Superdeformed and hyperdeformed states in Z=122 isotopes

S. K. Patra\(^1\), M. Bhuyan\(^1,2\), M. S. Mehta\(^3\) and Raj K. Gupta\(^3\)
\(^1\) Institute of Physics, Sachivalaya Marg, Bhubaneswar-751 005, India.
\(^2\) School of Physics, Sambalpur University, Jyoti Vishar, Burla-768 019, India.
\(^3\) Department of Physics, Panjab University, Chandigarh-160 014, India.
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We calculate the binding energy, root-mean-square radius and quadrupole deformation parameter for the recently observed superheavy mass region. The half-life of the nuclei is found to be \(T_{1/2} \geq 10^8 \text{ y} \) and abundance \((1-10) \times 10^{-12}\) relative to \(^{232}\text{Th}\). This possibility of an extremely heavy nucleus motivated us to see the structures of such nuclei in an isotopic mass chain. Therefore, based on the relativistic mean-field (RMF) and non-relativistic Skyrme Hartree-Fock (SHF) methods, we calculated the bulk properties of \(Z=122\) nucleus in an isotopic chain of mass \(A=282-320\). This choice of mass range covers both the predicted neutron magic numbers \(N=172\) and \(184\).

The paper is organised as follows: Section II gives a brief description of the relativistic and non-relativistic mean-field formalism. The effects of pairing for open shell nuclei, included in our calculations, are also discussed in this section. The results of our calculations are presented in Section III, and a summary of the results obtained, together with concluding remarks, are given in the last Section IV.

I. INTRODUCTION

The stability of nuclei in superheavy mass region was predicted in mid sixties \([1,2,3]\) when shell correction was added to the liquid drop binding energy and the possible shell closure was pointed out at \(Z=114\) and \(N=184\). Later, however, the spectroscopic studies of the nuclei beyond \(Z=100\) have become possible \([4,5]\), and the heaviest nucleus studied so far in this series of experiments \([6]\) is \(^{254}\text{No} (Z=102, N=152)\). Thus, 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.

Even though, experimentally, the elements up to \(Z=118\) have been synthesized to date, with half-lives ranging from minutes to milliseconds \([7,8]\), the above mentioned theoretically predicted center of island of stability could not be located precisely. Recently, more microscopic theoretical calculations have predicted various other regions of stability, namely, \(Z=120, N=172\) or \(184\) \([9,10,11]\) and \(Z=124\) or \(126, N=184\) \([12,13]\). Apparently, there is a need to design the new experiments to solve the outstanding problem of locating the precise island of stability for superheavy elements. In an effort in this direction, using inductively coupled plasma-sector field mass spectroscopy, Marinov et al. \([14]\) have observed some neutron-deficient Th isotopes in naturally occurring Thorium substances. Long-lived isomeric states, with estimated half-lives \(T_{1/2} \geq 10^8 \text{ y}\), have been identified in the neutron-deficient \(^{211,213,217,218}\text{Th} \), which are associated with the superdeformed (SD) or hyperdeformed (HD) states (minima) in potential energy surfaces (PES). In a similar search for long-lived, trans-actinides in natural materials, more recently, these authors \([15]\) obtained a possible evidence for the existence of a long-lived superheavy nucleus with mass number \(A=292\) and atomic number \(Z=122\) in natural Thorium.

The half life is again estimated to be the same as above, i.e. \(T_{1/2} \geq 10^8 \text{ y}\) and abundance \((1-10) \times 10^{-12}\) relative to \(^{232}\text{Th}\). This possibility of an extremely heavy Z nucleus motivated us to see the structures of such nuclei in an isotopic mass chain. Therefore, based on the relativistic mean-field (RMF) and non-relativistic Skyrme Hartree-Fock (SHF) methods, we calculated the bulk properties of \(Z=122\) nucleus in an isotopic chain of mass \(A=282-320\). This choice of mass range covers both the predicted neutron magic numbers \(N=172\) and \(184\).

II. THEORETICAL FRAMEWORK

A. The Skyrme Hartree-Fock (SHF) method

The general form of the Skyrme effective interaction, used in the mean-field models, can be expressed as an energy density functional \(\mathcal{H}\), given as a function of some empirical parameters \([16,17]\), as

\[
\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{eff} + \cdots
\]

where \(\mathcal{K}\) is the kinetic energy term, \(\mathcal{H}_0\) the zero range, \(\mathcal{H}_3\) the density dependent and \(\mathcal{H}_{eff}\) the effective-mass dependent terms, which are relevant for calculating the properties of nuclear matter. These are functions of 9 parameters \(t_i, x_i\).
of a finite nucleus with mass. The other terms, representing the surface contributions
The kinetic energy of the energy density functional
are published since 1972 (see, e.g., [18]). In most of the
Skyrme set with
The relativistic Lagrangian density for a nucleon-meson
The subscripts
The root mean square (rms) matter radius is defined as

Here, the total nucleon number density \( \rho = \rho_n + \rho_p \), the kinetic energy density \( \tau = \tau_n + \tau_p \), and the spin-orbit density \( \vec{J} = \vec{J}_n + \vec{J}_p \). The subscripts \( n \) and \( p \) refer to neutron and proton, respectively. The \( \vec{J}_q = 0, q = n \) or \( p \), for spin-saturated nuclei, i.e., for nuclei with major oscillator shells completely filled. The total binding energy (BE) of a nucleus is the integral of the energy density functional \( \mathcal{H} \).

At least eighty-seven parametrizations of the Skyrme interaction are published since 1972 (see, e.g., [18]). In most of the Skyrme parameter sets, the coefficients of the spin-orbit potential \( b_3 = b_4 = W_0 \) [19], but we have used here the Skyrme SkI4 set with \( b_4 \neq b_4' \) [20]. This parameter set is designed for considerations of proper spin-orbit interaction in finite nuclei, related to the isotope shifts in Pb region.

B. The relativistic mean-field (RMF) method

The relativistic Lagrangian density for a nucleon-meson many-body system [21] [22],

All the quantities have their usual well known meanings. From the above Lagrangian we obtain the field equations for the nucleons and mesons. These equations are solved by expanding the upper and lower components of the Dirac spinors and the boson fields in an axially deformed harmonic oscillator basis with an initial deformation \( \beta_0 \). The set of coupled equations is solved numerically by a self-consistent iteration method. The centre-of-mass motion energy correction is estimated by the usual harmonic oscillator formula

C. Pairing Effect

Pairing is a crucial quantity for open shell nuclei in determining the nuclear properties. The constant gap, BCS-pairing approach is reasonably valid for nuclei in the valley of \( \beta \)-stability line. However, this approach breaks down when the coupling of the continuum becomes important. In the present study, we deal with nuclei on the valley of stability line since the superheavy 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 super-heavy element possible to be synthesized, particularly when a combination of magic proton and neutron number happens to occur (largest shell correction). In order to take care of the pairing effects in these nuclei, we use the constant gap formula for proton and neutron, as given in [22]:

and

III. RESULTS AND DISCUSSION

Ground state properties using the SHF and RMF models: There exists a number of parameter sets for solving the stan-
standard SHF Hamiltonians and RMF Lagrangians. In many of our previous works and of other authors \[11, 22, 23, 27, 28, 29\] 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. It is found that, more or less, most of the recent parameter sets reproduce well the 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.

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 $^{292}_{122}$, is shown in Fig. 1. 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 minima. For SHF, the minima appear at around $\beta_2 = -0.459, -0.159$ and $0.511$. 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. The absolute value differ by a constant factor from one another, i.e., if we scale the lower curve by, say, a scaling factor $c = 1.0075$ then both the curves will coincide with each other. This difference in energy is also reflected in the binding energy calculations of this nucleus in an isotopic chain, which will be discussed in the following subsection.

**B. Binding energy and Two-neutron separation energy**

Fig. 2 shows the calculated binding energy, obtained in both the SHF and RMF formalisms. We notice that, similar to the PES, the binding energy obtained in the RMF model also over-estimates the SHF result by a constant factor. In other words, here also the multiplication by a constant factor ‘c’ will make the two curves overlap with one another. This means that a slight modification of the parameter set of one
TABLE I: The SHF(SkI4) and the RMF(NL3) results for binding energy $BE$, two-neutron separation energy $S_{2n}$ and the quadrupole deformation parameter $\beta_2$, compared with the Finite Range Droplet Model (FRDM) data [24]. The energy is in MeV.

| Nucleus | $BE$ (MeV) | $S_{2n}$ (MeV) | $\beta_2$ | Nucleus | $BE$ (MeV) | $S_{2n}$ (MeV) | $\beta_2$ | Nucleus | $BE$ (MeV) | $S_{2n}$ (MeV) | $\beta_2$ |
|---------|------------|---------------|----------|---------|------------|---------------|----------|---------|------------|---------------|----------|
| 294     | 2062.49    | 16.29         | 0.534    | 296     | 2078.46    | 15.94         | 0.529    | 300     | 2108.67    | 14.81         | 0.526    |
| 298     | 2093.81    | 15.34         | 0.526    | 302     | 2123.01    | 14.34         | 0.529    | 306     | 2150.03    | 13.20         | 0.556    |
| 300     | 2108.67    | 14.81         | 0.526    | 304     | 2136.83    | 13.82         | 0.545    | 308     | 2162.49    | 12.45         | 0.560    |
| 302     | 2123.01    | 14.34         | 0.529    | 306     | 2150.03    | 13.20         | 0.556    | 310     | 2174.49    | 12.00         | 0.571    |
| 306     | 2150.03    | 13.20         | 0.556    | 312     | 2187.10    | 12.62         | 0.584    | 314     | 2199.12    | 12.02         | 0.594    |
| 310     | 2174.49    | 12.00         | 0.571    | 314     | 2199.12    | 12.02         | 0.594    | 316     | 2210.49    | 11.37         | 0.595    |
| 312     | 2187.10    | 12.62         | 0.584    | 316     | 2210.49    | 11.37         | 0.595    | 318     | 2221.02    | 10.65         | 0.588    |
| 314     | 2199.12    | 12.02         | 0.594    | 318     | 2221.02    | 10.65         | 0.588    | 320     | 2231.23    | 10.21         | 0.575    |

The comparison of $S_{2n}$ for the SHF and RMF with the FRDM result are further shown in Fig. 3, which shows clearly that the two $S_{2n}$ values coincide remarkably well, except at mass $A=318$ which seems spurious due to some error somewhere in the case of FRDM. Apparently, the $S_{2n}$ decrease gradually with increase of neutron number, except for the noticeable kinks at $A=294$ ($N=172$) and $312$ ($N=190$) in RMF, and at $A=304$ ($N=182$) and $308$ ($N=186$) in FRDM. Interestingly, these neutron numbers are close to either $N=172$ or 184 magic numbers. However, the SHF results are smooth.

The binding energy per particle for the isotopic chain is also plotted in Fig. 4. We notice that here again the SHF and RMF curves could be overlapped with 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 $^{302}_{122}$ is the most stable element from the binding energy point of view. Interestingly, $^{302}_{122}$ 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.

Also, we have calculated the "free solutions" for the whole isotopic chain, both in prolate and oblate deformed configurations. In many cases, we find low lying excited states. As a measure of the energy difference between the ground band and the first excited state, we have plotted in Fig. 5 the binding energy difference $\triangle E$ between the two solutions, noting that the maximum binding energy solution refers to the ground state and all other solutions to the intrinsic excited state(s). From Fig. 5, we notice that in RMF calculations, the energy difference $\triangle E$ is small for neutron-deficient isotopes, but it increases with the increase of mass number $A$ in the isotopic series. On the other hand, in SHF formalism, $\triangle E$ value remains small throughout the isotopic series. 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 of the periodic table.
FIG. 4: The binding energy per particle BE/A for the superheavy isotopes $^{282–320}$122, obtained in SHF(SkI4) and RMF(NL3) formalisms, compared with the FRDM results [34], wherever available.

C. Quadrupole deformation parameter

The quadrapole deformation parameter $\beta_2$, for both the ground and first excited states, are also determined within the two formalisms. 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 [11, 14, 20, 21, 22, 23, 25, 35, 36]. We have seen in Fig. 1 that both the ground-state and intrinsic excited quadrapole deformation parameters for SHF and RMF results agree well with each other (the same is true for “free solutions”, not shown here). However, the ground-state (g.s.) quadrapole deformation parameter $\beta_2$ plotted in Fig. 6 for SHF and RMF, and compared with FRDM results [34], show that the FRDM results differ strongly. Both in the SHF and RMF results, we find highly deformed oblates solutions in the g.s. 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 in both SHF and RMF models. Interestingly, most of the isotopes are superdeformed in their g.s. configurations, and due to the shape co-existance properties of these isotopes, some time it is possible that the g.s. could be the hyperdeformed solution.

D. Nuclear radii

The root mean square (rms) radius for proton ($r_p$), neutron ($r_n$) and matter distribution ($r_m$), both in SHF and RMF formalisms, is shown in Fig. 7. The upper pannel is for the SHF and the lower one for the RMF 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, the value of $r_p$ also increase as shown in the figure. This trend is similar in both the formalisms. A minute inspection of the figure shows that, in RMF calculation, the radii show a jump at $A=312$ ($N=190$) after the monotonous increase of radii till $A=310$. Note that a similar trend was observed in RMF calculations for $S_{2n}$ (see, Fig. 3).
TABLE II: The $Q_\alpha$ and $T_\alpha$ calculated on the SHF(SkI4) and the RMF(NL3) models, and compared with the Finite Range Droplet Model (FRDM) results [34], wherever available. The energy is in MeV.

| Nucleus | $Z$ | $BE$ | $Q_\alpha$ | $T_\alpha$ | $BE$ | $Q_\alpha$ | $T_\alpha$ | FRDM results |
|---------|-----|------|------------|-----------|------|------------|-----------|--------------|
| 292     |    |      | 14.39      | 10^{-6.93} | 2046.19 | 13.83      | 10^{-6.93} | 2023.06 | 13.98 | 10^{-6.07} |
| 288     |    |      | 14.48      | 10^{-6.93} | 2031.75 | 12.35      | 10^{-6.10} | 1993.49 | 12.42 | 10^{-5.10} |
| 284     |    |      | 14.48      | 10^{-6.93} | 2015.80 | 12.87      | 10^{-6.10} | 1977.62 | 12.33 | 10^{-5.44} |
| 280     |    |      | 14.48      | 10^{-6.93} | 2000.37 | 12.92      | 10^{-6.10} | 1961.66 | 11.61 | 10^{-4.45} |
| 276     |    |      | 14.48      | 10^{-6.93} | 1984.99 | 11.82      | 10^{-6.10} | 1944.97 | 10.94 | 10^{-4.47} |
| 272     |    |      | 14.48      | 10^{-6.93} | 1968.51 | 11.45      | 10^{-6.10} | 1927.62 | 10.57 | 10^{-4.18} |
| 268     |    |      | 14.48      | 10^{-6.93} | 1951.66 | 10.92      | 10^{-6.10} | 1909.90 | 9.93  | 10^{-4.15} |
| 264     |    |      | 14.48      | 10^{-6.93} | 1934.29 | 10.25      | 10^{-6.10} | 1905.34 | 8.75  | 10^{-3.59} |
| 260     |    |      | 14.48      | 10^{-6.93} | 1916.17 | 9.98       | 10^{-6.10} | 1891.53 | 8.75  | 10^{-3.59} |
| 256     |    |      | 14.48      | 10^{-6.93} | 1897.85 | 7.53       | 10^{-6.10} | 1871.98 | 8.35  | 10^{-3.19} |
| 252     |    |      | 14.48      | 10^{-6.93} | 1877.08 | 8.02       | 10^{-6.10} | 1852.03 | 7.64  | 10^{-2.91} |
| 248     |    |      | 14.48      | 10^{-6.93} | 1856.80 | 7.18       | 10^{-6.10} | 1831.98 | 6.90  | 10^{-2.01} |
| 244     |    |      | 14.48      | 10^{-6.93} | 1835.68 | 6.85       | 10^{-6.10} | 1809.98 | 6.52  | 10^{-2.81} |
| 240     |    |      | 14.48      | 10^{-6.93} | 1814.23 | 5.91       | 10^{-6.10} | 1788.21 | 5.77  | 10^{-2.54} |
| 236     |    |      | 14.48      | 10^{-6.93} | 1791.84 | 5.64       | 10^{-6.10} | 1754.15 | 5.14  | 10^{+1.18} |
| 232     |    |      | 14.48      | 10^{-6.93} | 1768.19 | 5.54       | 10^{-6.10} | 1754.15 | 5.14  | 10^{+1.18} |

![Fig. 7: The rms radii of proton ($r_p$), neutron ($r_n$) and matter ($r_m$) distribution for $^{282-320}$ nuclei using nonrelativistic SHF(SkI4) and relativistic mean field formalism RMF(NL3).](image)

![Fig. 8: The half-life time $T_\alpha$ and the $Q_\alpha$ energy for $^{292}$ nuclei, using the non-relativistic SHF(SkI4), the relativistic mean field formalism RMF(NL3), and the FRDM data [34].](image)

E. The $Q_\alpha$ energy and the decay half-life $T_\alpha$

We choose the nucleus $^{292}$ (Z=122, N=170) for illustrating our calculations of the $\alpha$-decay chain and the half-life time $T_\alpha$. The $Q_\alpha$ energy is obtained from the relation [37]:

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

Here, $BE(N, Z)$ is the binding energy of the parent nucleus with neutron number $N$ and proton number $Z$, $BE(2, 2)$ is the binding energy of the $\alpha$-particle ($^4He$) 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 nuclei are obtained by using both the RMF and SHF formalisms. Our predicted results are compared in Table II with the finite range droplet model (FRDM) calculation of Ref. [34]. The $Q_\alpha$ values are then calculated, also shown in Table II and in lower panel of Fig. 8. Then, the half-life $Log_{10}T_\alpha(s)$ are estimated by using the phenomenological formula of Viola and Seaborg [38]:

$$Log_{10}T_\alpha(s) = aZ - b + (cZ + d)$$

where $Z$ is the atomic number of parent nucleus, $a=1.66175$, $b=0.85166$, $c=0.20228$, and $d=33.9069$. The calculated $Log_{10}T_\alpha(s)$ are also given in Table II and in upper panel of
From Fig. 8, we notice that the calculated values for both $Q_\alpha$ and $T_{\alpha_1}(s)$ agree quite well with the FRDM predictions. For example, the value of $T_{\alpha_1}$, in both the FRDM and RMF coincides for the $^{264}$Hs nucleus. Similarly, for $^{276}$Hg, the SHF prediction matches the FRDM result. Possible shell structure effects in $Q_\alpha$, as well as in $T_{\alpha_1}(s)$, are noticed for the daughter nucleus $A=256$ ($Z=104, N=152$) and $284$ ($Z=118, N=166$) in SHF and for $A=256$ ($A=104, N=152$) and $288$ ($Z=120, N=168$) in RMF calculations. Note that some of these proton or neutron numbers refer to either observed or predicted magic numbers.

IV. SUMMARY

Concluding, we have calculated the binding energy, rms radius and quadrupole deformation parameter for the possibly discovered $Z=122$ superheavy element recently. From the calculated binding energy, we also estimated the two-neutron separation energy for the isotopic chain. We have employed both the SHF and RMF formalisms in order to see the formalism dependence of the results. We found qualitatively similar predictions in both the techniques. A shape change from oblate to prolate deformation is observed with increase of isotopic mass number at $A=290$. The ground-state structures are highly deformed which are comparable to superdeformed or hyperdeformed solutions, in agreement with the observations of Ref. [15] for the superheavy region. From the binding energy analysis, we found that the most stable isotope in the series is $^{302}Z=122$, instead of the observed $^{292}Z=122$, considered to be a neutron-deficient nucleus. Our predicted $\alpha$-decay energy $Q_\alpha$ and half-life time $T_{\alpha}$ agree nicely with the FRDM calculations. Some shell structure is also observed in the calculated quantities at $N=172$ or 190 for RMF and at $N=182$-186 for SHF calculations for the various isotopes of $Z=122$ nucleus.

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