GROUND STATE PROPERTIES OF EXOTIC NUCLEI NEAR Z=40 IN THE RELATIVISTIC MEAN-FIELD THEORY

G.A. LALAZISSIS\(^1\) and M.M. SHARMA\(^2\)
\(^1\)Physik Department, Technische Universität München
D-85747 Garching, Germany
\(^2\)Max Planck Institut für Astrophysik, Karl-Schwarzschild-Strasse 1,
D-85740 Garching bei München, Germany

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Abstract

Study of the ground-state properties of Kr, Sr and Zr isotopes has been performed in the framework of the relativistic mean field (RMF) theory using the recently proposed relativistic parameter set NL-SH. It is shown that the RMF theory provides an unified and excellent description of the binding energies, isotope shifts and deformation properties of nuclei over a large range of isospin in the Z=40 region. It is observed that the RMF theory with the force NL-SH is able to describe the anomalous kinks in isotope shifts in Kr and Sr nuclei, the problem which has hitherto remained unresolved. This is in contrast with the density-dependent Skyrme Hartree-Fock approach which does not reproduce the behaviour of the isotope shifts about shell closure. On the Zr chain we predict that the isotope shifts exhibit a trend similar to that of the Kr and Sr nuclei. The RMF theory also predicts shape coexistence in heavy Sr isotopes. Several dramatic shape transitions in the isotopic chains are shown to be a general feature of nuclei in this region. A comparison of the properties with the available mass models shows that the results of the RMF theory are generally in accord with the predictions of the finite-range droplet model.
1 INTRODUCTION

The relativistic mean-field (RMF) theory [1] has received much attention recently due to its advantages over the non-relativistic density-dependent Skyrme approaches [2]. The RMF theory has been successful [3, 4] in describing the ground-state properties of nuclei about the line of stability. It has been demonstrated [5] that the RMF theory is able to describe nuclei also far away from the line of stability. With perpetual improvement in the techniques of producing radioactive beams, study of exotic nuclei [7, 8] very far away from the stability line has now become feasible. Interesting features such as neutron halos [9] in neutron-rich nuclei are being unravelled. As nuclei very far away from the stability line entail very large isospins, it is incumbent on theories to be able to provide and predict the properties of nuclei in these extreme regions. Microscopic theories which could fulfill these demands are much required. Availability of appropriate interactions to be able to do justice to these extreme conditions has been equally in demand. The RMF theory bears a potential to describing nuclei over a large range of charge and mass.

The RMF theory has been applied extensively to study the ground-state properties of nuclei along the stability line. The forces NL1 [3] and NL2 [10] were employed in most of the calculations [4]. NL1 and NL2 were the only available choice for realistic calculations. It was, however, observed [3] that both these parameter sets overestimate the neutron-skin thickness of nuclei with large neutron excess. A larger asymmetry energy of both NL1 and NL2 was found responsible for this problem. Recently, this problem has been remedied and a new force NL-SH was obtained by Sharma et al. [6]. This force has been shown to provide an excellent description of the ground state properties of spherical as well as deformed nuclei along the stability line. The description obtained for nuclei away from the stability line [3] and close to the neutron drip line [11] has also been successful. This is partly due to the fact that the force NL-SH has an appropriate \( \rho \)-meson coupling which leads to the correct asymmetry energy. It was shown [6] that NL-SH, which was obtained by adjusting the ground-state properties of only a few spherical nuclei, describes the binding energies and deformations of Xe isotopes over a large range of isospin on both the sides of the stability line.
The density-dependent Skyrme approaches [2] have, on the other hand, also been applied successfully to describing properties of nuclei mainly along the stability line. Properties of deformed nuclei have been predicted [12] satisfactorily using the Skyrme force SIII. The Skyrme approach, however, faces problems in providing an adequate description of nuclei across shell-closures. It is worth mentioning that the two approaches, one that of the RMF theory and the other of the Skyrme type have quite different underlying assumptions to generate the interaction. In the RMF theory the saturation and the density dependence of the nuclear interaction is provided by a balance between a large attractive scalar $\sigma$-meson field and a large repulsive vector $\omega$-meson field. The asymmetry component is provided by the isovector $\rho$ meson. The nuclear interaction is hence generated by the exchange of various mesons between nucleons. On the other hand, in the Skyrme approach, the nuclear interaction has a certain density dependence assumed at the outset, the latter being obtained from fits to empirical data. It may be reckoned that the structure of the force in the RMF theory and its density dependence differ from that of the Skyrme forces. Moreover, the spin-orbit interaction is added ad-hoc in the latter approach. It, however, arises naturally in the RMF theory as a result of the Dirac structure of nucleons. The density dependence of the spin-orbit interaction in the Skyrme theory also differs from its counterpart in the RMF theory. We have found that the isospin dependence of the spin-orbit interaction in the two approaches is different [13, 14].

The isotope shifts of nuclei have been measured since long. Precision measurements on isotope shifts of nuclei have been carried out extensively by the Mainz and other groups on several chains of nuclei. A detailed discussion of these properties has been provided in a review article by Otten [15]. As shown in this review, many isotopic chains exhibit anomalous kinks in the isotope shifts about neutron magic number. Such chains include the Pb isotopes which also have a closed proton shell. Other chains which also show such a behaviour include the isotopes of Sr and Kr among others. These isotopes do not have a magic proton number but encounter a closed neutron shell at N=50. The anomalous behaviour of the charge radii of nuclei about the shell-closure has been one of the long-standing problems. The empirical data which have reached considerable precision using laser
spectroscopic methods show this behaviour conspicuously. A kink in the isotope shifts in charge radii implies that the charge radii of the isotopes above the closed shell have a different trend in its variation with the neutron number as compared with their lighter counterparts. This suggests that neutrons in the unfilled-shell below the shell-closure behave differently than those which fill the next shell above it.

The problem of the anomalous kink in the empirical isotope shifts of Pb nuclei has until recently remained intractable. This problem was treated earlier using the Skyrme approach. It was shown by Sagawa et al. [16] that the isotope shifts only on one side of the neutron closed shell could be reproduced. A detailed investigation on it was also undertaken by Tajima et al. [17]. Employing several Skyrme interactions, it was shown [17] that the kink in the isotope shifts in Pb nuclei about N=126 could not be obtained within the Skyrme mean-field. Adding various correlations to the mean-field improved the situation only slightly. The kink in the isotope shifts could not, however, be reproduced by any of the Skyrme forces used in [17]. Recently, an attempt was made by Sharma et al. [18] to obtain the isotope shifts in Pb nuclei in the RMF theory. It was shown that the RMF theory with the force NL-SH is successful in reproducing the anomalous kink in the isotope shifts of Pb nuclei.

Nuclei in the region of Z=40 about the mass number 100 have been of particular interest in the nuclear structure due to predictions for the existence of highly deformed shapes. Properties of nuclei in this region have in the past been the focus of several detailed investigations both theoretically and experimentally. Extensive efforts devoted to studies in this region have been discussed in detail in [19]. On the experimental front, there exist high precision data on isotope shifts for Kr and Sr nuclei obtained by the Mainz group [20, 21] using laser spectroscopic methods. Measurements on the Sr chain were also carried out at the Daresbury Laboratory [22]. The data show an interesting feature that the magic nuclei $^{86}$Kr and $^{88}$Sr have the smallest rms charge radii in their respective chains, even when compared to nuclei ten mass numbers lower.

Theoretically, the isotope shifts and charge radii of nuclei in this region are still beyond a description. Extensive investigations were carried out by Bonche et al. [23]. Self-consistent calculations [23] including triaxial de-
mations in the Skyrme mean-field with the force SIII provide only a nearly linear response to the isotope shifts with mass number, in clear contradiction to the experimental trend. Furthermore, application of the method of generator coordinates\cite{24,25} to include triaxial deformations in Sr isotopes predicts spherical to deformed shape transitions. The isotope shifts could not, however, be reproduced by any means in the non-relativistic Skyrme approaches.

Attention has also been paid to the Sr and Zr isotopes\cite{26,27,28} in the RMF theory. However, because of the use of the force NL1\cite{3}, which has an asymmetry energy much larger than the empirical value, a good description for isotopes with a large neutron excess has been hindered. The RMF theory with NL1 has shown success primarily for nuclei along the line of the stability\cite{4}. Due to inadequacy of the force NL1 to extrapolations in the extreme regions, it has predicted spherical shapes for many Sr\cite{26} as well as Zr isotopes\cite{27}, in contradiction to the deformed shapes obtained empirically. With the advent of the force NL-SH, we study the ground state properties of Kr, Sr and Zr isotopes over a large range of isospin within the framework of the RMF theory in this paper. We focus especially upon the isotope shifts and deformation properties of these nuclei. The paper is organized as follows. Section II describes the details of the theoretical formalism employed in the RMF treatment of the deformed nuclei. Section III gives details on the procedure of our calculations. In section IV we present and discuss our results, where a comparison of our predictions with the empirical data is made. Comparison with other approaches is also made wherever possible. The last section summarizes our conclusions.

2 THE RELATIVISTIC MEAN-FIELD FORMALISM

The starting point of the RMF theory is a Lagrangian density\cite{1} which describes the nucleons as Dirac spinors interacting via the exchange of several mesons. The Lagrangian density can be written in the following form:

\[
\mathcal{L} = \bar{\psi}(i\slashed{\partial} - M)\psi + \frac{1}{2}\partial_{\mu}\sigma\partial^{\mu}\sigma - U(\sigma) - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega_{\mu}\omega^{\mu} - \frac{1}{4}R_{\mu\nu}R^{\mu\nu} + \frac{1}{2}m_{\rho}^{2}\rho_{\mu}\rho^{\mu} - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + g_{\sigma}\bar{\psi}\sigma\psi - g_{\omega}\bar{\psi}\omega\psi - g_{\rho}\bar{\psi}\rho\tau\psi - e\bar{\psi}\mathbf{A}\psi
\]

(1)
The meson fields are the isoscalar $\sigma$ meson, the isoscalar-vector $\omega$ meson and the isovector-vector $\rho$ meson. The latter provides the necessary isospin asymmetry. The bold-faced letters indicate the isovector quantities. The model contains also a non-linear scalar self-interaction of the $\sigma$ meson:

$$U(\sigma) = \frac{1}{2}m_\sigma^2 \sigma^2 + \frac{1}{3}g_2 \sigma^3 + \frac{1}{4}g_3 \sigma^4$$  \hspace{1cm} (2)

The scalar potential (2) introduced by Boguta and Bodmer [29] is essential for appropriate description of surface properties. $M$, $m_\sigma$, $m_\omega$ and $m_\rho$ are the nucleon-, the $\sigma$-, the $\omega$- and the $\rho$-meson masses respectively, while $g_\sigma$, $g_\omega$, $g_\rho$ and $e^2/4\pi = 1/137$ are the corresponding coupling constants for the mesons and the photon.

The field tensors of the vector mesons and of the electromagnetic field take the following form:

$$\Omega^{\mu\nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu$$

$$R^{\mu\nu} = \partial^\mu \rho^\nu - \partial^\nu \rho^\mu - g_\rho (\rho \times \rho)$$  \hspace{1cm} (3)

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$$

The classical variational principle gives the equations of motion. In our approach, where time reversal and charge conservation is considered, the Dirac equation is written as:

$$\{ -i\alpha \nabla + V(\mathbf{r}) + \beta[M + S(\mathbf{r})] \}$$  \hspace{1cm} (4)

where $V(\mathbf{r})$ represents the vector potential:

$$V(\mathbf{r}) = g_\omega \omega_0(\mathbf{r}) + g_\rho \tau_3 \rho_0(\mathbf{r}) + e \frac{1 + \tau_3}{2} A_0(\mathbf{r})$$  \hspace{1cm} (5)

and $S(\mathbf{r})$ the scalar potential:

$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r})$$  \hspace{1cm} (6)

the latter contributes to the effective mass as:

$$M^*(\mathbf{r}) = M + S(\mathbf{r})$$  \hspace{1cm} (7)
The Klein-Gordon equations for the meson fields are time-independent inhomogeneous equations with the nucleon densities as sources.

\[
\begin{align*}
\{-\Delta + m^2_\sigma\}\sigma(r) &= -g_\sigma \rho_s(r) - g_2 \sigma^2(r) - g_3^3(r) \\
\{-\Delta + m^2_\omega\}\omega_o(r) &= g_\omega \rho_v(r) \\
\{-\Delta + m^2_\rho\}\rho_0(r) &= g_\rho \rho_3(r) \\
-\Delta A_0(r) &= \epsilon \rho_c(r)
\end{align*}
\] (8)

The corresponding source terms are

\[
\begin{align*}
\rho_s &= \sum_{i=1}^{A} \bar{\psi}_i \psi_i \\
\rho_v &= \sum_{i=1}^{A} \psi_i^+ \psi_i \\
\rho_3 &= \sum_{p=1}^{Z} \psi_p^+ \psi_p - \sum_{n=1}^{N} \psi_n^+ \psi_n \\
\rho_c &= \sum_{p=1}^{Z} \psi_p^+ \psi_p
\end{align*}
\] (9)

where the sums are taken over the valence nucleons only. It should also be noted that the present approach neglects the contributions of negative-energy states (\(n\sigma - \text{sea} \) approximation), i.e. the vacuum is not polarized.

The Dirac equation is solved using the oscillator expansion method \cite{4}. For the determination of the basis wavefunctions an axially symmetric harmonic oscillator potential with size parameters

\[
\begin{align*}
b_z &= b_z(b_0, \beta_0) = \sqrt{\hbar / M \omega_z} \\
b_\perp &= b_\perp(b_0, \beta_0) = \sqrt{\hbar / M \omega_\perp}
\end{align*}
\] (10)

is employed. The basis is defined in terms of \(b_0\) and the deformation parameter \(\beta_0\). The volume conservation relates the quantities \(b_z\), \(b_\perp\) and \(b_0\) by

\[b_\perp^2 b_z = b_0^3\]

3 DETAILS OF THE CALCULATIONS

We have performed relativistic Hartree calculations for three isotopic chains. The isotopes of Kr \((Z=36)\), Sr \((Z=38)\) and Zr \((Z=40)\) have been considered.
here. As many nuclei in these chains are well deformed and involve several shape transitions, the calculations have been carried out for an axially deformed configuration for all the nuclei. Calculations for even Sr isotopes encompass mass numbers $A=70$ up to $A=110$, while the Kr isotopes cover the region between $A=72$ and $A=100$. We have also performed calculations for Zr nuclei in the region $80 \leq A \leq 110$. On the isotopic chains of Sr and Kr, several precision measurements \[15, 20, 21\] on isotopic shifts are available. For Zr isotopes, where measurements do not yet exist for the whole chain, our predictions serve to illustrate the comparison of the trend of the isotope shifts in this mass region.

For open shell nuclei, pairing has been included using the BCS formalism. In the BCS calculations we have used constant pairing gaps, which are taken from the empirical particle separation energies of neighbouring nuclei. The zero-point energy of a harmonic oscillator for the centre-of-mass energy is also included. In the present approach angular momentum and particle number projection as well as collective vibrations are neglected. It is estimated, however, that these additional features will have very small contributions.

The number of shells taken into account is 12 for both fermionic and bosonic wavefunctions. It should be noted that for convergence reasons 14 shells were also considered. It turned out, however, that the difference in the results is negligible and therefore all the calculations reported in the present work were performed in a 12 shells harmonic oscillator expansion.

In this paper we have used the recently proposed force NL-SH. This force has been shown to provide excellent results \[8\] for nuclei on both the sides of the stability line. The good value of the asymmetry energy of this force is partly responsible for a proper description of nuclei on both the proton rich and neutron rich sides. The parameters of the force NL-SH were provided in \[6\]. However, rounding off of some parameters to 3 decimal places as given in \[6\] overestimates the binding energies by a few MeV. The exact values of the force parameters were given in \[18\]. The parameters of the force NL-SH are:

\[
\begin{align*}
M &= 939.0 \text{ MeV; } m_\sigma = 526.059 \text{ MeV; } m_\omega = 783.0 \text{ MeV; } m_\rho = 763.0 \text{ MeV; } \\
g_\sigma &= 10.444; \quad g_\omega = 12.945; \quad g_\rho = 4.383; \quad g_2 = -6.9099 \text{ fm}^{-1}; \quad g_3 = -15.8337.
\end{align*}
\]

Here $g_2$ is in fm$^{-1}$ and $g_3$ is dimensionless. It should be pointed out that in refs.\[6, 18\] the dimensions of $g_2$ and $g_3$ were exchanged by mistake.
4 RESULTS AND DISCUSSION

4.1 Binding Energy

In Fig. 1 we show the binding energy per nucleon (E/A) for Kr, Sr and Zr nuclei using the force NL-SH in the RMF theory. The empirical values taken from the 1993 Atomic Mass Evaluation Tables [30] (expt.) are also shown. The figure also includes the predictions of the recent finite-range droplet model [31] (FRDM) and of the extended Thomas-Fermi with Strutinsky Integral (ETF-SI) model [32, 33] for comparison. The parabolic shapes of the binding energy per nucleon in all the three isotopic chains is depicted very well in the figure. The minimum in the binding energy is observed at the magic neutron number N=50 in the RMF as well as in the mass models. The RMF theory predicts binding energies which are in accord with the empirical values in almost all the cases. In Tables 1-3 we present the total binding energies obtained with the force NL-SH. For comparison, the empirical values [30] are also shown. The experimental binding energy of the nucleus $^{76}$Sr derives from the recent mass measurement [34] at the isotope on-line separator ISOLDE at CERN. The predicted values from the mass formulae FRDM and ETF-SI are also provided in the tables. We also show the values obtained with the RMF force NL1 and with the Skyrme force SIII [23] wherever available. In the latter case, triaxial deformations were also taken into account. The SIII results underestimate the binding of most of the nuclei by up to 6 MeV as one moves away from the closed neutron-shell nuclei.

The binding energies in the RMF are in overall agreement with the empirical data. Only for the light Kr isotopes does the RMF theory provide the binding energies which are at the most 3-4 MeV less than the empirical values. This disagreement amounts to 0.5% at the maximum. The empirical mass excess for many of the nuclei considered in our paper are not known. In the RMF theory, we predict the binding energies of these nuclei which lie mostly at the highly neutron deficient or neutron-rich sides of the isotopic chains. The calculated total binding energies in the RMF theory are also very close to those of FRDM and ETF-SI predictions within 1-2 MeV. That the FRDM and ETF-SI values are close to the empirical ones in understandable,
for these models have been fitted exhaustively to a large number of known data. In contrast, the agreement of the RMF theory with the empirical data and the model values is remarkable notwithstanding the fact that the force NL-SH was fitted only to 6 spherical nuclei at the stability line.

4.2 The Nuclear Radii and Isotope Shifts

In Fig. 2 we show the isotope shifts $r_c^2(A) - r_c^2(ref)$ for Kr, Sr and Zr nuclei calculated with respect to a reference nucleus in each chain. The semi-magic nuclei $^{86}$Kr, $^{88}$Sr and $^{90}$Zr serve as reference points. For the isotopic chains of Kr [21] and Sr [15, 20] the empirical data obtained from atomic laser spectroscopy are also shown. The experimental data for Kr and Sr nuclei exhibit a kink about the magic neutron number. This kink about the closed-shell is a characteristic feature of isotope shifts in many nuclei. This aspect has been clearly illustrated in [15]. A solution to this problem has eluded since long. It can be seen from the figure that the RMF theory is successful in reproducing this kink. In addition, the general trend which is exhibited by the data is reproduced well. That is, the magic isotopes $^{86}$Kr and $^{88}$Sr have the smallest rms charge radius in their respective chains, even when compared to nuclei 10 mass numbers lower. A similar behaviour is also predicted for Zr nuclei as can be seen from Fig. 2 (c), where empirical isotope shifts on this chain of nuclei are not known.

The absolute values of rms charge radii and neutron radii for all the three isotopic chains are presented in Fig. 3. On going from the lighter isotopes to the heavier ones, the charge radii exhibit a decreasing trend up to the magic isotopes. Clearly the lighter nuclei below the magic numbers possess higher charge radii than the heavier closed neutron-shell nucleus. This is consistent with the upward kink in the isotope shifts of lighter nuclei in Figure 2. The charge radii for nuclei heavier than the closed neutron-shell start increasing on adding further neutrons. The neutron radii, on the other hand, also show a kink about the neutron shell closure. However, the neutron radius for lighter isotopes in these chains is not higher than that of the respective closed-shell nucleus.

The isotope shifts for the Zr chain have not been measured. Here we only predict the behaviour of the isotope shifts in Zr nuclei. As seen in
Fig. 2, the isotope shifts in Zr nuclei also show a behaviour much similar to that shown by Sr and Kr nuclei. For, isotope shifts are closely related to shapes and deformation properties, all the three chains of nuclei seem to exhibit a similar pattern in their spatial properties. We will discuss the deformation properties in the ensuing subsection. Here we compare in Fig. 4 our predictions for the isotope shifts of Zr nuclei with those obtained with the Skyrme force SIII in [23]. The Skyrme approach gives practically a straight line. A similar feature was also observed [17] for the Pb isotopes both with SkM* and SIII. Thus, the Skyrme mean-field approach shows a trend very different from that of the empirical data and the RMF theory.

In Figure 5 we show the neutron skin thickness $r_n - r_p$ for Zr isotopes obtained in the RMF theory using the force NL-SH. We also compare these results with those from NL1. It may be noted that the force NL1 was used earlier in [27] to calculate the properties of neutron-rich Zr isotopes. Clear differences in the neutron-skin thickness for NL-SH and NL1 can be seen with an increase in neutron excess. This can be attributed primarily to the large asymmetry energy of 44 MeV of NL1. The asymmetry energy of NL-SH is 36 MeV, which is close to the empirical value of about 33 MeV. The kink seen in the neutron-skin thickness for the force NL1 at $A=100$ arises due to the spherical shapes predicted by NL1 about this mass.

In Fig. 5 we also show the neutron-skin thickness obtained from the density-dependent Skyrme force SIII, taken from [23]. For nuclei close to the symmetric nucleus $^{80}$Zr, SIII gives neutron-skin thickness similar to those of NL-SH and NL1. However, for nuclei with large neutron excess the values from SIII are much smaller than those of NL-SH and NL1. This is due to the fact that the force SIII provides neutron-rich Zr nuclei which have a larger charge radius and a smaller neutron radius as compared to the RMF forces.

### 4.3 Deformations

We have performed calculations in the RMF theory for both the prolate and oblate configurations. Our results predict deformed shapes for a large number of isotopes for all the three chains. The deformations of nuclei have been obtained from the relativistic Hartree minimization. We show in Fig. 6 the quadrupole deformation $\beta_2$ for the shape corresponding to the lowest
energy. The predictions of FRDM and ETF-SI are also shown for comparison. In all the three isotopic chains, the RMF theory gives a well-defined prolate shape for lighter isotopes. Further, an addition of a few neutrons below the closed neutron shell leads to an oblate shape in all the three cases. These shapes turn into spherical ones as nuclei approach the magic neutron number N=50. Nuclei above this magic number revert again to the prolate shape in the RMF theory. Thus, in all the three isotopic chains a shape transition from prolate-oblate-spherical-prolate is followed. Only in the Kr isotopes, the very heavy Kr nuclei assume an oblate shape. The very neutron-rich Sr and Zr nuclei, on the other hand, retain a highly deformed prolate shape.

In addition to the lowest minimum, several isotopes exhibit a second minimum, thus implying a shape-coexistence, i.e., the prolate and the oblate shapes differ in the energy only by a few hundred keV. These nuclei have been shown by squares surrounding the black circles. Our calculations predict two minima for several heavy Sr nuclei, the prolate shape results being a few hundreds keV lower in energy than the oblate one. This is displayed in Fig. 7, where the difference in the ground-state binding energy of the oblate and the prolate configurations is shown. It can be noticed that Sr isotopes beginning with A=92 acquire a prolate shape predominantly. For nuclei close to A=98, the prolate shape is lower than the oblate one only by about 300 keV. With a further increase in the neutron number the Sr isotopes take up the prolate minimum, the oblate shape being about 600-800 keV higher. The undulation in the prolate-oblate energy differences of neutron-rich Sr isotopes is a noteworthy feature of the RMF prediction.

As seen from Fig. 6 (b), most of the Sr isotopes acquire a deformed shape except those close to the neutron number N=50. This is in marked contrast with earlier calculations [26] using the force NL1, where spherical shapes were obtained for a large number of Sr nuclei. This has also been the case for many Zr isotopes in a previous work [27] with the force NL1 where spherical shapes were predicted. This is significantly different from the results of the Zr isotopes with the force NL-SH as shown in Fig. 6 (c), where large deformations and shape-transitions have been observed. Experimentally, nuclei in this region are susceptible to gaining very large deformations. Sr nuclei are a good case of such a property and the onset of deformation in nuclei close to A=100 is now well known [15]. The strong empirical onset of
deformation in the Mo chain [35] is being exhibited also by our Sr and Zr results with the force NL-SH.

A comparison of our results with those of the FRDM shows that by and large there is a reasonable agreement between the $\beta_2$ values of NL-SH and the predictions of FRDM. The striking difference between the two is that a shape transition from prolate to oblate in the lighter Sr and Zr nuclei in the RMF theory is not given by the FRDM. The FRDM, in contrast, provides a shape transition from prolate to about spherical on approaching the magic neutron number in these two chains. Nuclei heavier than semi-magic Sr and Zr isotopes are predicted to take up highly deformed prolate shapes in the FRDM. This is consistent with our results using NL-SH. The scenario with the Kr chain is slightly different from the other two. In the beginning of this chain at $A=72$, the RMF as well as FRDM show an additional shape transition from oblate to prolate. The shape transition from prolate-oblate-spherical-prolate is provided in both the RMF and the FRDM. Only for very heavy Kr isotopes, nuclei in the FRDM assume a highly deformed prolate shape, as against the oblate shape predicted by the RMF.

The ETF-SI model [36] also predicts deformation properties of a large number of nuclei all over the periodic table. The $\beta_2$ values for all the three isotopic chains are shown in Fig. 6. A peculiar feature of the ETF-SI predictions is that on going from light nuclei to the heavier ones, one encounters a shape transition from prolate to oblate, oblate to spherical, and then again spherical to oblate for both the Sr and Zr isotopic chains. The latter shape transition from spherical to oblate, which is predicted by ETF-SI in all the three chains, is not supported by our results nor by the predictions of the FRDM. For heavier nuclei, ETF-SI shows a transition from oblate to prolate directly without going first to a spherical shape. Moreover, for the very light Kr isotopes, ETF-SI provides only a very deformed oblate shape, in contrast with the results of RMF and FRDM. However, shape transition from prolate to oblate in the Kr chain at $A=92$ is consistent with the one obtained in the RMF theory. At this point, the FRDM predicts only a prolate shape for the heavy Kr nuclei. Thus, the significant discrepancy between the ETF-SI on one hand and RMF and FRDM on the other hand, lies in the shape transition from prolate to oblate for heavier isotopes in all the three chains in ETF-SI, which is not present in the other two approaches.
The \( \beta_2 \) values from NL-SH, FRDM and ETF-SI are shown in Tables 4-6. The \( \beta_2 \) values for the second minimum obtained for Kr and Sr isotopes with the force NL-SH are shown in the parentheses. A comparison of the magnitudes of the deformation for all the three isotopic chains shows that the three approaches provide values close to each other. In addition, we have also performed calculations with the RMF force NL1 for Sr and Zr isotopes. The resulting \( \beta_2 \) values are shown in Tables 5 and 6. Furthermore, we also include for comparison \( \beta_2 \) values available for Zr isotopes using the Skyrme force SIII and taken from [23]. The experimental quadrupole deformations obtained from BE(2) values taken from [35] are shown in the last columns of the tables. It may be noted that these empirical \( \beta_2 \) values do not indicate any signature as to ascertain the shape of a given nucleus. The absolute values, however, do compare well with the RMF predictions.

5 SUMMARY AND CONCLUSIONS

The RMF theory has been employed to obtain the ground-state properties of the isotopic chains of Kr, Sr and Zr nuclei. This region of nuclei which entails several dramatic transformations of shapes has not been amenable to an appropriate description in the conventional approaches such as the density-dependent Skyrme Hartree-Fock theory. Nuclei in this region exhibit anomalous behaviour in the isotope shifts, resulting in rms charge radii of lighter isotopes being larger than the heavier closed neutron-shell counterparts with \( N=50 \). This is a generic feature of many isotopic chains in this region, and is attributable primarily to the shape transitions very common in this region. The RMF theory with the force NL-SH renders a successful description of the general behaviour of the isotopic shifts in Kr and Sr chains. It also predicts a similar trend for Zr chain where empirical data do not yet exist and measurements are required. It is noteworthy that for the first time a microscopic theory is able to describe the empirical data on the isotope shifts. This success of the RMF theory should be viewed in conjunction with its ability to describe [18] also the kink in the isotope shifts across shell-closure in Pb nuclei.

A non-relativistic reduction of the RMF Hamiltonian shows [14] that the isospin dependence of the spin-orbit interaction which stems naturally in the
RMF theory as a consequence of the Lorentz covariance and Dirac structure of nucleons is not contained in the density-dependent Skyrme theory. Consequently all attempts in the Skyrme theory including a plausible influence of the ground-state correlations have failed to explain the anomalous kinks in the isotope shifts of Pb nuclei and nuclei in the Z=40 region.

Deformation properties of nuclei are pivotal to the successful description of the isotope shifts. The deformations which bring about the anomalous isotope shifts, are generally in good agreement with the $\beta_2$ values obtained from the BE(2) measurements. The RMF theory predicts prolate-oblate shape coexistence in heavy Sr nuclei. The shape-coexistence in a few Kr isotopes has also been shown. The RMF theory also predicts several shape transitions along the mass chains. Many of these shape changes are contained in either one or the other of the FRDM and ETF-SI mass formulae. ETF-SI deformations in many cases are just opposite to the predictions of the RMF and the FRDM. This fact is consequently reflected in the difficulty of the Skyrme approach to describe the isotope shifts on Sr and Kr nuclei.

The binding energies of nuclei in all the chains considered here have been described successfully in the RMF theory. The deviations in the binding energies from the empirical values are at the most 0.5%. The parabolic behaviour of the binding energy per nucleon has been obtained for all the chains. This is consistent with the empirical curves and also with the extensive mass fits of FRDM and ETF-SI. The agreement manifests the degree of the success of the RMF predictions even with a force obtained from a limited adjustment only on 6 nuclei. In conjunction with good description of the deformations and isotope shifts, the RMF theory provides a unified description of the ground-state properties of nuclei over a large range of isospin.

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Table 1: The binding energy (MeV) of Kr isotopes obtained with the force NL-SH. The predictions from the mass models FRDM [31] and ETF-SI [33] are also shown for comparison. A comparison has also been made with the binding energies in the Skyrme approach [23] with the force SIII, wherever available. The empirical values [30] are shown in the last column.

| A  | NL-SH   | FRDM   | ETF-SI  | SIII   | expt.   |
|----|---------|--------|---------|--------|---------|
| 70 | 575.87  | 578.33 | 577.28  | -      | 577.80  |
| 72 | 604.00  | 607.00 | 605.02  | -      | 607.11  |
| 74 | 628.49  | 631.99 | 630.13  | 626.42 | 631.28  |
| 76 | 651.64  | 654.82 | 653.56  | 648.90 | 654.23  |
| 78 | 672.69  | 675.56 | 675.23  | -      | 675.55  |
| 80 | 693.45  | 695.05 | 695.35  | -      | 695.43  |
| 82 | 713.39  | 714.57 | 714.26  | -      | 714.27  |
| 84 | 733.16  | 732.69 | 732.12  | -      | 732.26  |
| 86 | 750.06  | 748.97 | 748.79  | -      | 749.23  |
| 88 | 760.08  | 761.22 | 761.21  | -      | 761.80  |
| 90 | 769.89  | 771.95 | 772.60  | 769.42 | 773.21  |
| 92 | 779.84  | 782.35 | 782.25  | -      | 783.22  |
| 94 | 789.88  | 791.89 | 791.18  | -      | 791.76  |
| 96 | 799.46  | 800.85 | 799.33  | -      | 799.95  |
| 98 | 807.51  | 808.87 | 806.79  | 804.64 | -       |
| 100| 814.02  | 815.68 | 813.37  | 811.44 | -       |
Table 2: The binding energies for Sr isotopes. See the caption of Table 1 for details. In addition, the binding energies obtained in the RMF with the force NL1 are also shown.

| A   | NL-SH | NL1  | FRDM | ETF-SI | SIII | expt. |
|-----|-------|------|------|--------|------|-------|
| 70  | 542.39| -    | 543.98| 545.40 | -    | -     |
| 72  | 574.69| 579.51| 577.48| 577.70 | -    | -     |
| 74  | 606.74| 608.59| 609.17| 607.99 | 603.97| -     |
| 76  | 635.95| 638.35| 638.66| 636.47 | 633.56| 638.08|
| 78  | 661.71| 663.40| 663.90| 662.13 | 658.53| 663.01|
| 80  | 683.76| 688.35| 684.82| 685.56 | 680.74| 686.28|
| 82  | 705.86| 710.03| 707.62| 707.58 | -    | 708.13|
| 84  | 726.79| 730.51| 729.15| 728.51 | -    | 728.90|
| 86  | 748.81| 750.54| 749.43| 748.73 | 747.70| 748.92|
| 88  | 767.96| 768.84| 768.09| 767.88 | 768.99| 768.46|
| 90  | 779.76| 780.38| 781.81| 781.74 | 780.35| 782.63|
| 92  | 792.05| 791.60| 794.07| 794.85 | 791.05| 795.75|
| 94  | 803.83| 802.87| 806.53| 806.34 | 802.23| 807.81|
| 96  | 814.87| 813.74| 818.13| 817.16 | 813.41| 818.10|
| 98  | 826.60| 823.08| 828.98| 827.82 | 825.45| 827.87|
| 100 | 835.63| 832.09| 838.70| 837.22 | 834.77| 837.62|
| 102 | 844.71| 841.50| 847.24| 845.57 | 843.42| 846.62|
| 104 | 852.56| 848.80| 855.14| 852.79 | -    | -     |
| 106 | 859.77| -     | 862.58| 859.22 | -    | -     |
| 108 | 865.61| -     | 868.78| 864.69 | -    | -     |
| 110 | 870.50| -     | 873.46| 869.45 | -    | -     |
Table 3: The binding energies for Zr isotopes. See the caption of Table 2 for details.

| A  | NL-SH  | NL1   | FRDM  | ETF-SI | SIII  | expt. |
|----|--------|-------|-------|--------|-------|-------|
| 80 | 667.20 | 668.85| 669.26| 666.99 | 663.73| 669.75|
| 82 | 691.39 | 697.52| 692.30| 692.53 | 688.30| 694.74|
| 84 | 715.79 | 720.72| 717.23| 716.89 | 713.11| 718.19|
| 86 | 738.91 | 744.11| 740.80| 740.38 | 737.44| 740.65|
| 88 | 762.02 | 766.09| 763.18| 762.78 | 761.21| 762.61|
| 90 | 784.42 | 785.69| 784.11| 783.94 | 784.41| 783.89|
| 92 | 797.19 | 799.91| 799.43| 799.55 | 797.51| 799.72|
| 94 | 811.62 | 812.16| 813.42| 813.94 | 810.04| 814.68|
| 96 | 825.43 | 824.64| 827.25| 827.51 | 823.08| 828.99|
| 98 | 838.07 | 835.94| 840.74| 840.10 | 835.88| 840.96|
| 100| 851.40 | 847.98| 853.37| 852.43 | 849.25| 852.44|
| 102| 862.83 | 858.58| 864.82| 863.70 | 860.23| 863.72|
| 104| 872.79 | 868.44| 875.02| 873.82 | 870.61| 874.46|
| 106| 882.27 | 876.62| 884.43| 882.76 | -     | 884.45|
| 108| 891.00 | 884.68| 893.38| 890.75 | -     | -     |
| 110| 898.28 | 890.74| 901.17| 897.90 | -     | -     |
Table 4: The quadrupole deformations $\beta_2$ for Kr isotopes obtained in the RMF theory using the force NL-SH. The FRDM and ETF-SI predictions are also shown. The available empirical deformations (expt.) obtained from BE(2) values are also given in the last column. The experimental values do not depict the signature of the deformation. The deformations of nuclei showing a shape coexistence with a second minimum are given in the parentheses.

| A   | NL-SH   | FRDM   | ETF-SI | expt. |
|-----|---------|--------|--------|-------|
| 72  | -0.298  | -0.349 | -0.40  | -     |
| 74  | 0.441(-0.318) | 0.400 | -0.30  | 0.387 |
| 76  | 0.431(-0.267) | 0.400 | -0.30  | 0.408 |
| 78  | -0.222(0.339) | -0.232 | -0.30  | 0.343 |
| 80  | -0.204  | 0.002  | -0.30  | 0.265 |
| 82  | 0.110   | 0.071  | 0.18   | 0.202 |
| 84  | 0.0     | 0.062  | 0.15   | 0.149 |
| 86  | 0.0     | 0.053  | -0.04  | 0.145 |
| 88  | 0.049   | 0.062  | -0.13  | -     |
| 90  | 0.175(-0.175) | 0.162 | 0.15   | -     |
| 92  | 0.228(-0.224) | 0.228 | -0.21  | -     |
| 94  | -0.264  | 0.310  | -0.29  | -     |
| 96  | -0.298  | 0.337  | -0.31  | -     |
| 98  | -0.292  | 0.349  | 0.36   | -     |
| 100 | -0.284  | 0.350  | 0.38   | -     |
Table 5: The quadrupole deformations $\beta_2$ for Sr isotopes. See Table 4 for details. The values obtained from the RMF force NL1 are also shown here.

| A  | NL-SH | NL1   | FRDM | ETF-SI | expt. |
|----|-------|-------|------|--------|-------|
| 72 | 0.324 | -0.205| 0.371| -0.30  | -     |
| 74 | 0.430 | 0.432 | 0.400| 0.44   | -     |
| 76 | 0.450 | 0.464 | 0.421| 0.44   | -     |
| 78 | 0.450 | 0.456 | 0.421| 0.43   | 0.434 |
| 80 | 0.402 | 0.0   | 0.053| 0.40   | 0.377 |
| 82 | -0.200| 0.0   | 0.053| -0.30  | 0.290 |
| 84 | 0.089 | 0.0   | 0.053| 0.15   | 0.211 |
| 86 | 0.0   | 0.0   | 0.053| 0.00   | 0.128 |
| 88 | 0.0   | 0.0   | 0.045| 0.00   | 0.117 |
| 90 | 0.0   | 0.0   | 0.045| -0.11  | -     |
| 92 | 0.181(-0.165) | 0.097 | 0.080 | -0.15  | -     |
| 94 | 0.230(-0.218) | -0.187(0.180) | 0.255 | -0.19  | -     |
| 96 | 0.356(-0.275) | -0.242(0.207) | 0.338 | 0.35   | -     |
| 98 | 0.424(-0.309) | -0.218(0.459) | 0.357 | 0.39   | 0.354 |
| 100| 0.426(-0.314) | -0.194(0.439) | 0.368 | 0.38   | 0.372 |
| 102| 0.413(-0.295) | -0.172 | 0.369 | 0.40   | -     |
| 104| 0.403(-0.277) | -0.139 | 0.361 | 0.38   | -     |
Table 6: The quadrupole deformations $\beta_2$ for Zr isotopes. See Table 5 for details. The values from the Skyrme force SIII are also given.

| $^A$Zr | NL-SH | NL1 | SIII | FRDM | ETF-SI | expt. |
|-------|-------|-----|------|------|--------|-------|
| 80    | 0.463 | 0.466 | 0.490 | 0.433 | 0.45   | -     |
| 82    | 0.429 | 0.0  | -0.210 | 0.053 | 0.41   | -     |
| 84    | -0.201 | 0.0  | 0.0   | 0.053 | -0.26  | 0.250 |
| 86    | -0.145 | 0.0  | 0.0   | 0.053 | 0.00   | 0.149 |
| 88    | 0.0   | 0.0  | 0.0   | 0.053 | 0.00   | 0.187 |
| 90    | 0.0   | 0.0  | 0.0   | 0.035 | 0.00   | 0.091 |
| 92    | 0.099 | 0.0  | 0.0   | 0.053 | 0.00   | 0.102 |
| 94    | 0.197 | 0.0  | 0.232 | 0.062 | 0.02   | 0.090 |
| 96    | 0.243 | 0.0  | 0.232 | 0.217 | -0.19  | 0.081 |
| 98    | 0.337 | 0.0  | 0.344 | 0.330 | -0.27  | -     |
| 100   | 0.397 | 0.453 | 0.425 | 0.358 | 0.36   | 0.321 |
| 102   | 0.404 | 0.427 | 0.438 | 0.369 | 0.380  | 0.421 |
| 104   | 0.402 | 0.418 | 0.440 | 0.381 | 0.40   | -     |
Figure Captions.

**Fig. 1** The binding energy per nucleon for Kr, Sr and Zr isotopes in the RMF theory with the force NL-SH. The predictions from the mass models FRDM and ETF-SI are also shown for comparison. The RMF binding energies exhibit a clear parabolic behaviour with the mass number and compare reasonably well with the empirical data (expt).

**Fig. 2** The isotope shifts for Kr, Sr and Zr nuclei calculated with the force NL-SH. The experimental isotope shifts for Kr \(^{34}\) and Sr \(^{13,20}\) nuclei are also shown. The prediction for Zr isotope shifts is very similar to the behaviour of the Kr and Sr nuclei.

**Fig. 3.** The rms charge and neutron radii of Kr, Sr and Zr isotopic chains obtained in the RMF theory using the force NL-SH.

**Fig. 4.** The isotope shifts for Zr nuclei in the RMF theory compared with the prediction of the Skyrme force SIII.

**Fig. 5.** The neutron-skin thickness of Zr isotopes in the RMF theory with the forces NL-SH and NL1. The NL1 values are higher than those of NL-SH due to the correspondingly high asymmetry energy of NL1 as compared to that of NL-SH and the empirical value. The predictions of the Skyrme force SIII are even lower than the NL-SH values (see text for details).

**Fig. 6.** The quadrupole deformation \(\beta_2\) obtained from relativistic Hartree minimization for Kr, Sr and Zr isotopes using the force NL-SH. The predictions of the mass models FRDM and ETF-SI are displayed for comparison. Nuclei exhibiting a shape coexistence and thus a second minimum in the RMF theory are depicted by a square surrounding the \(\beta_2\) value of the lowest minimum. Several shape transitions in all the three isotopic chains emerge as the characteristic feature of the deformation properties in the RMF theory.

**Fig. 7.** The prolate-oblate shape coexistence for neutron-rich Sr isotopes predicted in the RMF theory. The energy difference in the prolate and oblate minima for Sr isotopes is shown. Most of the nuclei in the neutron-rich domain possess a prolate minimum. An oblate second minimum lies only a few hundred keV higher in energy.