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Ground state properties of rare earth nuclei of the astrophysical r-process

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Abstract: Self consistently Hartree-Fock-Bogolyubov calculations have been performed with Skyrme functional SLY6 parameter set to study the ground-state properties of stable and unstable isotopes of Ytterbium (Yb), Lutetium (Lu), Hafnium (Hf), Tantalum (Ta) and Tungsten (W) nuclei. Binding energy, Quadrupole deformation and Hexadecapole deformation of nuclei having Z=70-74, neutron number (N =100 - 112) and neutron rich nuclei (N=124 - 127) have been analysed with the help of their potential energy surface (PES). Ground-state binding energy and deformation have been compared with the experimental data and data available from other works in literature.

1. Introduction

In recent days, the structure of exotic nuclei is a leading topic in nuclear structure studies. The number of nuclei away from the valley of stability is very large and their structures are yet to be examined. Experimental data are not available for neutron drip line region. Alternately the ground state properties of the exotic nuclei can be determined with the help of relativistic or nonrelativistic mean field theory such as Hartree-Fock-Bogolyubov (HFB). Heavier elements were synthesized with the help of two astrophysical process of capturing free neutron namely the slow(s) process and the rapid(r) process. Exotic nuclei play an important role in the r-process nucleosynthesis. The abundance pattern of nuclei have played an important role in studies of origin of the elements [1, 2]. In r-process nucleosynthesis the equilibrium abundances for a given isotopic chain can be determined with the help of the neutron density, temperature and neutron separation energy by employing the Saha equation. This equilibrium suggests that the maximum abundance of participating elements will be described by similar neutron separation energies which can be found with g.s properties of nuclei. The s-process takes place during stellar evolution and passing through nuclei near stability in a time scale of hundreds to thousands of years. For most of the nuclei participating in the s-process, relevant experimental data are available [3, 4, 5]. The r-process operates over a time scale of seconds far from the stability valley in a high neutron density environment. Little experimental data or no data are available for many of the nuclei involved and search for its stellar origin involves a large number of speculations [6]. In order to fully understand the r-process, we need to know physical conditions such as temperature, neutron density as well as knowledge of nuclear properties such as masses, β decay life times and neutron-capture cross-section for a large number of extremely neutron-rich nuclei far from stability [6, 7, 8] in the astrophysical environment. Using nuclear mass model it has been shown that the required conditions can be determined mostly from the neutron-separation energies for a small number of critical nuclei with N=50, 82, 126 closed neutron shell [9]. Most of the relevant nuclear properties are still beyond the experimental capabilities and therefore it must be calculated from theoretical approach. Nuclei around mass number 195 are important for the r-process which include isotopes of Ytterbium (Yb), Lutetium (Lu), Hafnium (Hf), Tantalum (Ta) and Tungsten (W). We have first examined the isotopes of these nuclei for which relevant experimental data are available and then extended our calculation to the nuclei with neutron number around N = 126. Potential energy surface of unstable and stable isotopes have been examined under the efficient SLY6 interaction in HFB model. The outline of the paper is as follows. Theoretical models and calculation used in the present work are described in section 2. In section 3, we present our results for nuclear properties and conclusion is presented in section 4. This work has been acknowledged in section 5.

2. Theory and Calculation

The standard Hartree-Fock-Bogolyubov (HFB) theory is one of the most successful theories for describing the nuclear ground state properties of nuclei. Pairing correlation may be generally incorporated with the help of the BCS approximation [10] for nuclei lying close to stability but BCS approximation becomes unreliable for nuclei lying close to the drip lines due to the coupling between the bound and single particle states and is not treated [11, 12, 13] satisfactorily. HFB theory includes pairing correlation self consistently, allowing it to correctly treat the pairing effect. Skyrme HFB approximation is a successful theoretical approach to deal with finite nuclei around drip line [14]. The g.s $|\Phi>$ of the Hartree-Fock-Bogolyubov (HFB) method is obtained by minimization of the total energy

$$E =< \Psi|\hat{H}|\Psi >= E\,[\rho, \kappa, \kappa*] \tag{1}$$

where ρ is one-body density matrix and κ is a pair tensor, the minimization of the total Routhian $E^{\lambda} = E - \lambda_{q} < \Psi|\,\widehat{N_q}\,|\,\Psi > Nq$ leads to the HFB equation, which can be expressed in terms of the U and V transformation matrices.

$$H \begin{pmatrix} U_n \\ V_n \end{pmatrix} = e_n \begin{pmatrix} U_n \\ V_n \end{pmatrix} \tag{2}$$

$$H = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \tag{3}$$

Where the quasiparticle energies e_n are the Lagrangian multipliers introduced to constrain the orthonormalization of the quasiparticle states and Nq is constrained on neutron and proton number. The Hamiltonian is defined in standard form $\hat{H} = \hat{T} + \hat{V}$ where $\hat{V}$ is two-body interaction and $\hat{T}$ is the kinetic energy part. The matrix elements of the mean-field and gap Hamiltonians are given as

$$h_{ij} = T_{ij} + \sum_{kl} V_{ikjl\rho lk} \;,\; \Delta_{ij} = \frac{1}{2} \sum_{kl} V_{ijkl\kappa kl} \tag{4}$$

Where $V_{ikjl\rho lk}$ is the antisymmetrized two-body matrix element and Δ_{ij} is the pairing field. Equation (2) and (3) are the HFB equations. The calculation of HFB method can be employed in two steps, first diagonalization of $\hat{h}$ and then solving the HFB equations in the basis. In our calculation we have used the deformed harmonic oscillator basis to get the solution of HFB equations. In this work we have used the efficient SLY6 parameter set [15] with zero range Bogolyubov pairing interaction for nuclei.

The total energy E of the system [16, 17] can be defined as

$$E = \int dr\ \{H_{kin}\,(\tau_q) + H_{SK}\,(\rho_q\,, \tau_q\,,\ s_q\,,\ j_q\,,\ J_q\,,\ T_q) + H_{pair}\,(\chi_q) + H_C\,(\rho_p)\} - E_{CM} \quad (5)$$

It contains local time-even and time-odd densities, as well as the pairing density χ_q. Where ρ_q is density of nucleon, τ_q is kinetic energy, s_q is spin, j_q is current, J_q is Spin-Orbit part, T_q is Spin kinetic energy, χ_q is pairing density and q denotes proton and neutron. The total densities $\rho = \rho_p + \rho_n$ have no index. The parameters of the zero-range density dependent pairing force are defined by the pairing form factor

$$f(r) = V_0\ \left(1 - \left(\frac{\rho(r)}{\rho_0}\right)^{\alpha}\right) \quad (6)$$

Pairing force parameters V_0 used in our calculation are -249.8 MeV for neutron and -230.9 MeV for proton while the pairing cut-off energy is 60 MeV. Pairing force parameters used here has been achieved by fitting the experimental binding energy data. To explore the dependence of total nuclear energy on deformation, we have performed HFB calculations with constraint on the quadrupole moment. Numerical calculations have been carried out using the axially deformed Harmonic Oscillator (HO) basis state expansion to solve the HFB equations iteratively. The self-consistent calculation in this work has been performed by using the freely available code HFODD (V2.40h) [18]. The number of shells taken into account are 15. Detailed discussion about the numerical technique is available in [19, 20] and the references therein. We have calculated the ground-state properties of Yb (A=170-174, 175, 194-197), Lu (A=175, 195-197), Hf (A=176-180, 196-198), Ta (A=180, 181, 195-199) and W (A=182-184, 186, 198-200) isotopes.

3. Results

In this section we present the results obtained in our work. We discussed the results for stable isotopes of Yb, Hf, Lu, Ta and W nuclei first followed by the results of unstable isotopes of nuclei under investigation.

3.1. Binding Energy and Deformation of Stable Nuclei

Table 1: Binding Energy and Quadrupole deformation of stable isotopes.

Isotope	B.E(MeV)(HFB)	B.E(MeV)(EXP)	β_2 (HFB)	β_2 [22]	β_2 [21]
Yb^{170}	-1380.636	-1378.124	0.3109	0.3239	0.287
Yb^{171}	-1387.626	-1384.737	0.3097	-	0.299
Yb^{172}	-1394.373	-1392.758	0.3076	0.3315	0.300
Yb^{173}	-1400.921	-1399.125	0.3050	-	0.300
Yb^{174}	-1407.272	-1406.591	0.3020	0.3226	0.289
Yb^{176}	-1419.403	-1419.277	0.2956	0.3014	0.289
Lu^{175}	-1414.055	-1412.101	0.2957	-	0.289
Hf^{176}	-1420.263	-1418.801	0.2874	0.299	0.278
Hf^{177}	-1426.977	-1425.177	0.2828	-	0.277
Hf^{178}	-1433.501	-1432.803	0.2782	0.2779	0.278
Hf^{179}	-1439.851	-1438.902	0.2732	-	0.267
Hf^{180}	-1445.990	-1446.289	0.2690	0.2731	0.267
Ta^{180}	-1446.386	-1444.622	0.2506	-	0.255
W^{182}	-1459.146	-1459.333	0.2337	0.2485	0.232
W^{183}	-1465.688	-1465.524	0.2284	-	0.243
W^{184}	-1472.066	-1472.93	0.2223	0.2339	0.232
W^{186}	-1484.332	-1485.882	0.2063	0.2257	0.221

Table-1 shows the binding energy and quadrupole deformation of isotopes of different nuclei. We compared our result with experimental values where are available and with other works available in literature [21, 22]. We have taken experimental values from nndc website [23]. In this calculation we have not taken odd-even mass difference into consideration. Our results are close to the experimental values and are quite satisfactory.

In this work we have done restrained calculation to get the deformation of rare earth nuclei under consideration which are mostly deformed in their ground state. In Figure 1 we plotted the ground state binding energy with the quadrupole deformation to obtain the potential energy surface (PES). PES of stable nuclei have been obtained in the frame work of axially symmetric calculations. These surfaces are sensitive to the effective nuclear force in both Relativistic [24] and Nonrelativistic [25, 26] fields as well as in pairing calculation [27, 25, 26]. The potential energy surface for the stable isotopes of all five elements are presented in Figure. 1. From Figure 1 we can observe that all nuclei are prolate in shape and their quadrupole deformations are given in Table-1. We have chosen these nuclei as they are very stable and these nuclei of Z=70-74 produced r-process peak at N=126. We have taken isotopes of rare earth nuclei Yb, Lu, Hf, Ta and W to observe their g.s deformation. All these nuclei show shape transition when we move from neutron deficient to neutron rich isotope. In near future author will do these calculation. It can be easily observed that the quadrupole deformation values for all stable isotopes lie between 0.31 to 0.20 that is all stable isotopes of Yb, Hf, Lu, Ta and W are deformed and have prolate shape in their ground states. When we move from neutron deficient to neutron rich isotopes shape may change and will have oblate deformation. It is also clear from the Figure 1 that difference between prolate and oblate minimum decreases as proton number increases from 70 to 74. It is also important to observe that the energy barriers at zero deformation decrease linearly with increase in neutron and proton number as shown in Figure 1.

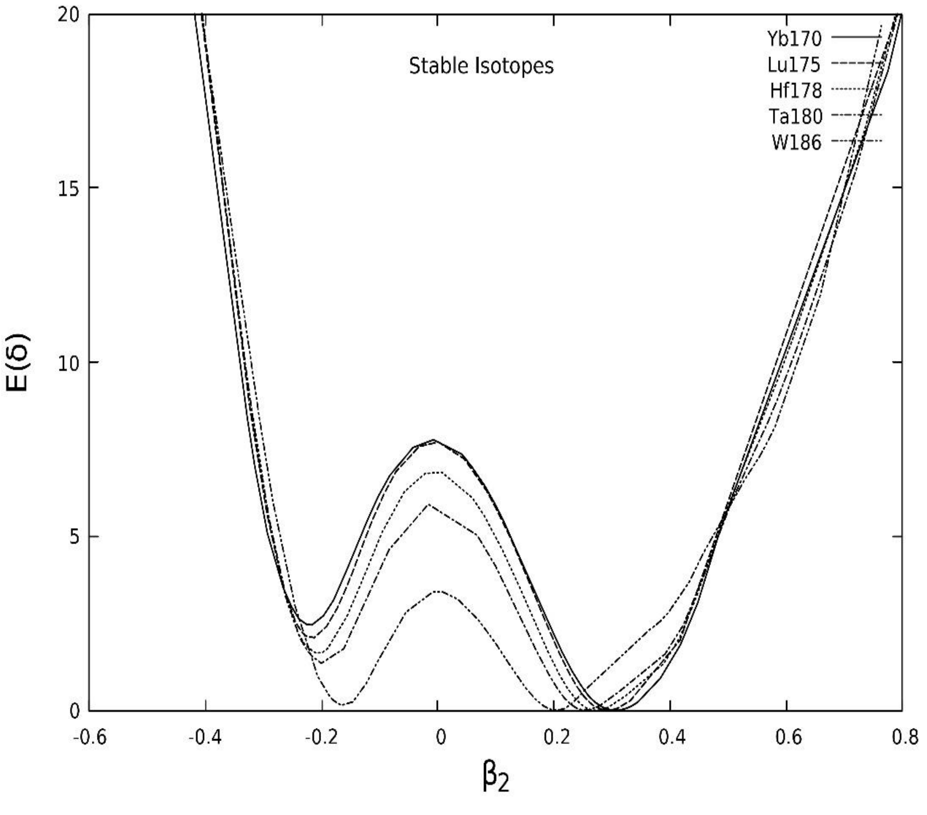

Figure 1: Potential Energy Surface of Stable Isotopes of Nuclei under investigation.

Table 2: Hexadecapole deformation of stable isotopes.

Isotope	β_4	Isotope	β_4	Isotope	β_4
Yb^{170}	0.0445	Lu^{175}	0.0160	Hf^{176}	0.0165
Yb^{171}	0.0389	Ta^{180}	-0.0134	Hf^{177}	0.0081

In Table 2 we present our results of hexadecapole deformation for the stable isotopes of few of representative nuclei. Hexadecapole deformation of stable isotopes have small values while all the isotopes having neutron number near about magic number N=126 have zero hexadecapole deformation.

3.2. Binding Energy and Quadrupole deformation of Unstable Nuclei

The ground state binding energies and quadrupole deformations of unstable isotopes for Z = 70 − 74 nuclei around the N = 126 shell closure have been calculated with the same HFB parameters as we did for stable isotopes of nuclei under consideration. We did not compare our results with experiment as data are very scarce in this region. It can be seen from the Figure 2 that all unstable nuclei with N = 126 are spherical. Quadrupole deformation of isotopes of nuclei under study is nearly zero. This clearly is an effect of the shell closure at N = 126. In Table- 3 we present our results for ground-state binding energy and quadrupole deformation of all unstable isotopes under investigation. These neutron rich nuclei are important in r-process where the neutron capture time is much shorter than the β-decay rate.

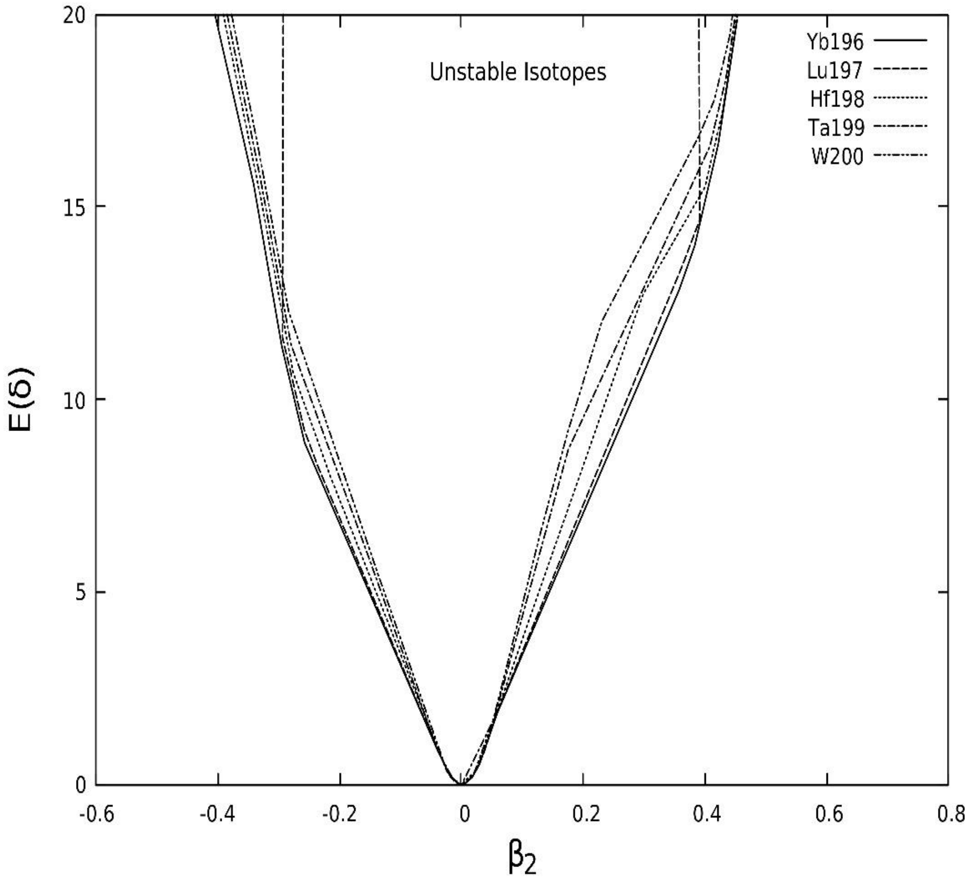

Figure 2: Potential Energy Surface of Neutron rich Unstable Isotopes.

Table 3: Binding energy and Quadrupole deformation of unstable Isotopes

Isotope	B.E(MeV)(HFB)	β_2 (HFB)	Isotope	B.E(MeV)(HFB)	β_2 (HFB)
Yb^{190}	-1486.250	0.0831	Hf^{200}	-1540.780	-0.0016
Yb^{191}	-1490.365	0.0007	Hf^{201}	-1542.817	-0.0027
Yb^{192}	-1494.761	0.0014	Hf^{202}	-1544.710	-0.0042
Yb^{193}	-1499.020	0.001	Hf^{203}	-1546.481	-0.0063
Yb^{194}	-1503.124	0.001	Hf^{204}	-1548.149	-0.0095
Yb^{195}	-1507.036	0.0003	Hf^{205}	-1549.728	-0.0151
Yb^{196}	-1510.651	0.0003	Hf^{206}	-1551.243	-0.0246
Yb^{197}	-1512.733	-0.0002	Ta^{190}	-1504.312	-0.123
Yb^{198}	-1514.518	-0.001	Ta^{191}	-1509.424	-0.115
Yb^{199}	-1516.120	0.0018	Ta^{192}	-1514.451	-0.099
Yb^{200}	-1517.578	0.0030	Ta^{193}	-1519.386	-0.0846
Yb^{201}	-1518.917	0.0048	Ta^{194}	-1524.151	-0.0252
Yb^{202}	-1520.153	0.0077	Ta^{195}	-1529.283	-0.0012
Yb^{203}	-1521.301	0.0128	Ta^{196}	-1534.269	-0.001
Lu^{190}	-1493.370	0.1023	Ta^{197}	-1539.096	-0.0004
Lu^{191}	-1497.771	0.0850	Ta^{198}	-1543.729	-0.001
Lu^{192}	-1502.065	0.0187	Ta^{199}	-1548.076	-0.0002
Lu^{193}	-1506.714	0.0003	Ta^{200}	-1550.804	-0.0010
Lu^{194}	-1511.216	0.0004	Ta^{201}	-1553.243	-0.002
Lu^{195}	-1515.562	0.0003	Ta^{202}	-1555.498	-0.0031
Lu^{196}	-1519.714	-0.0001	Ta^{203}	-1557.609	-0.0046
Lu^{197}	-1523.574	0.0001	Ta^{204}	-1559.598	-0.0067
Lu^{198}	-1525.871	0.001	Ta^{205}	-1561.481	-0.0100
Lu^{199}	-1527.874	0.0013	Ta^{206}	-1563.275	-0.0151
Lu^{200}	-1529.693	0.0023	W^{192}	-1518.967	-0.107
Lu^{201}	-1531.368	0.0036	W^{193}	-1524.278	-0.0963
Lu^{202}	-1532.923	0.0056	W^{194}	-1529.481	-0.0825
Lu^{203}	-1534.374	0.0088	W^{195}	-1534.539	-0.0167
Lu^{204}	-1535.562	0.0145	W^{196}	-1539.909	-0.0018
Hf^{190}	-1499.408	-0.1150	W^{197}	-1545.135	-0.0011
Hf^{191}	-1504.149	-0.1010	W^{198}	-1550.203	-0.001
Hf^{192}	-1508.816	-0.0854	W^{199}	-1555.075	-0.001
Hf^{193}	-1513.328	-0.0257	W^{200}	-1559.664	-0.0004
Hf^{194}	-1518.220	-0.0004	W^{201}	-1562.608	-0.0013
Hf^{195}	-1522.964	-0.0001	W^{202}	-1565.266	-0.0022
Hf^{196}	-1527.550	-0.0001	W^{203}	-1567.741	-0.0034
Hf^{197}	-1531.944	-0.0004	W^{204}	-1570.069	-0.0049
Hf^{198}	-1536.048	-0.0001	W^{205}	-1572.275	-0.0070
Hf^{199}	-1538.559	-0.001	W^{206}	-1574.375	-0.010

4. Conclusion

Isotopes of rare earth nuclei have been studied in the HFB approach using the energy functional SLY6 in the present work. Pairing strength has been obtained by fitting the binding energy and quadrupole deformation. Good agreement has been obtained for ground state properties such as binding energy, quadrupole deformation and hexadecapole deformation. A long list of study remains to be done in the near future, and this calculation can be viewed as a triggering point for a more aspiring work. A more systematic study is required to understand the g.s properties of r- process nuclei with different Skyrme forces and pairing correlation. Systematic calculation of r- process nuclei with N=50, 82 and N=126 closed shell has to be performed for better understanding of required condition for nucleosynthesis of r process nuclei i.e temperature and neutron density in Solar pattern. Nuclear g.s properties of extremely neutron rich nuclei are important in order to fully understand the r- process which is responsible for nucleosynthesis of element heavier then Fe. Nuclear properties can be studied by performing the restrained calculation of the isotopic chain of the nuclei. PES calculation may give the shape coexistence clearly as well as triaxial deformation when we go from neutron deficient to neutron rich nuclei. We intend to carry out shape transition, parametric studies of r-process nuclei based on more detailed and more realistic nuclear astrophysical model with different Skyrme functional. High spin state calculation of rare earth nuclei is also required to understand more precisely astrophysical r- process of nucleosynthesis.

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