lighter and relatively heavier clusters, like <sup>14</sup>N and <sup>35</sup>Cl, <sup>36</sup>Ar, respectively, whereas the same for the g.s. of <sup>118–122</sup>Ba are predicted to be only the relatively heavier ones like  ${}^{42}Ca$  and  ${}^{43}Ca$ . Furthermore, the oblate state (e.s.I) and hyper-deformed state in  $^{112-116}$ Ba also show the presence of heavier cluster  $^{103}{\rm Sn},~^{105}{\rm Sn},~^{104}{\rm In},~^{95}{\rm Pd},~^{96}{\rm Pd}$  and  $^{103}{\rm Cd},$  respectively. Note that these heavier clusters have less probability to decay from the interior of the parent nucleus. The important point to note here is that <sup>12</sup>C cluster is formed inside the Ba nuclei, and not from the outer region. In other words, <sup>12</sup>C does constitute the cluster structure both in ground and excited states of some Ba isotopes, particularly in <sup>112,114,116</sup>Ba and <sup>118,120,122</sup>Ba, respectively. The hyper-deformed solutions ( $\beta_2 \sim 1.2$ ) are obtained only for the <sup>112–116</sup>Ba isotopes, i.e., there are no such hyper-deformed states predicted for  $^{118-122}$ Ba isotopes. In other words,  $^{118-122}$ Ba nuclei show no clustering configuration at such large deformations. Some of the calculations for clustering on lighter mass regions are already carried out by using recent RMF (NL3\* and NL075) force parameters. Some

of the results are also included in above subsection but the counting of nucleons for the Mg isotopes are are not included in the thesis [14].

### 6.3 Summary and Conclusion

Concluding, we have calculated the gross nuclear properties and the nucleon density distributions for the isotopic chain  $^{112-122}$ Ba using the deformed relativistic mean field formalism with NL3 parameter set. The gross properties, like the binding energy, deformation parameter  $\beta_2$  and the charge radius  $r_c$ , show qualitative similarity between the experimental and RMF calculated values. Analyzing the nuclear density distributions, we get the internal or sub-structure of clusters in Ba isotopes. We find the prolate ground and first-excited oblate states of some Ba isotopes, specifically, the <sup>112,114,116</sup>Ba and <sup>118,120,122</sup>Ba, respectively, which consist of <sup>12</sup>C cluster. The ground-state solutions also support the cluster configurations of other light and the relatively heavier nuclei such as H, N, Cl, Ar and Ca. Some g.s. solutions also contain light particles like <sup>1,2,3</sup>H. This is an interesting result of the RMF(NL3) technique for nuclear structure physics. It is relevant to mention here that, in view of our earlier [179] as well as the recent calculation [14], the above results on clustering are not expected to change much by changing of the RMF parametrization. For example, the clustering phenomenona remains almost similar with NL3 and another force parameters NL-SV1, NL3\* and NL075 [177, 178, 14], though these results are more apparent and universal for the RMF approach. Also, the pairing effect on cauterization picture is examined. We notice that there is no change at all in the clustering of a nucleus with and without pairing correlations. Some times, the solutions which appeared in the zero-pairing case, were washed out when pairing interaction was allowed. However, the cluster structure of a nucleus remained unaffected as long as the solution for that nucleus existed.

As already pointed out in the Introduction, clustering is also important for the decay of excited compound nuclei formed in nuclear reactions. Todate, the decay of <sup>116,118,122</sup>Ba<sup>\*</sup> compound nuclei in to the intermediate mass fragments (IMFs), and symmetric and near-symmetric fission fragments are measured[190, 191, 192, 193, 194]. The fusionevaporation residues are not yet identified. <sup>12</sup>C as one of the IMFs measured with the largest yield is shown in RMF (NL3) calculation to arise from the interior of Ba nuclei, and not from the outer region. Finally, the present RMF model, used for the calculation of clustering structure in nuclei, has still some scope to take into account the parity reflection symmetry and correlations beyond the mean field in the formalism, which may at present be a limitation.

### Chapter 7

# Summary and conclusion

In this thesis we analyze the nuclear potential as well as the nuclear structure and internal sub-structure for both stable and drip-line nuclei over the nuclear chart. We have applied the well known and widely used effective mean-field theories such as relativistic mean field, Effective Field Theory motivated relativistic mean field and Skyrme Hartee-Fock approach to study the basic gross nuclear properties of a nucleus such as the binding energy (BE), root mean square charge  $r_{ch}$ , neutron  $r_n$ , proton  $r_p$ , matter radius  $r_m$  and the quadrupole deformation parameter  $\beta_2$  for ground and intrinsic excited (or isomeric) states. Mainly, our studies are directed towards the exotic drip-lines and super-heavy nuclei in the nuclear landscape.

In Chapter 2, we have presented both non-relativistic Skryme-Hartree-Fock (SHF) and relativistic mean field (RMF) theories in detail. The SHF model is generated by the interactions between all the constituent nucleons in the nucleus as described by the nucleon-nucleon potential. This leads to the ansatz for the Hartree-Fock approximation that the ground-state trial wave-function of a nucleus containing 'A' nucleons is written as a Slater determinant, or antisymmetrised product of occupied states. The full manybody Hamiltonian, written in terms of an one-body kinetic energy term and a two-body force for nucleons. The expectation value of the total Hamiltonian with respect to the Hartree-Fock wavefunction gives an approximation to the ground-state energy. In case

of relativistic mean field theory, the interaction between the nucleons introduced by different mesons. The Lagrangian density that introduces nucleon field  $\psi$ , isoscalar scalar meson field  $\sigma$ , isoscalar vector meson field  $\omega$ , isovector vector meson field  $\rho$  and isovector scalar meson field  $\delta$ . The Euler-Lagrange equation reproduced the field equations for different fields and these are solved self-consistently. The total energy of the nucleus comes from the energy contribution from nucleon and mesons. The BCS pairing correlation for open shell nuclei is included in this sections. The fixation of parameters as well as different forces are also discussed in this chapter. This chapter contains all mathematical derivations and parametrizations, which are used in the calculation and further predictions.

In Chapter 3, we have discussed microscopic origin of nucleon-nucleon NN potential derived from linear and non-linear relativistic mean field Lagrangian density. This potential is entitled as R3Y and is presented eloquently in terms of the well known inbuilt RMF theory parameters. In other word, the potential can be expressed in terms of meson masses  $(m_{\sigma}, m_{\omega}, m_{\rho} \text{ and } m_{\delta})$  and their coupling constants  $(g_{\sigma}, g_{\omega}, g_{\rho} \text{ and } g_{\delta})$  for different fields. This NN potential could replace the phenomenological M3Y interaction for most of the calculations of nuclear observables. The results obtained from different force parameters are compared with M3Y potentials. To show the applicability of the microscopic origin of R3Y potential, we have studied the cluster radioactivity. This make a bridge between R3Y and the phenomenological M3Y in terms of optical potential and explaining the cluster decay property of the nuclei. Exploring such R3Y potential from RMF theory being considered as a unified formalism for studying a number of nuclear phenomena or at least one step forward in our understanding of NN-interaction.

In **Chapter 4**, we have studied the nuclear structure for ground and intrinsic excited (or isomeric) states of superheavy nuclei in the frame work of relativistic and non-relativistic effective interactions. The axially deformed relativistic mean field and non-relativistic Skryme-Hartree-Fock theory are employed to investigate the bulk properties of recently synthesized super-heavy nuclei such as Z=115, 117, 120 and 122 and their isotopic chains. First of all, the potential energy surfaces (PES) as a function of

quadrupole deformation parameter  $\beta_2$  is calculated by using both the RMF and SHF theories in a constrained method. Thus, from the PES curve, one can found the ground as well as the intrinsic excited state solutions of a given nucleus. The gross properties, such as binding energy (BE), root mean square charge radius  $r_{ch}$ , proton radius  $r_p$ , neutron radius  $r_n$ , matter radius  $r_m$  and quadrupole deformation parameter  $\beta_2$  are calculated using various forces. From the calculated binding energy, we also estimated the twoneutron separation energy  $S_{2n}$  for the isotopic chain. The pairing energy  $E_{pair}$  and the shape co-existence  $\Delta E$  are evaluated for all atomic nuclei. Closed shell structures are observed at N = 172 or 184 and N = 182 from the analysis of binding energy per particle BE/A and the  $S_{2n}$  energy in an isotopic chain for RMF and SHF calculations. We found spherical and super-deformed or hyper-deformed ground state solution for Z=115, 117 and Z=120,122, respectively. The  $\alpha$ -decay energy  $Q_{\alpha}$ , half-life time  $T_{\alpha}$  and mean-life  $\tau$ are also estimated for  $^{287,288}115$ ,  $^{293,294}117$ ,  $^{292,304}120$  and  $^{292}122$  series. Our predicted observables for  $\alpha$ -decay chains agree nicely with the FRDM calculations and available experimental data for all isotopic series. Both SHF and RMF formalisms are employed to see the force dependence of the results. We found qualitatively similar predictions in both the techniques.

According to the previous calculation (Chapter-3), we found some closed shell structure at N=172,182 or 184 for all atomic nuclei, which enhanced our curiosity to find a suitable combination of neutron and proton number at superheavy island with magic properties. In **Chapter 5**, the main aim of this work is to identify the next double closed shell nucleus beyond <sup>208</sup>Pb, which may be a possible candidate for the experimentalists to look for. In this context, we have a wide range of nuclei starting from the the proton-rich to the neutron-rich region in the superheavy valley (Z=112-130). Two well established distinct approaches such as non-relativistic SHF and relativistic mean field formalism with various force parameters are used in this calculations. The recently developed effective field theory motivated relativistic mean field forces G1 and G2 are also involved. To our knowledge, this is one of the first such extensive and rigorous calculation in both SHF and RMF models using a large number of parameter sets. Based on the four important observables such as average pairing gap (for proton  $\Delta_p$  and neutron  $\Delta_n$ ), two neutron separation energy  $S_{2n}$ , shell correction energy  $E_{shell}$  and single-particle energy spectra  $\epsilon_{n,p}$ , we have concluded that the general set of magic numbers beyond <sup>208</sup>Pb are Z=120 and N=172, 182/184. The highly discussed proton magic number Z = 114 (from last four decades) is found to be feebly magic in nature.

In Chapter 6, we extend the idea of nuclear structure to sub-structure, i.e. the internal configuration (clustering) of a nucleus. The aim of this work is to discuss the possibility of existence (preformation) of cluster (s) inside the parent nucleus and identify them. The recent experiment at GANIL, motivated us to see the interesting clusters of Ba isotopes in the ground and/ or excited states with well developed and microscopic model. Here, we have used relativistic mean-field formalism with successful NL3 force for the present study. First of all, we have calculated the gross nuclear properties like binding energy, deformation parameter  $\beta_2$ , the charge radius  $r_c$  and the nucleon density distributions  $\rho_{n,p}$  for the isotopic chain <sup>112–122</sup>Ba using the deformed relativistic mean field theory. The obtained bulk properties from RMF show a qualitative as well as quantitative similarity to the experimental values. The internal configuration of these nuclei are analyzed from nucleonic density distributions. The most important step in this calculation is to count the number of nucleons inside the cluster (s) region. Here we are using a straight forward method to find the number of nucleons (proton and neutron separately) for a cluster region. Using this method, we found the prolate ground and first-excited oblate states of some Ba isotopes, specifically, <sup>112,114,116</sup>Ba and <sup>118,120,122</sup>Ba, respectively. The cluster mostly consist of <sup>12</sup>C nucleus and also support the cluster configurations of other light and the relatively heavier nuclei such as H, N, Cl, Ar and Ca. Some g.s. solutions also contain light particles like  $^{1,2,3}$ H. This is an interesting result of the RMF(NL3) technique for nuclear structure physics. It is relevant to mention here that, the above results on clustering are not expected to change much by changing of the RMF parametrization.

In concluding this thesis we would like to say that, the main objective behind the present effort has been to see how far the effective interaction can account the diverse properties of nuclei in normal as well as exotic situations. The reasons behind the choice of the SHF and RMF theory for the study of nuclear properties are multifarious. One of the important reasons, is the simplicity and self-consistent solution involved in calculations. These approaches become feasible over nuclear chart including superheavy nuclei. It has been possible to describe successfully many important observables like binding energy, root mean square charge and matter radius, quadrupole deformation parameter, single particle energy, pairing energy, average pairing gap for nucleons, the shell correction energy, single particle energy levels and other related related properties with popular set of forces such as FIT-Z, SIII, SKMP, SkI4, SLY4 (for SHF) and NL-SH, NL3, NL3<sup>\*</sup>, G1 and G2 (for RMF).

**Future Prospects:** The studies of nuclei far from the valley of stability broaden the opportunities of research in the area of both nuclear structure and reaction physics. This is also an indirect impact to the atomic physics as well as in astrophysics and material science. In nuclear physics there are a number of exciting and crucial topics to be addressed. Some of the topics which we are intending to pursue in immediate future are as follow:

- The nuclear structure near the drip-line is one of the important research area in present day nuclear physics. A lot of exotic phenomena like halo and skin structure exhibit due to the large isospin in such nuclei. A detail analysis is needed within the availability of nuclear models taking into account the necessity of the problem. This can also be extended to superheavy nuclei, which is again an important area. More explanations are needed to understand the super-deformed / hyper-deformed (β<sub>2</sub> ~ 0.5) ground state in case of exotic nuclei including superheavy. Further modification is important in the method of calculation of half-life t<sup>α</sup><sub>1/2</sub> and mean-life τ<sup>α</sup> of nucleus.
- In the intermediate region, the nuclei far away from the  $\beta$ -stable region or near to drip-line showing some magicity, i.e. the half-life of these nuclei higher in magnitude than that of neighbor. This motivates us to explore such special features are important topic at the present status of nuclear physics. Further more explanation

needed for the crucial feature such as *Island of Inversion* in an isotopic chain of atomic nuclei.

- The experimental proton drip-line is known up to Z=82. However, to reach the neutron drip-line experimentally is much more tricky, and the present experimental status to reach the theoretical prediction of neutron drip-line is up to the Mg-isotopes. Many interesting physics has been evolved in recent past near the proton and neutron drip lines. The proton and neutron halo and skin is one among the exciting discoveries. More work in this direction are needed.
- The application of these models in nucleon-nucleus and nucleus-nucleus reaction also plays significant roles to understand the observables like differential reaction cross-section  $d\sigma/d\Omega$ , total reaction cross-section  $\sigma_t$ , analyzing power  $A_y$  and the spin rotation parameter Q - value. We have already dedicated some efforts in this directions, which can be available in Ref. [195] but more clarification and deep understanding is important.
- We have already undertaken some modification in the relativistic mean field Lagrangian keeping in view for a complete Lagrangian. At present, we have introduced some extra terms like the cross-coupling of  $\omega$  and  $\rho$  with new coupling constant  $\Lambda_v$  in ERMF and applied this to the study of nuclear matter [196]. The extension of this modified Langagian to the study of finite nuclei under rudimentary stage.

Here we have mention some work, which are already taken care in our plan for the current or near future study. Also, there are so many highly interesting works are already there to explore in the nuclear structure study. Again, an unified description both for nuclear matter under extreme conditions and the properties of finite nuclei starting from the beta stable to drip-line and superheavy nuclei using simple effective interaction is one step forward in nuclear physic and also in progress.

# Appendix A

### Eigen functions and its components

The Dirac equation with the eigen values  $E_i$  and eigen function  $Psi_i(r)$  are given by,

$$h\Psi_i(r) = E_i\Psi_i(r),\tag{A.1}$$

with the normalization condition,

$$\int d^3 r \Psi_i^{\dagger}(r) \Psi_i(r) = 1.$$
(A.2)

The eigen functions in Eqns (A.1-A.2) for a spherically symmetric nuclei is given by [8, 73],

$$\Psi_i(r) = \Psi_{n,k,m,t} = \begin{bmatrix} \frac{i}{r} G_a(r) \Phi_{km} \\ \frac{i}{r} F_a(r) \Phi_{-km} \end{bmatrix} \zeta_t,$$
(A.3)

where,  $G_a$  and  $F_a$  are the upper and lower component of the wavefunction  $\Psi_i(r)$  with a = (n, k, m), respectively. The  $\Phi_{km}$  is the spin harmonics. The values  $t = \frac{1}{2}$  and  $\frac{-1}{2}$  for proton and neutron, respectively. The radial equations for  $F_a$  and  $G_a$  are given by,

$$\left(\frac{d}{dr} + \frac{k}{r}\right)G_a(r) - \left[E_a - U_1(r) + U_2(r)\right]F_a(r) - U_3G_a(r) = 0,$$
(A.4)

and

$$\left(\frac{d}{dr} - \frac{k}{r}\right)F_a(r) - \left[E_a - U_1(r) - U_2(r)\right]G_a(r) - U_3F_a(r) = 0.$$
(A.5)

Here,  $U_1$  (r),  $U_2$  (r) and  $U_3$  (r) the single particle potentials and they defined as:

$$U_1(r) = W(r) + t_a R(r) + \left(t_a + \frac{1}{2}\right) A(r) + \frac{1}{2M^2} \left(\beta_s + 2t_a \beta_v\right) \nabla^2 A(r),$$
(A.6)

$$U_2(r) = M - \Phi(r),$$

$$U_{3}(r) = \frac{1}{2M} \left[ f_{v}W'(r) + t_{a}f_{\rho}R'(r) + A'(r)\left(\frac{(\lambda_{p} + \lambda_{n})}{2} + t_{a}(\lambda_{p} - \lambda_{n})\right) \right].$$
(A.8)

The prime (') denotes the first derivative of the field with respect to the radial component of the co-ordinates.

(A.7)

# Appendix B

# The Hartree-Fock potential

The explicity form of the Hartree-Fock equation (see Eqn. 2.41) can be written as,

$$\epsilon_i \phi_i(\mathbf{r}) = -\frac{\hbar^2}{2m} + \sum_{j>i}^A \int \phi_j^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}) \phi_j(\mathbf{r}') d\mathbf{r}' - \sum_{j>i}^A \int \phi_j^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}') \phi_j(\mathbf{r}) d\mathbf{r}'.$$
(B.1)

Here, the second term in the above expression is known *direct* or *Hartree* term,

$$U_H^{(i)}(\mathbf{r} = \sum_{j>i}^A \int \phi_j^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \phi_j(\mathbf{r}') d\mathbf{r}', \qquad (B.2)$$

which is a local potential that depends only on the one-body density,

$$\rho(\mathbf{r}) = \sum_{i=j}^{A} \phi_j^*(\mathbf{r}) \phi_j(\mathbf{r}).$$
(B.3)

The third term of the Eqn. (B.1) is called as *exchange* or *Fock* potential,

$$U_H^{(i)}(\mathbf{r} = \sum_{j>i}^A \phi_j^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \phi_j(\mathbf{r})$$
(B.4)

which comes from the antisymmetrisation of the many-body wave function, which is non-local potential. Its non-local density matrix is given by,

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^{A} \phi_i^*(\mathbf{r}') \phi_i(\mathbf{r}).$$
(B.5)

This leads to a simplified form for the Hartree-Fock equation given as:

$$\epsilon_i = -\frac{\hbar^2}{2m} + U_H^{(i)}(\mathbf{r})\phi_i(\mathbf{r}) - \int U_F^{(i)}(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}')d\mathbf{r}'.$$
(B.6)

Hence, within the Hartree-Fock approach, a particular system under investigation is specified by choosing the relevant two-body potential. The Coulomb and kinetic interactions are universal functions for all systems and also independent of  $V(\mathbf{r}, \mathbf{r}')$ .

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