The structural evolution in transitional nuclei of mass $80 \leq A \leq 132$

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In this theoretical study, we report an investigation on the behavior of two neutron separation energy, differential variation of the separation energy and the abnormality in nuclear charge radius along the isotopic and isotonic chains of transition nuclei. We have used relativistic mean field formalism with NL3 and NL3$^*$ forces for this present analysis. The study refers to even-even nuclei such as Zr, Mo, Ru and Pd with $N = 40–86$, where a rich collective phenomena such as proton radioactivity, cluster or nucleus radioactivity, exotic shapes, Island of Inversion and etc. are observed. These non-monotonic aspects over the isotopic chain are mainly correlated with the structural properties like shell/sub-shell closures, shape transition, clustering and magicity etc. In addition to these, we have shown the internal configuration of these nuclei to get a further insight into the reason for these discrepancies.

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I. INTRODUCTION

Nowadays, one of the most sensitive and crucial region in the nuclear chart for investigation is laying in between $Z=35–64$ and $A=82–132$. This region reveals a large number of interesting discoveries of new phenomena, such as proton radioactivity [11–13], cluster or nucleus radioactivity [4–5], exotic shapes [7, 8], Island of Inversion [9, 10], abnormal variation of major shell closures (i.e. extra stability near drip-line) [11–13] and giant halo near neutron drip-line region [14] etc. These crucial features may be due to the rapid growing possibility of neutron-proton ratio ($N/Z$) in a nucleus. From last few decades, it is possible to study these exotic nuclei by using the radioactive isotope beams (RIB) facilities. This reveals the new concept entitled as aforementioned magic number. In other word, the confirmation of magic number near $\beta$–stability line are not mandatorily universal [15–17]. Further, the structural properties of nuclei far away from the $\beta$–stability line are also an active areas of research in both theories and experiments [11–14, 18]. In particular, the neutron-rich Zr–, Mo–, Ru– and Pd– with mass numbers $A=100–130$ are of special interest for various reasons. For example, they lie far away from $\beta$–stable region of Nuclear Landscape, result in a well established deformation, but close enough in magnitude of microscopic excitations to compete with collectivity of double shell closure nuclei [14, 19, 20]. Moreover, these nuclei are also holding an active participation in the nucleosynthesis of heavy nuclei in astrophysical $r$–process. The mass and decay properties are quite essential ingredient to build up the path, the isotopic abundances and the time period of these process [21].

In addition to that the nuclear structure of these nuclei are characterized by a strong competition between various shapes, which gives rise to the shape instabilities that lead to coexistence nuclear shape transitions in the isotopic chains [22]. This could be understood from the the potential energy surface at different deformations. Elaborately, the occurrence of two (or more) nearly equally deep minima in the potential energy surface at different deformations shows the signature for nuclear shape coexistence. Hence, one can say the nuclear shape are not only vary with the nucleon number but also with the excitation energy and spin. It is well known that the binding energy of a nucleus is one of the most precise measured observable from the experiments [23, 24]. Several nuclear observables which are highly relevant for understanding various features of nuclear structure can be computed from its mass such as the average nuclear field, nucleon-nucleon (NN) potential, single particle energy etc. The correlations among these fundamental quantities are emended to explain the deformed ground states, low lying isomeric states and few derived quantities like moments of inertia and vibrational excitation energy etc [25, 26]. It is acknowledged that the energy involved in removal of fermions from a strongly correlated system of identical fermions must be a good indicator for the stability of the system. This magnitude of this energy have much higher values for systems with even number of particles than odd one, if the pairing is a dominant component in the binary fermion–fermion interaction.

In this present work, the quantities of interest are the nuclear potential energy surface, nuclear shape, nuclear binding energy, two neutron separation energies ($S_{2n}$), the differential variation of neutron separation energy $\Delta S_{2n}$ and the root-mean-square charge distribution $r_{ch}$ for the even-even mass transition nuclei. Base on these decisive observables, we have focused on the evolution on the structural properties of transition nuclei. The paper is organized as follows: Section II gives a brief description of the relativistic mean field formalism. The results of our calculation along with discussions are presented in Section III. Section IV includes a short summary along with few concluding remarks.

II. THE RELATIVISTIC MEAN-FIELD (RMF) METHOD

The microscopic self consistent mean-field calculations are the standard tool for the investigation of nuclear structure phenomena. The relativistic mean field (RMF) theory is one of the most popular and widely used formalism among them.
It starts with the basic Lagrangian that describes nucleons as Dirac spinors interacting through different meson fields. The original Lagrangian of Walecka has taken several modifications to take care of various limitations and the successful relativistic Lagrangian density for a nucleon-meson many body system [29, 39] is expressed as:

\[
\mathcal{L} = \psi_i \{ i \gamma^\mu \partial_\mu - M \} \psi_i + \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m^2 \sigma^2 - \frac{1}{3} \gamma^\mu \gamma^\nu \gamma^\rho \partial_\mu \sigma \partial_\nu \sigma \partial_\rho \sigma + \frac{1}{4} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \partial_\mu \sigma \partial_\nu \sigma \partial_\rho \sigma \partial_\sigma \sigma + \frac{1}{2} m^2 \nu \nu \nu - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} \bar{\psi} \gamma^\mu V^\mu \psi - \frac{1}{4} \bar{\psi} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \bar{\psi} \gamma^\sigma \gamma^\rho \gamma^\nu \gamma^\mu \psi + \frac{1}{2} m^2 \nu \nu \nu - \frac{1}{4} \bar{\psi} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \bar{\psi} \gamma^\sigma \gamma^\rho \gamma^\nu \gamma^\mu \psi - \frac{1}{4} F^{\mu\nu} F_{\mu\nu} - c \bar{\psi} \gamma^\mu (1 - \tau_3) \psi A^\mu \psi.
\]

(1)

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 are solved numerically by a self-consistent iteration method [40–43]. The centre-of-mass motion energy correction is estimated by the usual harmonic oscillator formula \( E_{\text{c.m.}} = \frac{1}{2} (41A^{-1/3}) \). The total quadrupole deformation parameter \( \beta_2 \) is evaluated from the resulting proton and neutron quadrupole moments, as

\[
Q = Q_n + Q_p = \sqrt{\frac{16\pi}{5}} \left( \frac{3}{4\pi} AR^2 \beta_2 \right).
\]

(2)

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

\[
\langle r_m^2 \rangle = \frac{1}{A} \int \rho(r_\perp, z) r^2 \, dr, \tag{3}
\]

where \( A \) is the mass number, and \( \rho(r_\perp, z) \) is the axially deformed density. The total binding energy and other observables are also obtained by using the standard relations, given in [29]. In order to take care of the pairing effects in the present study, we have used the constant gap for proton and neutron, as given in [44, 45], which are valid for nuclei both on or away from the stability line (more details in Ref. [32]).

### III. DETAILS OF CALCULATION AND RESULTS DISCUSSION

The mean-field equations are solved self-consistently by taking different inputs of the initial deformation called \( \beta_0 \) [29, 32, 46–48]. For a normal ground state solution of the considered mass region, the desire number of major shells for fermions and bosons are \( N_F = N_B = 12 \). To verify the convergence of the solutions, few calculations are done with \( N_F = N_B = 12-16 \). The variation of these solutions are \( \leq 0.002\% \) on binding energy and 0.001\% on nuclear radii over the range of major shell. This implies that the used model space is good enough for the considered mass regions. However, the number of mesh points for Gauss-Hermite and Gauss-Lagurre integration are 20 and 24, respectively. Here, we have used the well known NL3 [46] and recent developed NL3* [47] force parameters, which are able to reproduce the properties of the stable nuclei as well as the nuclei away from the \( \beta \)-stability line. We obtain the calculation for different potentials, nuclear densities (for protons and neutrons), single-particle energy for nucleons, nuclear radii, deformation parameter and binding energies etc. For a given nucleus, there are more than one solutions. In this case, the solution corresponding to maximum binding energy is treated as ground state for a given nucleus and other solutions are the intrinsic excited states (see FIG. 1).

### A. Potential energy surface

Conventionally, in case of a quantum mechanical system, the path followed by the different solutions at various deformation defines a potential barrier or potential energy surface, which can be used for the determination of the ground state of a nucleus. More elaborately, from the potential energy surface (PES) obtained from a self-consistent relativistic mean field theory, one can regulate the reasonable results for the ground state similar to the non-relativistic calculations [49]. Since quadrupole deformation plays the most important and dominant part, we have neglected the other deformation coordinates in the present study for simplicity and low computation time cost. Here, the potential energy curve is calculated microscopically by the constrained RMF theory [32, 33, 50–52]. The expectation value of the Hamiltonian [48, 51, 53] at
TABLE I: The binding energy per particle $E_b/A$ and the quadrupole deformation parameter $\beta_2$ for the ground states of transition nuclei compare with the experimental data [54], wherever available.

| N  | RMF (NL3) | RMF (NL3*) | Experiment |
|----|-----------|------------|------------|
|    | BE $r_{ch}$ | $\beta_2$ | BE $r_{ch}$ | $\beta_2$ | BE $r_{ch}$ | $\beta_2$ | Experiment |
| 42 | 691.3      | 4.29       | 0.197      | 690.9      | 4.29       | 0.192      | 0.367 |
| 44 | 715.7      | 4.29       | 0.188      | 715.8      | 4.27       | 0.001      | 0.251 |
| 46 | 739.2      | 4.28       | 0.001      | 739.2      | 4.27       | 0.001      | 0.151 |
| 48 | 762.6      | 4.28       | 0.001      | 761.9      | 4.28       | 0.001      | 0.185 |
| 50 | 783.9      | 4.28       | 0.001      | 783.1      | 4.28       | 0.000      | 0.089 |
| 52 | 797.8      | 4.29       | 0.001      | 797.2      | 4.28       | 0.000      | 0.102 |
| 54 | 810.5      | 4.34       | 0.169      | 808.9      | 4.31       | 0.002      | 0.090 |
| 56 | 824.5      | 4.38       | 0.243      | 822.9      | 4.38       | 0.233      | 0.088 |
| 58 | 837.0      | 4.42       | 0.318      | 834.9      | 4.40       | 0.274      | 0.074 |
| 60 | 849.8      | 4.48       | 0.432      | 847.6      | 4.49       | 0.453      | 0.355 |
| 62 | 860.6      | 4.50       | 0.428      | 858.2      | 4.50       | 0.428      | 0.427 |
| 64 | 870.6      | 4.52       | 0.427      | 868.0      | 4.52       | 0.424      | 0.38  |
| 66 | 880.4      | 4.54       | 0.419      | 877.6      | 4.54       | 0.418      | 0.292 |
| 68 | 889.8      | 4.56       | 0.416      | 886.8      | 4.56       | 0.419      | 0.306 |
| 70 | 897.2      | 4.59       | 0.445      | 893.9      | 4.59       | 0.461      | 0.38  |
| 72 | 904.1      | 4.62       | 0.478      | 900.4      | 4.62       | 0.479      | 0.33  |
| 74 | 911.8      | 4.52       | 0.170      | 908.8      | 4.52       | 0.166      | 0.176 |
| 76 | 917.7      | 4.52       | 0.109      | 914.5      | 4.52       | 0.095      | 0.167 |
| 78 | 923.4      | 4.52       | 0.065      | 920.0      | 4.52       | 0.043      | 0.043 |
| 80 | 929.5      | 4.54       | 0.002      | 925.7      | 4.53       | 0.002      | 0.074 |
| 82 | 935.5      | 4.55       | 0.000      | 931.0      | 4.55       | 0.001      | 0.001 |
| 84 | 936.3      | 4.56       | 0.003      | 931.8      | 4.56       | 0.009      | 0.009 |
| 86 | 936.9      | 4.57       | 0.062      | 932.5      | 4.57       | 0.067      | 0.139 |

The potential energy surface as a function of deformation parameter $\beta_2$, for the proton rich nucleus $^{82}$Zr, the double magic nucleus $^{90}$Zr and the neutron rich nucleus $^{110,120}$Zr are shown in Fig. 1, as a representative case. All other Mo−, Ru− and Pd− isotopes are also showing the similar behaviors, which are not given here. The energy ($E_b = E_{g.s} - E_{e.s}$) on the $Y$−axis is the difference between the ground state energy to other constraint energy solutions. The solid and dotted line in the figure are for NL3 and NL3* force, respectively. The calculated PES for both the cases are shown for a wide range from oblate to prolate deformations. We notice from the figure that there are more than one minima appear at different $\beta_2$. The magnitude of binding energy for the corresponding minima shows that the ground state solution appear at a certain deformation is given as,

$$H' = \sum_{ij} \frac{\langle \psi_i | H_0 - \lambda Q^2 | \psi_j \rangle}{\langle \psi_i | \psi_j \rangle}$$

where $\lambda$ is the constraint multiplier and $H_0$ is the Dirac mean field Hamiltonian. The convergence of the numerical solutions on the binding energy and the deformation are not very much sensitive to the deformation parameter $\beta_0$ of the harmonic oscillator basis for the considered range due to the large basis. Thus the deformation parameter $\beta_0$ of the harmonic oscillator basis is chosen near the expected deformation to obtain high accuracy and less computation time period.
TABLE II: Same as Table I, only for $^{86-114}$Mo and $^{86-114}$Pd isotopes.

| N   | RMF (NL3) BE $r_{ch}$ $\beta_2$ | RMF (NL3*) BE $r_{ch}$ $\beta_2$ | Experiment | RMF (NL3) BE $r_{ch}$ $\beta_2$ | RMF (NL3*) BE $r_{ch}$ $\beta_2$ | Experiment |
|-----|---------------------------------|---------------------------------|------------|---------------------------------|---------------------------------|------------|
| 42  | 696.7 4.34 -0.206 696.2 4.34 -0.203 | 697.8 4.42 0.002 697.8 4.42 0.002 | |
| 44  | 722.2 4.32 0.001 719.5 4.32 0.002 725.8 | 730.0 4.44 0.094 729.9 4.44 0.095 | |
| 46  | 748.2 4.33 0.003 748.2 4.33 0.003 750.1 | 760.9 4.43 0.101 760.7 4.43 0.104 | |
| 48  | 773.4 4.33 0.001 773.1 4.33 0.001 773.7 | 789.5 4.42 0.004 789.1 4.42 0.005 | |
| 50  | 796.9 4.33 0.001 796.4 4.33 0.001 796.5 4.3156 0.1058 | 817.4 4.42 0.001 816.8 4.41 0.001 815.0 | |
| 52  | 812.7 4.34 0.001 812.2 4.34 0.001 814.2 4.3518 0.1509 | 836.9 4.43 0.003 836.3 4.42 0.004 836.3 | |
| 54  | 828.1 4.38 0.174 827.1 4.37 0.158 830.8 4.3841 0.1720 | 855.9 4.46 0.136 855.4 4.46 0.139 856.4 | |
| 56  | 843.5 4.42 0.230 842.2 4.41 0.220 846.2 4.4088 0.1683 | 874.2 4.48 0.176 873.6 4.48 0.177 875.3 4.4839 0.196 | |
| 58  | 857.2 4.45 0.268 855.7 4.43 0.246 860.5 4.4458 0.2309 | 891.1 4.51 0.189 890.5 4.50 0.188 892.8 4.5086 0.209 | |
| 60  | 871.2 4.50 0.366 869.1 4.49 0.356 873.9 0.311 | 906.9 4.52 0.187 906.2 4.52 0.184 909.5 4.5322 0.229 | |
| 62  | 883.6 4.53 0.386 881.4 4.52 0.382 886.9 0.362 | 921.8 4.53 0.190 921.1 4.53 0.179 925.2 4.5563 0.243 | |
| 64  | 895.4 4.49 -0.234 894.0 4.49 -0.228 898.9 0.354 | 936.1 4.57 0.240 934.9 4.54 0.165 940.2 4.5776 0.257 | |
| 895.2 4.54 0.379 893.9 4.54 0.377 | 951.8 4.59 -0.231 950.4 4.58 -0.229 954.3 0.220 | |
| 66  | 907.4 4.51 -0.236 905.7 4.51 -0.233 0.38 | 905.3 4.60 0.292 949.5 4.60 0.290 77 | |
| 906.5 4.56 0.374 904.9 4.55 0.373 | 963.5 4.62 -0.234 963.9 4.60 -0.234 967.6 0.164 | |
| 68  | 918.1 4.53 -0.241 915.9 4.53 -0.239 | 967.5 4.62 0.304 961.9 4.60 0.301 | |
| 70  | 927.0 4.55 -0.231 924.6 4.54 -0.223 | 977.9 4.63 -0.221 975.8 4.61 -0.226 0.207 | |
| 72  | 935.7 4.55 -0.197 933.2 4.55 -0.190 | 975.3 4.60 0.216 974.1 4.59 0.216 | |
| 74  | 944.6 4.57 -0.180 941.7 4.56 -0.179 | 989.1 4.63 -0.198 986.8 4.62 -0.184 | |
| 76  | 951.8 4.58 -0.172 948.4 4.58 -0.171 | 1000.6 4.63 -0.163 998.1 4.62 -0.151 | |
| 78  | 958.3 4.57 0.114 955.0 4.56 0.094 | 1011.8 4.63 0.115 1009.8 4.62 0.1147 | |
| 80  | 965.0 4.58 0.041 961.4 4.57 0.037 | 1021.0 4.63 -0.054 1018.5 4.63 -0.053 | |
| 82  | 972.2 4.59 0.001 967.9 4.59 0.001 | 1032.4 4.65 0.073 1029.3 4.64 0.0757 | |
| 84  | 973.6 4.60 0.005 969.4 4.60 0.014 | 1041.5 4.65 0.001 1037.8 4.65 0.0017 | |
| 86  | 975.5 4.62 0.118 971.3 4.61 0.109 | 1044.5 4.66 0.027 1040.9 4.67 0.0427 | |
| 1086.4 4.69 0.130 1044.9 4.69 0.1317 | | |

The calculations mainly explain the nuclear structure as well as the sub-structure properties, based on the basic ingredients such as binding energy ($E_B$), quadrupole moment $Q_{20}$, nucleonic density distribution $\rho_n(r_{+}, z)$, and $rms$ nuclear radii etc. Nevertheless, the present study demonstrates the applicability of RMF on the nuclear structure study for transition nuclei near neutron drip-line. The obtained results for binding energy $BE$, quadrupole deformation parameter $\beta_2$ and the charge radius $r_{ch}$ for NL3 and NL3* force parameter for the isotopic chain of Zr, Mo, Ru and Pd are listed in Table-I along with the experimental data. We notice on the binding energy and the $rms$ $r_{ch}$ for all nuclei over the isotopic chain from RMF agree well with the experimental values. Quantitatively, the mean deviation of $BE$ and $r_{ch}$ between the calculated result and the available experimental data over the isotopic chain are $\sim 0.01$ and $0.004$, respectively. Further, the quadrupole deformation parameter $\beta_2$, for both ground (g.s.) and selective excited states (e.s.) are also given in Table I. In some of the earlier RMF and
Skyrme Hartree-Fock (SHF) calculations, it was shown that the quadrupole moment obtained from these theories reproduce the experimental data pretty well [30, 32, 33, 46, 48, 55–57]. From the table, one can find that the shape of few nuclei are not consistent with the experimental observed shape. In this context, we have also estimated the first excited state solutions in these nuclei are almost degenerate and might have large shape fluctuations. For example, in $^{92}_{40}\text{Zr}$ the two solutions for $\beta_2 = -0.197$ and $\beta_2 = 0.25$ are completely degenerate with binding energies of 691.3 and 691.0 MeV, respectively. Hence, 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. Similar behavior are also observed for few other nucleus are listed in Table- I. Such phenomenon is known to exist in many other regions [58, 59] of the nuclear chart.

C. Two neutron separation energy $S_{2n}(Z,N)$

Two neutron separation energy $S_{2n}(Z,N)$, can be estimated from the ground state nuclear binding energies of $BE(Z,N)$, $BE(Z,N-2)$ and the neutron mass $m_n$ with the relation:

$$S_{2n}(Z,N) = -BE(Z,N) + BE(Z,N-2) + 2m_n,$$  \hspace{1cm} (5)

The $BE$ of the $^A X_Z$ and $^A Z$ are calculated from RMF for NL3 and NL3* force parameters. It is essential to have very precise mass measurements to predict the correct estimation of the neutron separation energy $S_{2n}$. The calculated $S_{2n}$ energy from RMF as a function of neutron number for Zr, Mo, Ru and Pd isotopes are compared with latest experimental data [54], shown in the Fig. 2. From the figure it is clear that in an isotopic chain, the $S_{2n}$ energy shows the well-known regularities for a given atomic number i.e. the $S_{2n}$ decreases smoothly as the number of neutron increases in an isotopic chain. A sharp discontinuities (in other word kinks) appears at neutron magic numbers at $N = 50$ and 82. In energy terminology, one can write, the energy necessary to remove two neutrons from a nucleus ($Z, N_{magic}+2$) is much smaller than that to remove two neutrons from the nucleus ($Z, N_{magic}$), which breaks the regular trend.

D. Differential variation of two neutron separation energy

The differential variation of the two neutron separation energy ($S_{2n}$) with respect to neutron number ($N$) i.e. $dS_{2n}(N,Z)$ is defined as

$$dS_{2n}(Z,N) = \frac{S_{2n}(Z,N+2) - S_{2n}(Z,N)}{2}.$$

The $dS_{2n}(N,Z)$ is one of the key quantity to explore the rate of change of separation energy with respect to the neutron number in an isotopic chain. Here, we have calculated the $dS_{2n}(N,Z)$ for NL3 & NL3* force parameter. Further, we have also estimated the $dS_{2n}(N,Z)$ energy from the experimental $S_{2n}$ energy. In Fig. 3, we are compared the experimental values with our calculation for Zr, Mo, Ru and Pd isotopes. In general, the large sharp deep fall in the $dS_{2n}$ over an isotopic chain shows the signature of neutron shell closure. In other word, this deviation in the general trend may disclose some additional nuclear structure features. From the figure, we observed the same characteristics for all $Z=38-46$. 

FIG. 2: (Color online) The two neutron separation energy as a function of neutron number from RMF theory with NL3 and NL3* force parameter for $^{82-126}_{38-40}\text{Zr}$, $^{84-128}_{40-48}\text{Mo}$, $^{86-130}_{40-48}\text{Ru}$ and $^{88-132}_{50-56}\text{Pd}$ nuclei are compared with the experimental data [54].

FIG. 3: (Color online) The differential variation of the two neutron separation energy $dS_{2n}$ as a function of neutron number from RMF theory with NL3 and NL3* force parameter for $^{82-126}_{38-40}\text{Zr}$, $^{84-128}_{40-48}\text{Mo}$, $^{86-130}_{40-48}\text{Ru}$ and $^{88-132}_{50-56}\text{Pd}$ nuclei are compared with the experimental data [54].
E. The root-mean-square charge distributions

The root mean square (rms) matter radius from relativistic mean field theory can be expressed as:

\[ \langle r^2 \rangle = \frac{1}{A} \int \rho(r, z)r^2 dr, \]  

(7)

where \( A \) is the mass number and \( \rho(r, z) \) is the axially deformed density. The rms charge radius can be calculated from the rms proton radius \( \langle r^2_p \rangle \) with simple algebraic relation,

\[ \langle r^2_{ch} \rangle = \langle r^2_p \rangle + 0.64. \]  

(8)

From the theoretical point of view, the macroscopic-microscopic models [60] and microscopic mean-field formulations using effective interactions are most sophisticated approaches to determine the rms charge radius in comparison with experimental data [61]. In this present work, we have shown the variations or fluctuations of the charge radii on the top of a fairly smooth average behavior in an isotopic chain. The results from RMF approaches for NL3 and NL3* parameters along with the available experimental data are shown in Fig. 4. From the figure it is clear that the obtained radii from RMF for \(^{82-126}\)Zr, \(^{84-128}\)Mo, \(^{86-130}\)Ru and \(^{88-132}\)Pd follows closely the experimental data [61]. For most of the nuclei, the experimental values are unavailable, the RMF prediction are made for the charge radii of such a nucleus that awaits experimental confirmation. The circle, square and triangle symbols indicate the ground state data for NL3, NL3* and experiment. Further, the solid circle and solid square symbols indicate the shapes corresponds to the first intrinsic excited states obtained from NL3 and NL3* force, respectively. From the figure, one can observe the smooth behavior for lighter isotopes, then there is a small fall in the charge radii for Zr, Mo, and Pd at about \( N = 62, 64, 72 \) and 74. These fall corresponds to the transition from the prolate to the oblate and vice versa. But the magnitude for both the states are different, i.e., the oblate deformation is at \( \beta_2 \sim 0 \), while the prolate one appears with \( \beta_2 \sim 0.4 \). In case of Pb isotope, the change is the radii only at one place i.e. at \( N = 74 \). Further, one can notice that the tiny change in the calculation can lead to the first intrinsic excited state as ground state (see Fig. 1). In other word, we can practically degenerate the ground state binding energy for the deformation corresponding to the first intrinsic excited state. Thus, the inconsistency in the \( r^2 \) could be explain in terms of configuration mixing i.e. the actual ground state is not only the spherical configuration but also from the neighbor deformed intrinsic excited states.

F. The contour plot of the axially deformed density distributions

In the above figures and tables, we have shown the results for few structural observables such as binding energy, quadrupole deformation, rms radius, separation energy and differential separation energy in comparison with the experimental data [54, 61]. Based on the experimental data, we have focused on the ground of \(^{82-126}\)Zr, \(^{84-128}\)Mo, \(^{86-130}\)Ru and \(^{88-132}\)Pd nuclei along with few selective excited states. Overall, we found some significant signature of shell closure at \( N = 50 \) and 82 in the isotopic chains. Further, the abnormal variation of \( S_{2n} \) and \( dS_{2n} \) near \( N \sim 64 \) and 74 in Zr,
**Mo and Ru isotopes suggests a shape co-existence.** A more careful inspection shows that the tendency of abnormality in the \(S_{2n}\) and \(dS_{2n}\) are decreased in the isotonic chain. In other word, we get a smoother behavior in neutron separation energy for \(Pd\) nuclei in comparison to \(Zr\) isotopes. The divergence can be cut down by taking the dynamical correlations beyond mean field \([62, 64]\).

To get a complete picture into the reason behind such discrepancy over the isotopic chain, we have shown the contour plot of axially deformed density of proton and neutron of these nuclei. In FIG. 4, we have displayed the distribution of \(Zr\) isotopes for \(N=42, 50, 60\) and \(82\) as representative cases. All the isotopes of \(Mo, Ru\) and \(Pd\) also showing similar behavior as \(Zr\) as shown in FIG. 4. From the figure, one can clearly identify the spherical, oblate, prolate shapes corresponding to their \(\beta_2\) values as the local minima in the PECs. Similar calculations can also be found in Ref. \([65, 66]\). In these figures we can see that the transition from oblate to prolate at \(N=42\), then change to the spherical structure at \(N=50\) and further changing the deformations to prolate one. Even the proton number is fixed in the isotopic chain, still we found a little change in the density distribution due to the the influence of excess neutron number. Following the color code, the red and light grey color corresponding to the high density (\(\sim 0.09 \text{ fm}^{-3}\)) and low density (\(\sim 0.001 \text{ fm}^{-3}\)), respectively. More inspection on the figures shows that the central density of the proton increases as compared to the neutron with respect to the neutron number. In this region, few isotopes of \(Mo\) (for \(^{116-118}\text{Mo}\)) are triaxial shape in their ground state, which is very close to the axial solutions \([66]\). In other word, the location of minima for triaxial solution for these isotopes of \(Mo\) are almost same as the minima appear for axial prolate axial solution. Hence, we have used the simple axial deformed calculation, which is good enough for the a qualitative descriptions of structural observables in this mass region.

**IV. SUMMARY AND CONCLUSIONS**

We have used self-consistent relativistic mean field theory with most popular \(NL3\) and recent \(NL3^*\) force parameters to study the structural evolution in transition nuclei. The conjecture has been made from the neutron separation energies, differential variation of separation energy and the root-mean-square charge radii of these nuclei. In the present calculations we have shown that \(Zr, Mo\) and \(Sr\) isotopes undergo a transition from oblate to prolate shapes at \(N \sim 64\) and \(74\). But, in case of \(Pd\) follows a smooth pattern through out the isotopic chain. We have also shown the dependence of nuclear charge radii on deformation also play an crucial role on their structural transition. Further, we have also observed a large shell gap at \(N=82\), almost same in magnitude at \(N=50\) for these considered nuclei, which is a well-known feature for mean-field calculation. We have also demonstrated the efficiency of RMF theory calculations to reproduce those features and therefore to make predictions in unexplored regions.

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