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A pilgrimage through superheavy valley

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Abstract. We searched for the shell closure proton and neutron numbers in the superheavy region beyond $Z = 82$ and $N = 126$ within the framework of non-relativistic Skryme–Hartree–Fock (SHF) with FITZ, SIII, SkMP and SLy4 interactions. We have calculated the average proton pairing gap Δ_p, average neutron pairing gap Δ_n, two-nucleon separation energy S_{2q} and shell correction energy E_{shell} for the isotopic chain of $Z = 112$–126. Based on these observables, $Z = 120$ with $N = 182$ is suggested to be the magic numbers in the present approach.

Keywords. Skyrme–Hartree–Fock (SHF); binding energies; nucleon separation energy; pairing energy; average pairing gap; shell correction energy; single-particle energy.

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1. Introduction

The search for new elements is an important issue in nuclear science for more than a century after the discovery of elements beyond the last heaviest naturally occurring element ^{238}U. The discovery of transuranium elements (neptunium, plutonium and other 14 elements), gave a new look to the periodic table. This enhancement in the modern periodic table raises a few questions in our mind: whether there is only a limited number of elements that can coexist in nature or whether new elements can be produced by artificial synthesis using modern techniques? what is the maximum number of protons and neutrons inside a nucleus? and, what is the next double shell closure nuclei after ^{208}Pb.

To answer these questions, first, we have to know the observable(s) which is(are) responsible to sustain the nucleus against Coulomb repulsion. The obvious reply is the shell energy, which stabilizes the nucleus against the Coulomb disintegration [1]. With the development of heavy-ion beam it was possible to make some progress in the superheavy region. Recent theoretical calculations for superheavy elements have generated quite an excitement where new magic numbers are predicted for both protons and neutrons. Many theoretical models predict the magic shells at $Z = 114$ and $N = 184$ [2–5], which could have surprisingly long lifetime, even of the order of a million years [6–8].

Some other such predictions of shell-closure for superheavy regions within the relativistic and non-relativistic theories, have some impact in this direction [9,10]. At present, $Z = 114$ nucleus is already synthesized, but only for a lighter isotope $^{289}114$ [11]. The α-decay properties are also observed and decay energies or Q_α values are estimated from RMF formalisms [12]. Recent experiments [11,13–22] gave some signature for nuclei, even closure to the expected island of stability in superheavy valley. Hence, it is an inherent interest for nuclear theorist as well as experimentalist to see the *Island of Stability* in superheavy valley. Here, we have scanned the superheavy region using recently developed and successful microscopic models to find some signature of shell closures for protons and neutrons.

This paper is organized as follows: the details of theoretical formalism for calculations are given in §2. The obtained results with a brief discussion are included in §3. A summary of the results together with concluding remarks are given in §4.

2. The Skyrme–Hartree–Fock (SHF) method

The general form of the Skyrme effective interaction can be expressed in terms of energy density functional $\mathcal{H}$ [23,24], as

$$\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \cdots , \tag{1}$$

where $\mathcal{K} = (\hbar^2/2m)\tau$ is the kinetic energy term with m as the nucleon mass, $\mathcal{H}_0$ the zero range, $\mathcal{H}_3$ the density-dependent and $\mathcal{H}_{\text{eff}}$ the effective mass-dependent terms, relevant for calculating the properties of nuclear matter, are functions of nine parameters t_i, x_i ($i = 0, 1, 2, 3$) and η, given as

$$\mathcal{H}_0 = \frac{1}{4} t_0 \left[(2 + x_0)\rho^2 - (2x_0 + 1)\left(\rho_{\text{p}}^2 + \rho_{\text{n}}^2\right)\right], \tag{2}$$

$$\mathcal{H}_3 = \frac{1}{24} t_3 \rho^\eta \left[(2 + x_3)\rho^2 - (2x_3 + 1)\left(\rho_{\text{p}}^2 + \rho_{\text{n}}^2\right)\right], \tag{3}$$

$$\begin{aligned}\mathcal{H}_{\text{eff}} = {} & \frac{1}{8}\left[t_1(2 + x_1) + t_2(2 + x_2)\right]\tau\rho \\ & + \frac{1}{8}\left[t_2(2x_2 + 1) - t_1(2x_1 + 1)\right](\tau_{\text{p}}\rho_{\text{p}} + \tau_{\text{n}}\rho_{\text{n}}).\end{aligned} \tag{4}$$

The surface contributions of a finite nucleus with b_4 and b_4' as additional parameters, are

$$\begin{aligned}\mathcal{H}_{S\rho} = {} & \frac{1}{16}\left[3t_1\left(1 + \frac{1}{2}x_1\right) - t_2\left(1 + \frac{1}{2}x_2\right)\right](\vec{\nabla}\rho)^2 \\ & - \frac{1}{16}\left[3t_1\left(x_1 + \frac{1}{2}\right) + t_2\left(x_2 + \frac{1}{2}\right)\right] \\ & \times \left[(\vec{\nabla}\rho_{\text{n}})^2 + (\vec{\nabla}\rho_{\text{p}})^2\right]\end{aligned} \tag{5}$$

and

$$\mathcal{H}_{S\vec{J}} = -\frac{1}{2}\left[b_4\rho\vec{\nabla}\cdot\vec{J} + b_4'\left(\rho_{\text{n}}\vec{\nabla}\cdot\vec{J}_{\text{n}} + \rho_{\text{p}}\vec{\nabla}\cdot\vec{J}_{\text{p}}\right)\right]. \tag{6}$$

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

To deal with the open shell nuclei in determining the nuclear properties, the constant gap BCS-pairing approach is included in the present calculation. In the present study, we deal with nuclei on or near the valley of stability line since the superheavy elements, though very exotic in nature, lie on the β-stability line. Apparently, in a given nucleus, for a constant pairing gap $\triangle$, the pairing energy E_{pair} is not constant as it depends on the occupation probabilities and, hence on the deformation parameter β_2, particularly near the Fermi surface. This type of prescription for pairing effects in SHF, has already been used by us and many others [25].

3. Result and discussion

A well-defined approach such as non-relativistic Skryme–Hartree–Fock (SHF) with FITZ, SIII, SkMP and SLy4 interactions [23,24,26] is used in the present study. The present study has appeared as a powerful tool to study the shapes and collective properties of nuclei, which is mainly connected with the stability of a nucleus. In order to get magic numbers for protons and neutrons in the superheavy valley, we have first established the basic magic properties. It is well understood that the magic number for a nucleus has the following characteristics:

(1) The average pairing gap for proton Δ_p and neutron Δ_n at the magic number is minimum.
(2) The binding energy per particle is maximum compared to the neighbouring one, i.e., there must be a sudden decrease (jump) in two-neutrons (or two-protons) separation energy S_{2n}, just after the magic number in an isotopic or isotonic chain.
(3) At the magic number, the shell correction energy E_{shell} is negative to the maximum, i.e., a pronounced energy gap in the single-particle levels.

Here, we focus on the shell closure properties based on the above important observables and identify the magic proton and neutron numbers in the superheavy region. A wide range of nuclei starting from the proton-rich to neutron-rich region is scanned in the superheavy valley ($Z = 112$–126).

3.1 *Average pairing gap*

The average pairing gap is defined by [27,28],

$$\Delta_q = G_q \sum_{\alpha_q} \left[n_{\alpha_q} \left(1 - n_{\alpha_q} \right) \right]^{-1/2}. \tag{7}$$

Here, q is neutron or proton, n_{α_q} is the occupation probability of a state with quantum numbers $\alpha_q = nljm$. The quantity G_q stands for pairing strength and the sum is restricted

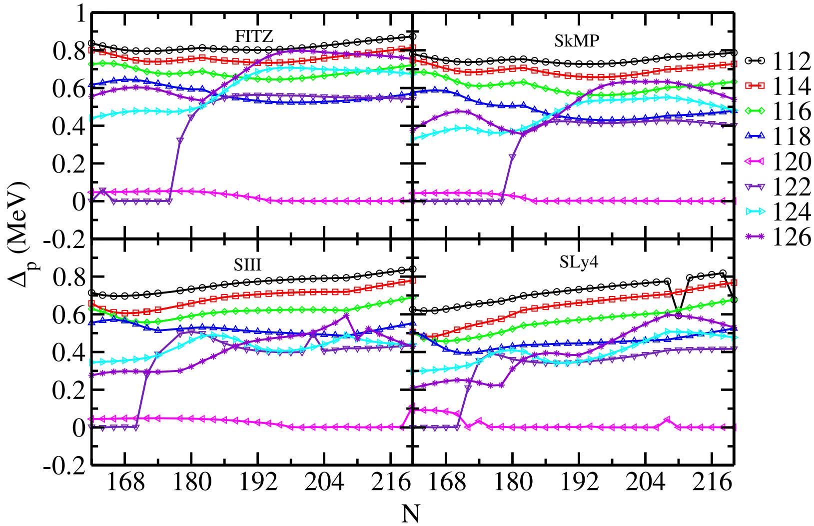

Figure 1. The proton average pairing gap Δ_p for Z=112–126 with N=162–220 and Z=112–130 with N=162–260

to positive values of m. This simple approach is used to calculate the average pairing gap for proton (Δ_p) and neutron (Δ_n). The curves for Δ_p are displayed in figure 1 obtained by SHF with FITZ, SIII, SLy4 and SkMP parameters. Analysing the figure carefully, it is clear that the value of Δ_p is almost zero for the whole isotopic chain $Z = 120$ for all the forces. For example, $\Delta_p \sim 0.0001$ for all isotopes of $Z = 120$ and $0.1 \leq \Delta_p \leq 0.8$ for all other atomic numbers.

To predict the corresponding neutron shell closure of the magic number $Z = 120$, we have estimated the neutron pairing gap Δ_n for all elements of $Z = 112-126$ with their corresponding isotopic chain. As a result, the calculated Δ_n for the whole isotopic chain are displayed in figure 2. We have obtained an arc-like structure with vanishing Δ_n at $N = 182$, 208 for SHF for the parameter sets considered. This minimization in the pairing gap indicates the close shell structure of the nucleus. Hence, the average pairing gap for proton and neutron for all force parameters are directing $Z = 120$ to be the next magic number after $Z = 82$ with $N = 182$, 208.

3.2 *Two-neutron separation energy*

The two nucleon separation energy of a nucleus is defined as

$$S_{2q}|_{q=n,p} = BE(N_q) - BE(N_q - 2), \tag{8}$$

where N_q is the number of neutrons (protons) for a given nucleus. A sharp fall in the S_{2q} value means that a very small amount of energy is required to remove two nucleons as compared to its magic neighbour. Thus, the nucleus is significantly stable compared to the daughter, which is the basic characteristic of a magic number. This lowering in two-neutron separation energy is a conclusive test for shell closure investigation. Figure 3

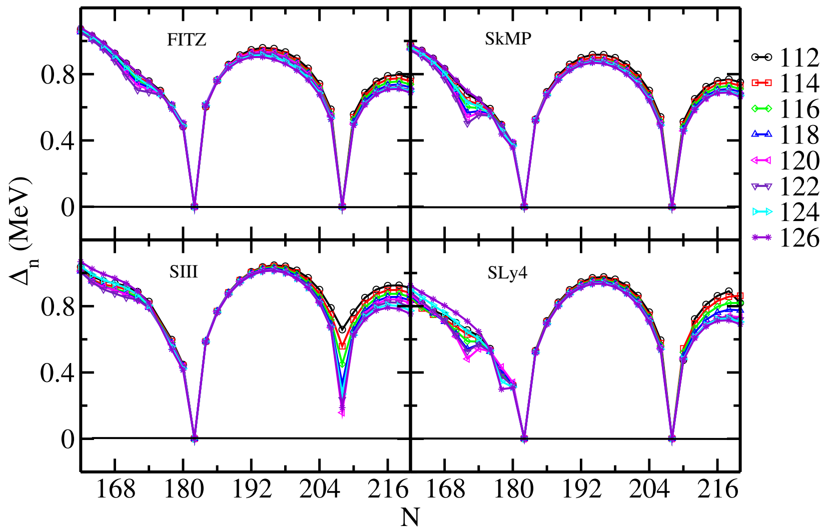

Figure 2. Same as figure 1 but for neutron average pairing gap Δ_n.

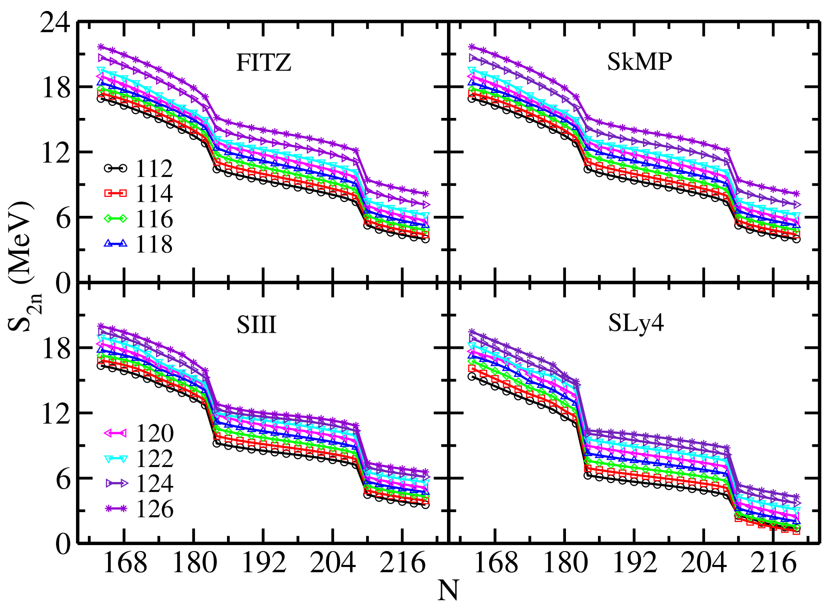

Figure 3. The two-neutron separation energy S_{2n} for $Z = 112$–126 and $N = 162$–220 in the framework of SHF theory.

shows S_{2n} as a function of mass number for all isotopic chains of the considered elements for SHF formalisms. From this figure, we notice such an effect, i.e., jump in two-neutron separation energy at $N = 182$ or 208.

3.3 *The shell correction energy*

According to Strutinsky energy theorem on liquid-drop model [29,30], the total quantal energy can be divided into two parts:

$$E_{\mathrm{tot}} = E_{\mathrm{avg}} + E_{\mathrm{shell}}, \tag{9}$$

where E_{tot}, E_{avg} and E_{shell} are the total, average and shell correction energy, respectively. With the addition of shell correction contribution to the total energy, the whole scenario of liquid properties is converted to shell structure which can explain the magic shell even in the framework of liquid-drop model. The values of n_α is 1 and 0 for occupied and empty states, respectively. This implies that the shell correction energy is the difference between the exact energy and average energy and is given by

$$E_{\mathrm{shell}} = \sum_{\alpha} (n_\alpha - \bar{n}_\alpha)\, \varepsilon_\alpha, \tag{10}$$

with ε_α being the energy eigenvalues of the nuclear potential. Hence, the shell correction energy E_{shell}, is a key quantity to determine the shell closure of nucleon. The magnitude of total (proton + neutron) E_{shell} energy is dictated by the level density around the Fermi level. A positive E_{shell} reduces the binding energy and a negative shell correction energy increases the stability of the nucleus. We have illustrated the SHF result of E_{shell} in figure 4, which clearly shows the extra stability of $^{302,328}120$.

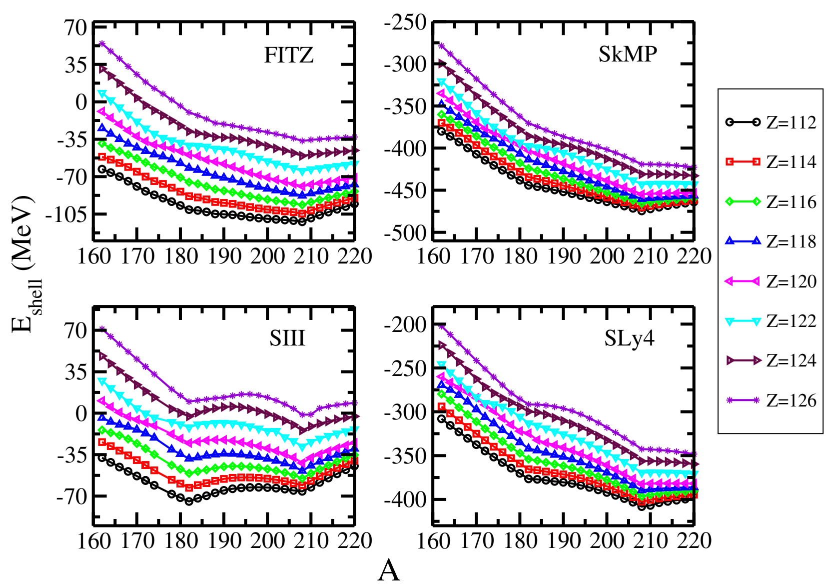

Figure 4. The shell correction energy E_{shell} for $Z = 112$–126 and $N = 162$–220 in the framework of SHF theory.

4. Summary and conclusion

In summary, we have analysed the pairing gaps Δ_p and Δ_n, two-neutron separation energy S_{2n} and shell correction energy E_{shell} for the $Z = 112$–126 region covering the proton-rich to neutron-rich isotopes. To our knowledge, this is one of the first such extensive and rigorous calculation in SHF using a large number of parameter sets. Although the results depend slightly on the forces used, the general set of magic numbers beyond ^{208}Pb are $Z = 120$ and $N = 182$ or 208. The highly discussed proton magic number $Z = 114$ in the past (last four decades) is found to be feebly magic in nature.

Acknowledgements

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