Multi-deformed Configurations and Shape Coexistence for Superheavy Elements *

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Abstract

We use the considered axial deformed relativistic mean field theory to perform systematical calculations for $Z = 112$ and 104 isotopic chains with force parameters NL3, NL-SH and NL-Z2 sets. Three deformed chains (oblate, moderate prolate and super-deformed chain) are found for $Z = 112$ and 104 isotopic chains. It is found that there is a chain of super-deformed nuclei which can increase the stability of superheavy nuclei in the $Z = 112$ isotopic chain. Shape coexistence is found for $Z = 112, 104$ isotopic chain and the position is defined. For moderate prolate deformed chains of $Z = 112$ and 104, there is shell closure at $N = 184$ for moderate prolate deformed chain. For oblate deformed chain of $Z = 112$, the shell closure appears around at $N = 176$. For super-deformed chains of $Z = 112$ and 104, the position of shell closure have strong parameter dependence. There is shell anomalism for oblate or superdeformed nuclei.

Key words: relativistic mean field, superheavy element, deformed configuration, shape coexistence, superdeformed chain

1 Introduction

Since the possible existence of superheavy elements was predicted in 1960s by nuclear theoreticians, the search of superheavy elements in nature has become a hot topic for scientists. Empirically, many heavy elements were identified by nuclear synthesis. At first, the elements $Z = 105 \sim 108$ were successfully produced and both physicists and chemists agree on the existence of these elements although their half-lives are not very long. During 1995 $\sim$ 1996, because of the participating of more and more large laboratories in researches of new elements, the elements $Z = 110 \sim 112$ were produced by Hofmann et al. at GSI in Germany[1-3]. $Z = 114$ was produced by Oganessian et al. at Dubna in Russia in 1999[4,5]. One year later it was again reported that $Z = 116$ was synthesized at Dubna[6]. Recently, $^{288}115$ and $^{287}115$ were synthesized at FLNR, JINR[7]. The achievement in producing new elements speeds up the researches on superheavy nuclei not only in experiment but also in theory. Theoretically, several models have been used and many aspects such as the collisions, structure, and stability have been investigated [8-18] for heavy and superheavy elements.

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Recently, there are systematically calculations for superheavy elements within the framework of deformed relativistic mean-field (RMF) theory \[21-23\]. These calculations predicted that there are shape coexistence and super-deformation in the ground state of superheavy nuclei and deformation can be an important cause for the stability of superheavy nuclei based on a constraint RMF calculation. The conclusion changes the usual conception that the existence of superheavy elements is due to their spherical shell structure and makes people recognize that deformed configurations are as important as the spherical one for stability of superheavy elements in theory.

However, the constraint RMF calculation consumes much time, thus the calculation is very limited. Although there are many systematical calculations for superheavy nuclei which find there are a moderate prolate solution, an oblate solution, and a superdeformed prolate solution for the same element \[22, 23\], there is no calculation which can give out deformed configurations of a whole isotopic chain. No information tells us that whether there are two or more deformed configurations for most of the nuclei in a whole isotopic chain or only exist in a few nuclei in the isotopic chain. Our aim is to study these properties in a long isotopic chain. Thus, we select \( Z = 104 \) and \( Z = 112 \) isotopic chains and carry out systematical calculation within the framework of deformed relativistic mean-field (RMF) theory. The binding energy, quadrupole deformation, root mean square radii, shape coexistence and shell closure are the investigative projects.

2 The formalism of the relativistic mean-field theory

The relativistic mean-field theory has been widely used to describe finite nuclei, in the RMF method, the local Lagrangian density is given as\[24, 25\]

\[
\mathcal{L} = \bar{\psi} (i \gamma^\mu \partial_\mu - M) \psi - g_\sigma \bar{\psi} \gamma^\mu \sigma \psi - g_\omega \bar{\psi} \gamma^\mu \omega \psi - g_\rho \bar{\psi} \gamma^\mu \rho \psi \\
+ \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{3} g_2 \sigma^3 - \frac{1}{4} g_3 \sigma^4 \\
- \frac{1}{4} \Omega^{\mu \nu} \Omega_{\mu \nu} + \frac{1}{2} m_\omega \omega^{\mu \nu} \omega_\mu - \frac{1}{4} R^{a \mu \nu} R^a_{\mu \nu} + \frac{1}{2} m_\rho \rho^{a \mu} \rho^a_\mu \\
- \frac{1}{4} F^{\mu \nu} F_{\mu \nu} - e \bar{\psi} \gamma^0 A^0 \frac{1}{2} (1 - \tau^3) \psi. (1)
\]

The meson fields included are the isoscalar \( \sigma \) meson, the isoscalar-vector \( \omega \) meson and the isovector-vector \( \rho \) meson. \( M, m_\sigma, m_\omega \) 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 isospin Pauli matrices are written as \( \tau^a, \tau^3 \) being the third component of \( \tau^a \). The field tensors of the vector mesons and of the electromagnetic fields take the following form:

\[
\Omega^{\mu \nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu, \\
R^{a \mu \nu} = \partial^\mu \rho^{a \nu} - \partial^\nu \rho^{a \mu}, \\
F^{\mu \nu} = \partial^\mu A^\nu - \partial^\nu A^\mu. (2)
\]

The variational principle gives the equations of motion. For the static case the meson fields and photon field operators are assumed to be classical fields and they are time independent. They are replaced by their expectation values. The symmetries of the system simplify the calculations considerably. In all the systems considered in this work, there exists time reversal symmetry, so there are no currents in the nucleus and therefore the spatial vector components of \( \omega^\mu, \rho^{a \mu} \) and \( A^\mu \) vanish. This leaves only the time-like components, \( \omega^0, \rho^{0 \mu} \) and \( A^0 \). Charge
conservation guarantees that only the 3-component of the isovector \( \rho^{00} \) survives. Finally we have the following Dirac equation for the nucleon:

\[
\{-i\alpha \nabla + V(r) + \beta [M + S(r)]\} \psi_i = \varepsilon_i \psi_i, \tag{3}
\]

where \( V(r) \) is the vector potential

\[
V(r) = g_\omega \omega^0(r) + g_\rho \tau^3 \rho^{00} + e \frac{1 + \tau^3}{2} A^0(r), \tag{4}
\]

and \( S(r) \) is the scalar potential

\[
S(r) = g_\sigma \sigma(r). \tag{5}
\]

The Klein-Gordon equations for the mesons and the electromagnetic fields with the densities as sources are

\[
\{-\Delta + m^2\} \sigma(r) = -g_\sigma \rho_s(r) - g_2 \sigma^2(r) - g_3 \sigma^3(r), \tag{6}
\]

\[
\{-\Delta + m^2\} \omega_0(r) = g_\omega \rho_v(r), \tag{7}
\]

\[
\{-\Delta + m^2\} \rho_{00}(r) = g_\rho \rho_3(r), \tag{8}
\]

\[-\Delta A^0(r) = e \rho_c(r). \tag{9}\]

The corresponding densities are

\[
\rho_s(r) = \sum_{i=1}^A \bar{\psi}_i(r) \psi_i(r), \tag{10}
\]

\[
\rho_v(r) = \sum_{i=1}^A \psi_i^\dagger(r) \psi_i(r), \tag{11}
\]

\[
\rho_3(r) = \sum_{i=1}^A \psi_i^\dagger(r) \tau^3 \psi_i(r), \tag{12}
\]

\[
\rho_c(r) = \sum_{i=1}^A \psi_i^\dagger(r) ((1 - \tau^3)/2) \psi_i(r). \tag{13}
\]

Now we have a set of coupled equations for mesons and nucleons and they will be solved consistently by iterations.

### 3 Numerical calculation and analysis

The validity of deformed relativistic mean-field (RMF) theory in the calculation for superheavy nuclei is tested in previous papers\cite{21-23}, so we do not test the validity any more in our work. In the process calculation, three typical sets of force parameters NL3\cite{19}, NL-SH\cite{20}, and NL-Z2\cite{10} in RMF model are chosen. The method of harmonic basis expansions is used in solving the coupled RMF equations. The number of bases is chosen as \( N_f = 12, N_b = 20 \). Pairing has been included using the BCS formalism. In the BCS calculations we have used constant pairing gaps \( \Delta_n = \Delta_p = 11.2/\sqrt{A} \text{ MeV}^{[30]} \). This input of pairing gaps is used in nuclear physics for many years. Although the BCS model may fail for light neutron-rich nuclei, the nuclei studied here are not light neutron-rich nuclei and the RMF results with BCS treatment should be reliable. The different inputs of \( \beta_0 \) lead to different iteration numbers of the self-consistent calculation and different computational time, but physical quantities such as the binding energy and the deformation do not change much, which is tested in Ref.\cite{22}. Thus, when we carry out calculation, we only choose a proper initial \( \beta_0 \) and neglect its effect on our results.

3
3.1 Quadrupole deformation

The quadrupole deformation of isotopic chain $Z = 112$, $160 \leq N \leq 200$ with the force parameters NL3, NL-SH and NL-Z2 are listed in figure 1. There are three deformed chains 1, 2 and 3, denoted with circle, triangle and star respectively, which can be seen for all the force parameters NL3, NL-SH and NL-Z2 in figure 1. 1 is an oblate chain, the quantities of quadrupole deformation $\beta_2 \leq -0.3$. 2 is a moderate or light prolate deformed chain except that there is light oblate deformation in the NL-Z2 calculation when $N \geq 186$. It is very interesting that 3 is a super-deformed chain with $\beta_2 \geq 0.4$. The phenomenon of several deformed configurations for a single superheavy element is predicted in Refs.[22, 23] with constraint RMF calculation. In our work, it is the first time to obtain several deformed chains in a isotopic chain without using any constraint RMF calculations at all.

Is it a general phenomenon that there are several deformed chains for a isotopic chain of superheavy elements? To answer this question, we also perform RMF calculation for $Z = 104$, $152 \leq N \leq 198$ isotopic chain. The results are shown in figure 1 as well. All the results of the force parameters (NL3, NL-SH, and NL-Z2) show three deformed chains (oblate, moderate prolate and super-deformed prolate deformation ) for the $Z = 104$ isotopic chain as well as $Z = 112$. Although there are three deformed bands for the $Z = 104$ isotopic chain, the super-deformed configurations appear with neutron number $N \geq 168$ (for NL3 and NL-Z2 calculation) or $N \geq 170$ (for NL-SH calculation). The oblate deformation appears in the region of $N \leq 168$ for NL3 calculation, $N \leq 170$ for NL-SH calculation, however, it appears in the whole region of $Z = 104$ isotopic chain for the NL-Z2 calculation. Why oblate deformation does not appear in the whole region for NL3 and NL-SH calculations? Obleate deformed configurations which are predicted by NL-Z2 set but not by NL3 and NL-SH sets in the region. Are they physical solutions? In figure 1, we see there is a sudden change at $N = 176$ in the oblate chain for the NL-Z2 calculation, when $N \geq 178$ the oblate deformation changes gradually with the variation of the neutron number. It indicates that the results of NL-Z2 calculation in the region $N \geq 178$ are physical solutions. The NL-Z2 set may be better than the other parameters in describing the deformation in larger neutron region. From the above mentioned analysis, we conclude that it is a general phenomenon that there are several deformed configurations for a isotopic chain of superheavy elements, and that the super-deformed nuclei can exist in the superheavy elements. Since there are several deformed configurations for the superheavy elements, is there shape coexistence in a superheavy element? This phenomenon will be discussed in the subsection 3.3 in detail.

From figure 1, we can see there are minima or maxima in the deformed chains. In super-deformed chain of $Z = 112$, the minimum appears at $N = 172$ for NL3, $N = 168$ for NL-SH and $N = 176$ for NL-Z2, and the maximum appears at $N = 182$ for all the force parameters. And in super-deformed chain of $Z = 104$, there is no minima for NL3; for NL-SH, the minimum is at $N = 188$; for NL-Z2, sudden changes occur at $N = 182, 184$, which is the very minimum. In the moderate deformed chain of both $Z = 112$ and $Z = 104$, the minimum appears at around $N = 184$ for all the three parameters. In oblate chain of $Z = 112$, there is a maximum at $N = 176$ for all the force parameters. There is no obvious kink for NL3 and NL-SH calculation in oblate chain of $Z = 104$, but there is a large peak at $N = 176$ and a small peak at $N = 190$ for NL-Z2 calculation. Generally the minimum of the prolate deformed chain and the maximum or peak of oblate deformed chain correspond to shell closure. In the moderate deformed chain, the minimum ($\beta_2 \approx 0$) appears at $N \simeq 184$, which agrees with the prediction in refs.[10, 31–35] that spherical neutron shell closures occur at $N = 184$. For superdeformed heavy nuclei the shell closures depend on the force parameters. There is strong trend that shell closure occurs
at $N = 176$ for $Z = 112$ in the oblate deformed chain, for all the parameters giving a peak at $N = 176$. If the minimum or maximum is the sign of shell closure, the above analysis indicates that the positions of shell closure for the super-deformed and oblate deformed nuclei are different from that of spherical nuclei and have strong parameter dependence. We believe that there may be shell anomalism in oblate and super-deformed prolate superheavy nuclei. In fact, the phenomenon of shell anomalism is predicted in some Refs.$^{[36-38]}$.

3.2 Root mean square radii (rms)

The root mean square (rms) radii are the project of investigation, for they contain a lot of important information of ground state properties. In figure 2, the rms radii of oblate, moderate prolate and super-deformed prolate configurations with NL3, NL-SH and NL-Z2 for the isotopic chains of $Z = 112, 104$ are listed. The solid symbol stands for neutron and empty symbol stands for proton radii. The circles, up triangles and down triangles denote the oblate, moderate prolate and super-deformed configuration respectively.

In figure 2, it is seen that there is a gap $0.15 \sim 0.38 fm$ for $Z = 112$ and $0.17 \sim 0.45 fm$ for $Z = 104$ isotopic chain between neutron rms radii and proton rms radii of the same deformed configuration for all the force parameters. The gap become larger and larger with the increasing of the neutron number. For the three parameters NL3, NL-SH and NL-Z2, if we select the rms radii of NL3 as the standard, the NL-SH calculation underestimates the rms radii about $0.05 fm$ and the NL-Z2 calculation overestimates the rms radii about $0.1 fm$ in the same deformed configuration for both $Z = 112$ and $Z = 104$ isotopes. We also can see three obvious chains of rms radii for the three deformed configurations respectively in figure 2.

For $Z = 112 \ (160 \leq N \leq 200)$ isotopic chain, NL3, NL-SH and NL-Z2 calculations show that the rms radii of moderate prolate deformed configuration are the smallest among the three deformed ones, and the rms radii of super-deformed one are the largest in the region $N \leq 190$, namely, nuclei with large absolute values $\beta_2$ tend to have larger rms radii in this region, however, when $N \geq 192$ the rms radii of oblate deformation are the largest. The gap of rms radii between the different deformed configurations is about $0.1 \sim 0.2 fm$ in general. For moderate prolate deformed configuration, there are obvious kinks in the proton rms radii at $N = 184$, which agrees with the results in subsection 3.1 that there is shell closure at $N=184$. For oblate deformed one, the calculation of NL3, NL-SH and NL-Z2 shows kink in the proton rms radii at $N = 176$, but the NL-Z2 calculation is not very obvious. Together with the prediction of subsection 3.1, we are convinced that there is shell closure at $N = 176$ for oblate deformed configuration. Finally, for super-deformed configuration, the NL3 and NL-SH calculations show kinks at $N \simeq 168, 184$ in the proton rms radii, and the kink appears at $N \simeq 190$ for NL-Z2, there also are obvious kinks at $N \simeq 186$ for NL3 and NL-SH at $N \simeq 192$ in proton rms radii. In summary, the characters of shell closure for super-deformed configuration are not very obvious in the region $N < 184$, and have strong parameter dependence. There are some sudden changes at $N = 198, 200$ for moderate prolate deformed configuration, at $N = 196, 198, 200$ for super-deformed one with NL-SH calculation and at $N = 198, 200$ for oblate deformed configuration with NL-Z2 calculation. The anomalism maybe come from the validity of the force parameter in these regions.

For $Z = 104 \ (152 \leq N \leq 198)$ isotopic chain, figure 2 shows that the rms radii of moderate prolate deformed configuration are larger than those of oblate one for both NL3 and NL-SH calculations. The gap between them is about $0.03 \sim 0.07 fm$. For NL-Z2 calculation, it scarcely shows any gap in the rms radii between moderate prolate and oblate deformed configuration when $152 \leq N \leq 176$ in figure 2. All the calculations of NL3, NL-SH and NL-Z2 indicate that the radii of super-deformed configuration are larger than that of the moderate. The radii
of oblate deformed configuration for NL-Z2 in the region $N \geq 178$ lie between the radii of super-deformed configuration and the moderate one. When $N \geq 186$, it is very close to the super-deformed configuration’s. As a whole, nuclei with large absolute values $\beta_2$ tend to have larger rms radii. In figure 2, obvious kinks can be seen at $N = 184$ in the proton rms radii for moderate deformed configuration of all the parameters, which consists with the prediction in subsection 3.1 that $N = 184$ is a magic number and shell closure exists there. Then we see the results for superdeformed configuration in figure 2. The rms radii suddenly become small at $N = 172$ with NL3 calculation. $N = 172$ is a magic number for spherical nuclei in many Refs.[8,10]. Is $N = 172$ still a magic number for superdeformed configuration, and does the sudden change come from the shell closure at $N = 172$ as well? It is very difficult to answer the question, because the other two force parameters NL-SH and NL-Z2 can not reproduce that phenomenon. There is also sudden change at $N = 194$ with NL3 calculation. The NL-SH calculation shows that the rms radii change gradually with the variation of neutron number and there is a kink at $N = 176$, from which the radii increases much more slowly with the increasing of neutron. It is seen that the rms radii suddenly become small at $N = 182$ and 184 with NL-Z2 calculation. Is it caused by the shell closure at around $N = 184$? However, it is not predicted by NL3 and NL-SH calculations. Finally, let’s see the results of oblate deformed configuration. We only list the results in the region $152 \leq N \leq 168$ for NL3 and $152 \leq N \leq 170$ for NL-SH, because when we perform calculation with NL3 at $N = 170$ and with NL-SH at $N = 172$, the results suddenly change to moderate deformed configuration’s. The calculation with NL-Z2 set shows there is sudden change at $N=176$. In summary, it is a very strange region in $N = 168 \sim 178$, there maybe exist complicate shell structure.

From the analysis for the rms radii of $Z = 112$ and 104 isotopes, we find that there is strong parameter dependence in predicting the position of shell closure for oblate and super-deformed configuration. Shell anomalism maybe occur in the oblate and super-deformed configuration.

Table 1: Binding energies for $Z = 112$ isotopic chains with calculation of NL3, NL-SH and NL-Z2 sets. $B_1, B_2$ and $B_3$ denote the binding energies of oblate, moderate prolate and super-deformed prolate configurations. $N$ is the neutron number.

| $N$ | $B_1$(MeV) | $B_2$(MeV) | $B_3$(MeV) | $B_1$(MeV) | $B_2$(MeV) | $B_3$(MeV) | $B_1$(MeV) | $B_2$(MeV) | $B_3$(MeV) |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 160 | 1946.55     | 1958.84     | 1953.41     | 1948.74     | 1962.90     | 1955.63     | 1946.60     | 1955.60     | 1952.48     |
| 162 | 1961.41     | 1973.53     | 1968.65     | 1963.73     | 1977.47     | 1970.63     | 1960.83     | 1970.81     | 1967.61     |
| 164 | 1975.69     | 1987.53     | 1982.56     | 1978.47     | 1991.75     | 1984.57     | 1975.06     | 1984.51     | 1981.87     |
| 166 | 1989.47     | 2001.13     | 1995.92     | 1992.56     | 2005.42     | 1998.00     | 1988.91     | 1997.96     | 1995.55     |
| 168 | 2002.88     | 2014.09     | 2009.13     | 2006.83     | 2017.59     | 2011.23     | 2002.49     | 2011.19     | 2008.79     |
| 170 | 2015.93     | 2026.18     | 2022.19     | 2018.61     | 2028.06     | 2024.43     | 2015.78     | 2023.79     | 2021.84     |
| 172 | 2028.60     | 2037.76     | 2035.05     | 2031.03     | 2040.07     | 2037.43     | 2028.69     | 2036.09     | 2034.51     |
| 174 | 2040.84     | 2049.03     | 2047.34     | 2043.28     | 2051.35     | 2049.84     | 2041.13     | 2047.98     | 2046.75     |
| 176 | 2052.75     | 2059.90     | 2058.66     | 2054.83     | 2062.30     | 2060.72     | 2053.22     | 2058.94     | 2058.62     |
| 178 | 2064.00     | 2070.54     | 2069.42     | 2065.97     | 2072.74     | 2070.93     | 2065.05     | 2070.14     | 2070.03     |
| 180 | 2074.84     | 2080.39     | 2079.65     | 2076.35     | 2082.60     | 2080.87     | 2076.62     | 2080.34     | 2080.93     |
| 182 | 2085.21     | 2090.59     | 2089.50     | 2086.11     | 2092.27     | 2090.59     | 2087.72     | 2090.29     | 2091.18     |
| 184 | 2094.79     | 2100.68     | 2099.03     | 2095.33     | 2101.54     | 2099.97     | 2097.96     | 2100.84     | 2100.90     |
| 186 | 2103.90     | 2108.92     | 2108.07     | 2104.13     | 2109.80     | 2108.89     | 2107.68     | 2109.50     | 2110.45     |
| 188 | 2112.76     | 2116.72     | 2116.79     | 2112.56     | 2118.12     | 2117.82     | 2117.09     | 2117.75     | 2119.70     |
| 190 | 2121.26     | 2124.88     | 2125.48     | 2120.50     | 2126.36     | 2126.67     | 2126.22     | 2125.67     | 2128.76     |
| 192 | 2129.42     | 2132.67     | 2134.31     | 2128.10     | 2134.23     | 2135.18     | 2135.07     | 2133.36     | 2137.73     |
| 194 | 2137.31     | 2139.97     | 2142.95     | 2135.52     | 2141.62     | 2143.35     | 2143.66     | 2141.01     | 2146.74     |
| 196 | 2144.84     | 2146.65     | 2151.09     | 2142.76     | 2148.55     | 2151.00     | 2151.76     | 2148.87     | 2155.49     |
| 198 | 2151.98     | 2152.87     | 2158.68     | 2149.67     | 2152.87     | 2158.97     | 2159.33     | 2156.53     | 2163.79     |
| 200 | 2158.78     | 2165.98     | 2165.99     | 2156.29     | 2161.52     | 2166.40     | 2167.00     | 2163.21     | 2171.58     |
Table 2: Binding energies for \( Z = 104 \) isotopic chains with calculation of NL3, NL-SH and NL-Z2 sets. \( B_1, B_2 \) and \( B_3 \) denote the binding energies of oblate, moderate prolate and super-deformed prolate configurations. \( N \) is the neutron number.

|   | NL3 |   | NL-SH |   | NL-Z2 |
|---|-----|---|-------|---|-------|
| \( N \) | \( B_1 \) (MeV) | \( B_2 \) (MeV) | \( B_3 \) (MeV) | \( B_1 \) (MeV) | \( B_2 \) (MeV) | \( B_3 \) (MeV) |
| 152 | 1876.43 | 1889.25 | 1878.83 | 1892.57 | 1875.29 | 1887.03 |
| 154 | 1890.14 | 1902.90 | 1892.08 | 1906.31 | 1899.64 | 1909.00 |
| 156 | 1903.29 | 1915.89 | 1904.97 | 1919.03 | 1902.92 | 1913.95 |
| 158 | 1915.93 | 1928.35 | 1917.46 | 1931.35 | 1915.50 | 1926.77 |
| 160 | 1928.13 | 1940.28 | 1929.56 | 1943.22 | 1927.78 | 1938.71 |
| 162 | 1939.99 | 1951.40 | 1941.38 | 1953.99 | 1940.00 | 1950.02 |
| 164 | 1951.44 | 1961.15 | 1952.84 | 1964.21 | 1954.00 | 1962.09 |
| 166 | 1692.32 | 1970.77 | 1963.94 | 1974.32 | 1963.39 | 1969.74 |
| 168 | 1972.60 | 1980.32 | 1976.98 | 1984.01 | 1978.43 | 1980.00 |
| 170 | 1989.86 | 1996.94 | 1985.01 | 1993.13 | 1986.82 | 1998.72 |
| 172 | 1999.24 | 1997.96 | 2003.14 | 1997.96 | 1997.78 | 1999.55 |
| 174 | 2008.53 | 2005.61 | 2012.32 | 2006.88 | 2008.14 | 2009.02 |
| 176 | 2017.68 | 2014.23 | 2021.20 | 2015.58 | 2018.38 | 2017.68 |
| 178 | 2026.58 | 2022.61 | 2029.66 | 2023.68 | 2024.41 | 2027.31 |
| 180 | 2034.82 | 2030.82 | 2037.56 | 2033.36 | 2033.09 | 2035.74 |
| 182 | 2042.81 | 2038.60 | 2045.37 | 2038.75 | 2041.30 | 2044.36 |
| 184 | 2050.54 | 2045.89 | 2052.65 | 2045.97 | 2049.34 | 2052.73 |
| 186 | 2056.40 | 2052.80 | 2058.30 | 2051.94 | 2056.83 | 2059.16 |
| 188 | 2061.92 | 2059.48 | 2063.67 | 2058.63 | 2063.97 | 2065.98 |
| 190 | 2069.40 | 2066.02 | 2069.59 | 2065.06 | 2071.20 | 2073.86 |
| 192 | 2075.42 | 2072.37 | 2075.05 | 2071.31 | 2078.14 | 2080.90 |
| 194 | 2081.42 | 2079.81 | 2079.84 | 2077.46 | 2084.85 | 2087.56 |
| 196 | 2087.61 | 2085.75 | 2086.46 | 2083.17 | 2091.27 | 2093.73 |
| 198 | 2093.75 | 2091.22 | 2092.22 | 2098.35 | 2097.51 | 2100.33 |

### 3.3 Binding energy

In the above subsections, we have discussed the deformation and root mean square radii of \( Z = 112, 104 \) isotopic chains, and find that there are three deformed chains for each isotopic chain. Since there are multi-deformed configurations for the superheavy nuclei, is there shape coexistence in them? In this subsection, we will discuss it in detail. The binding energies of the three deformed chains with the force parameters NL3, NL-SH and NL-Z2 are listed in table 1 and table 2 for \( Z = 112, 104 \) respectively. \( B_1, B_2 \) and \( B_3 \) denote the binding energies of oblate, moderate prolate and super-deformed prolate configurations respectively. The binding energies with NL3, NL-SH and NL-Z2 in the same deformed chain are very close, the difference between them is not larger than 0.05 percent (about 10 MeV). One of the important conditions for the shape coexistence is that the deference of binding energies between two deformed configurations is very small, usually less than 1 MeV. If it is larger than 1 MeV, the translation between two different configurations is very difficult and the probability of shape coexistence is very little. To find the sign of shape coexistence, we compare the binding energies of different deformed chain with each other, and list the results in figure 3. The circle denotes the values of \( B_1 - B_2 \), triangle is for \( B_2 - B_3 \) and star is for \( B_1 - B_3 \). In figure 3, it is seen that all the values of \( B_1 - B_2, B_2 - B_3 \) and \( B_1 - B_3 \) are in the region \(-14.5 \sim 8 \) MeV. It is obvious that the abstract values of them decrease with the increasing of the neutron number until to a certain region \((N \sim 184)\) and the trend changes when \( N > 184 \) for \( Z = 112 \) isotopic chain. For \( Z = 104 \) isotopic chain, the phenomenon is less clear than that of \( Z = 112 \). It is interesting that these values are very close to the fission barriers as high as \( 8 \sim 12 \) MeV around the double-shell closure \( Z = 114, N = 184^{[27-29]} \). This means the deformation is important for the stability of superheavy nuclei. From figure 3, we can also clearly find in which region the shape coexistence exists and what kind of shape coexistence is in the long isotopic chain.
For $Z = 112$ isotopic chain, from table 1 and figure 3, we can see $B_2$ is always the largest one and $B_1$ is the smallest among $B_1, B_2$ and $B_3$ in the region $N \leq 186$ for NL3, $N \leq 188$ for NL-SH and $N \leq 178$ for NL-Z2 calculation respectively. It indicates that the moderate prolate deformed configuration is the ground state of nuclei $N \leq 186$ for NL3, $N \leq 188$ for NL-SH and $N \leq 178$ for NL-Z2 calculation and the oblate or superdeformed configuration is the exciting state of them. The most distinct character is that $B_3$ is the largest one when $N \geq 188$ for NL3, $N \geq 190$ for NL-SH and $N \geq 180$ for NL-Z2 calculation, namely, there is a chain of super-deformed configurations which become the ground state and are more stable than the other deformed configurations. Although there are some differences with the different force parameters in predicting the region of super-deformation, all the parameters’ calculation show there is a more stable super-deformed region in the $Z = 112$ isotopic chain. It agrees with the Bohr and Mottelson’ suggestion\cite{26} that deformation can increase the stability of the heavy nuclei. But it should be noted that it is not for all heavy nuclei that deformation can increase the stability. This phenomenon appears only in special region of superdeformed chain. Figure 3 also shows that the results with NL3, NL-SH and NL-Z2 set are different in some details, but the total trend is consistent. In figure 3, the star is below and far from the dotted line $\delta E=-1$ MeV, it means that it is impossible for oblate and super-deformed prolate deformation to coexist in $Z = 112$ isotopes. There is no shape coexistence in the region $N \leq 172$, for no symbols in the region $1$ MeV $\leq \delta E \leq -1$ MeV as shown in figure 3. The NL3 results show there maybe exist moderate- and super-deformed shape coexistence in the region $176 \leq N \leq 190$ of $Z = 112$ isotopes, for the value of $B_2 - B_3$ (triangles) is around $1$ MeV or within $1$ MeV. Although the NL-SH results for $B_2 - B_3$ (triangles) are larger than $1$ MeV in the region $174 \leq N \leq 184$, they are very close to $1$ MeV, together with the values within $1$ MeV, we believe that moderate- and super-deformed shape coexistence maybe occur in $174 \leq N \leq 192$. The NL-Z2 results predict the moderate- and super-deformed shape coexistence should occur in $174 \leq N \leq 186$. It is interesting that all the regions of shape coexistence predicted by the parameters NL3, NL-SH and NL-Z2 contain the magic number N=184. It maybe have some trends that shape coexistence occur usually at around the magic number. NL3 calculation also shows moderate prolate and oblate deformation coexist at $N = 198, Z = 112$, and NL-Z2 shows moderate prolate and oblate deformation coexist at $N = 188, 190$. The calculation of Ref.\cite{23} predicts $N = 172, Z = 112$ exists shape coexistence, but our result does not indicate there is any shape coexistence.

On the other hand, for $Z = 104$ isotopic chain, from table 2 and figure 3, we can find there is no super-deformed configuration until $N \geq 168$ and no oblate deformed configuration when $N \geq 168$ for NL3, $N \geq 170$ for NL-SH calculation. $B_2$ is always larger than $B_3$ except $N = 198$ for NL-SH calculation. It may be an anomaly or un-physical solution. Thus, for $Z = 104$ isotopic chain, the moderate prolate deformed configuration may be the ground state, and the deformation can not increase the stability in this case at all. In figure 3, the results of NL3 and NL-SH are very close, the triangles, circles or stars are not in the region $-1$ MeV $\leq \delta E \leq 1$ MeV. It indicates there is no shape coexistence for $Z = 104$ isotopes with NL3 and NL-SH calculations. But the results that NL-Z2 parameter shows are very different from those of NL3 and NL-SH sets. It predicts moderate prolate and oblate deformation maybe coexist at $N = 172, 174$ and $176$, moderate prolate and super-deformation maybe coexist in $168 \leq N \leq 180$ and oblate and super-deformation maybe coexist at $N = 172, 174$ and in the region $182 \leq N \leq 198$. The shape coexistence also occurs around the magic number $N = 174$ and 184.
4 Summary

We use the considered axial deformed relativistic mean field theory to perform systematical calculations for $Z = 112$ and 104 isotopic chains with force parameters NL3, NL-SH and NL-Z2 sets. First, three deformed chains (oblate, moderate prolate and super-deformed chain) are found for $Z = 112$ and 104 isotopic chains. Second, a super-deformed chain can be the ground states for $Z = 112$ isotopic chain when $N \geq 188$ with NL3, $N \geq 190$ with NL-SH and $N \geq 180$ with NL-Z2 calculation. This confirms that the deformation can increase the stability of some superheavy nuclei. Third, although shape coexistence is a general phenomenon for superheavy nuclei, it only appears in some special regions of an isotopic chain, and only some special kinds of shape coexistence can exist. For $Z = 112$ isotopic chain, it is predicted that moderate prolate and super-deformation coexist in the region $174 \leq N \leq 184$ for NL3 set, $174 \leq N \leq 192$ for NL-SH set, $174 \leq N \leq 186$ for NL-Z2 set. There is no other kind of shape coexistence for $Z = 112$ isotopic chain except moderate prolate and oblate deformation at $N = 198$ for NL3 set, moderate prolate and oblate deformation at $N = 188, 190$ for NL-Z2 set. For $Z = 104$ isotopic chain, there is no shape coexistence with NL3 and NL-SH calculations. However, the NL-Z2 calculation predicts that moderate prolate and oblate deformation maybe coexist at $N = 172, 174$ and 176, moderate prolate and super-deformation maybe coexist in $168 \leq N \leq 180$ and oblate and super-deformation maybe coexist at $N = 172, 174$ and in the region $182 \leq N \leq 198$. We predict that shape coexistence maybe occur around the magic number. Finally, it is found that there is shell closure at $N = 184$ ($\beta_2 \approx 0$) for moderate prolate deformed chains of $Z = 112$ and 104, at $N = 176$ for oblate deformed chain of $Z = 112$, the position of shell closure have strong parameter dependence for super-deformed chains of $Z = 112$ and 104. It is confirmed the prediction that there is shell anomalous for oblate or superdeformed nuclei.

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Figure 1: The parameter of quadrupole deformation $\beta_2$ for $Z = 112$ and 104 isotopic chains with calculation of NL3, NL-SH and NL-Z2 sets. Empty circle, empty triangle and empty star denote oblate, moderate prolate and super deformation respectively.
Figure 2: The root mean square radii for $Z = 112$ and 104 isotopic chains with calculation of NL3, NL-SH and NL-Z2 sets. Circle, up-triangle and down-triangle denote oblate, moderate prolate and super deformed configuration respectively. The solid symbol stands for neutron and empty symbol stands for proton.
Figure 3: The energy differences for $Z = 112$ and 104 isotopic chains with calculation of NL3, NL-SH and NL-Z2 sets. $B_1$, $B_2$ and $B_3$ denote the binding energies of oblate, moderate prolate and super-deformed prolate configurations. The circle denotes the values of $B_1 - B_2$, triangle stands for $B_2 - B_3$ and star stands for $B_1 - B_3$. 
