

A Skyrme Hartree-Fock-Bogoliubov approach to Ground state properties of Selenium isotopes

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Introduction

Understanding nuclear stability of various nuclei through ground state properties is crucial for understanding nuclear physics and its applications. Studying the ground state properties of nuclei is essential for understanding the atomic structure. With the increasing interest in exotic nuclei, particularly those near the neutron drip line, the inevitability of accurate computational methods has emerged[1]. Despite the progress in nuclear physics, the exact nature of strong nuclear force and the behavior of exotic nuclei far from stability still remain a major mystery. These unresolved issues reflect the complexity of the field and drive ongoing research efforts. The HFB theory approximates the interactions among nucleons, by assuming each moving in a mean field created by the rest. Using the variational principle, the wave functions are represented as Slater determinants incorporating all correlations within a single particle framework[2].

This research employs HFBTHO code to calculate the ground state properties of Selenium isotopes ranging from mass number 63 to 97 with the aid of Skyrme-Hartree-Fock Bogoliubov calculations for all isotopes, with SLY4 as the Skyrme functional. Further, the obtained results were compared with experimental data from National Nuclear Data Centre (NNDC)[3].

Formalism

The success of shell model, which utilizes the mean field approximation, asserts that the nucleons occupy discrete energy levels, and they move freely in an average potential created by other nucleons. From the two-body interactions in the mean field, potential of a single particle can be extracted through variational minimization on Hartree-Fock energy, with Slater determinants as trial wave functions. The

Hartree-Fock equation thus obtained incorporates a density dependent self-consistent field along with the term for kinetic energy, which is then solved through iterative methods.

As Hartree-Fock method neglects correlation effects, employing Hartree-Fock-Bogoliubov (HFB) approach, ensures these effects are accounted by the introduction of quasi-particles in a pairing potential. In HFB theory, the ground state of the system is treated as a vacuum consisting of quasi-particles. It can be considered as a superposition of particles and holes reflecting the pairing correlations. Hamiltonian consisting of both kinetic energy and pairing correlations are used by the HFB equations where Lagrange multipliers ensure the particle number symmetry[2].

HFB matrix is solved by HFBTHO code, which utilizes transformed harmonic oscillator basis[1]. The HFB matrix is given by:

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} \cdot E_k \quad (1)$$

The code iteratively updates the pairing matrix and Hamiltonian to find self-consistent solutions. The quasi-particle blocking was involved in proceeding the calculations for odd isotopes. Pairing interaction is given as

$$V_{pairing}^{(n,p)}(r) = V_0^{(n,p)} \left(1 - \frac{\alpha p(r)}{\rho_0} \right) \delta(r - r') \quad (2)$$

A quasi-particle cut off of 60 MeV was used along with a pairing force of 0.5. The oscillator length was set to be 2.2 fm. The number of shells were limited to 20 and the pairing strength for both neutrons and protons were set to be 300 MeV.

Results and Discussion

The binding energy per nucleon (BE/A) for Selenium isotopes with mass numbers 63 to 97 is computed and is then compared with the available experimental data as depicted in Fig.1.

The results show that HFB calculations follow a similar trend to the experimental values with clear evidence of odd-even staggering in both even-even and odd-even isotopes. The given plot has a parabolic shape as expected from the experimental calculations. The peak binding energy at $A=78$ is due to the filling of $2p^{1/2}$ shell.

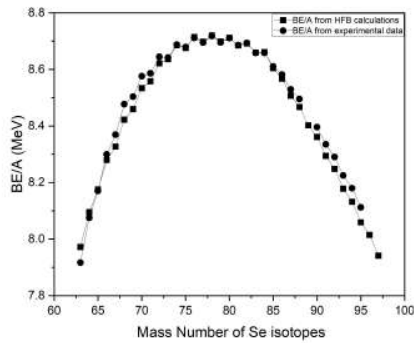


Fig. 1 BE/A plot for Selenium isotopes. The energy for single (S_n) and two (S_{2n}) neutron separations is also calculated using (3) and (4)

$$S_n = BE(Z, N) - BE(Z, N - 1) \quad (3)$$

$$S_{2n} = BE(Z, N) - BE(Z, N - 2) \quad (4)$$

The obtained results of these separation energy values are also compared with the available experimental values.

As the isotopes approach neutron drip line, the separation energy decreases. The comparative analysis with the experimental data as shown in the fig 2, holds positive of this statement.

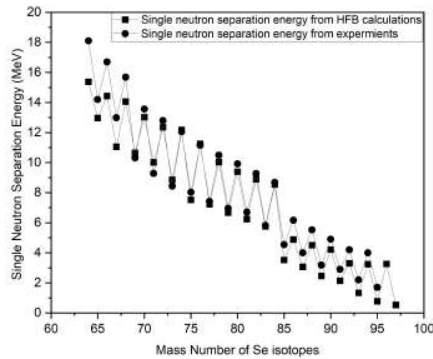


Fig. 2 Single-neutron separation energy plotted against mass number of Se isotopes.

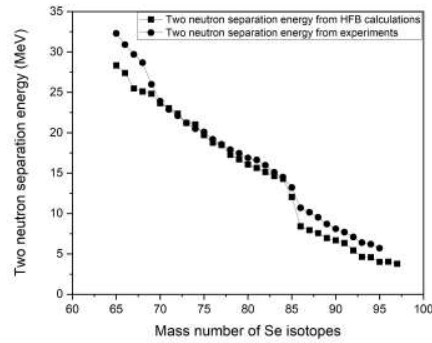


Fig. 3 Two-neutron separation energy plotted against mass number of Se isotopes.

The unpaired neutron present in the odd isotopes is held responsible for the lower separation energy of those isotopes compared to their even counterparts as seen from Fig 2 and 3. The plot of the two-neutron separation energy is also found in agreement with the experimental data.

References

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- [3] “NNDC | National Nuclear Data Center.” Accessed: Oct. 14, 2024. [Online]. Available: <https://www.nndc.bnl.gov/>