Neutron and Proton Separation Energies of Fe isotopes using Hartree-Fock-Bogoliubov approach

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Introduction

The ground state properties such as neutron and proton separation energies of Fe nuclei are of great significance because Fe^{56}plays the role of the most stable nucleus in the binding energy per nucleon curve. The change in these properties with variation of neutron number readily influences other parameters. Even though much information regarding these are available in the literature, mostly for even-even Fe isotopes, here we have made an attempt to understand more on these, including both even-even and even-odd systems.

In the present work, we have investigated some of the ground state properties of the Fe nuclides in a wide range with mass number A varying from 45 to 76. Generally, the nuclei beyond Fe^{56} are synthesized in supernova explosions. The enhanced stability around the nuclei of Fe^{56} could be attributed to the shell effects. [1] Here, we have employed the Hartree-Fock-Bogoliubov (HFB) self-consistent mean-field model with transformed harmonic oscillator basis, which takes pairing fields into consideration by the quasi-particle transformation through Bogoliubov equations. The short range of the nuclear interaction and the longer wavelength limits of the single particle states make one to use the effective interactions as energy density functional, namely Skyrme interactions. For this analysis, we have used the standard code HFBTHO version 2.00d. [2]

The separation energy of the nucleons is one of the most important properties determining the nuclear structure. The stability of a nucleus could be predicted by studying the separation energies. A nucleus is considered to be stable if it is stable against the emission of a single neutron and a single proton. Here, we have extended our study also to the stability of nuclei with respect to the two-neutron emission.

Formalism

The mean-field theory has played a vital role in the study of many-particle system, by reducing the complex many-body Schrödinger equation to a single particle problem. The Hartree-Fock-Bogoliubov (HFB) theory is the successor to the Hartree-Fock (HF) formalism and it incorporates the pairing correlations as perturbation to the mean-field Hamiltonian. The Bogoliubov transformation act as a useful trick in representing the ground state of the pair-wise interacting particles as a gas of non-interacting quasi-particles[3]. The HFB theory with effective zero-range pairing force is the best tool to study the ground state properties of nuclei which are on and off the dripline. The introduction of quasi-particle basis makes the HFB equation in the configuration space as

$$\begin{bmatrix} h & \Delta \\ -\Delta^* & -h^* \end{bmatrix} \begin{bmatrix} U_k \\ V_k \end{bmatrix} = E_k \begin{bmatrix} U_k \\ V_k \end{bmatrix} \qquad (1)$$

The program HFBTHO (v 2.00d) iteratively diagonalizes the HFB Hamiltonian till a self-consistent solution is obtained, by using the Skyrme forces and pairing interactions. The local nature of the Skyrme interaction makes the structure of direct and exchange terms similar, thus considerably reducing the number of calculations in the Skyrme HFB equations.

Here, we have employed SLY4 Skyrme functional as the effective interaction in the HFB calculations. The general form of the nucleon-nucleon interaction could be found in [3]. In this study, we have used mixed surface-volume pairing force in the pairing interaction with quasi-particle cut off at 60MeV by keeping the oscillator length of the basis as 2.2 fm. Pairing strength for both protons and neutrons have been fixed to be 300MeV. The calculation for even-odd and odd-odd isotopes are carried out by the blocking of the quasi-particle levels by the equal filling approximation [2].

Results and Discussion

The separation energies of the isotopes of Fe ranging from mass number A=45 to A=76 were calculated by the HFB approach and are then compared with the values of the mass table[4]. Fig.1 shows the variation of one-proton separation energy with mass number of Fe isotopes and its comparison with values of mass table. It can be seen that the separation energies of all the isotopes remain positive and are stable against one-proton emission. Note that, for the isotopes Fe^{46}, Fe^{54} and Fe^{76}, the one-proton separation energy shows an increase which is a sign of the magicity. In addition to these isotopes Fe^{51} and Fe^{74} also show an increase in proton separation energies due to the filling of the $1f_{7/2}$ and $1g_{9/2}$ subshells.

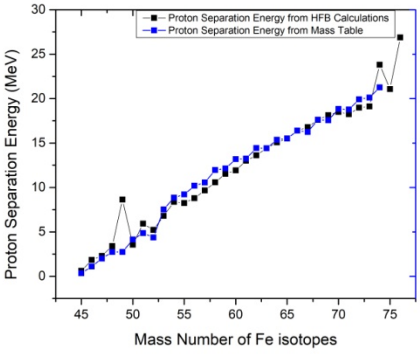

Fig.1 Plot of one-proton separation energy against mass number of Fe isotopes.

By considering the variation of one-neutron separation energies,

$$S_n = BE(Z,N) - BE(Z,N-1) \qquad (2)$$

of the isotopes of Fe, as shown in Fig.2, one can find a good agreement of HFB calculations with the values taken from the mass table [4]. All the isotopes show positive values for one-neutron separation energies, which indicate the stability against single neutron emission. The one-neutron separation energies of Fe isotopes with odd mass numbers is found to be lower than that of the isotopes with even mass numbers, manifesting odd-even effects in the isotopic chain.

The two-neutron separation energy could be calculated as,

$$S_{2n} = BE(Z,N) - BE(Z,N-2) \qquad (3)$$

The S_{2n} values from the HFB calculations are in good agreement and consistent with that of the values from the mass table, as evident from Fig.3. The two-neutron separation energy values are found to decrease with the increase in the mass number and it could also be seen that there is a rapid decrease starting from Fe^{54}, which is magic.

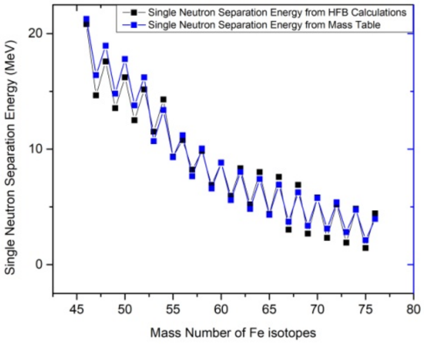

Fig.2 Plot of single neutron separation energy against mass number of Fe isotopes.

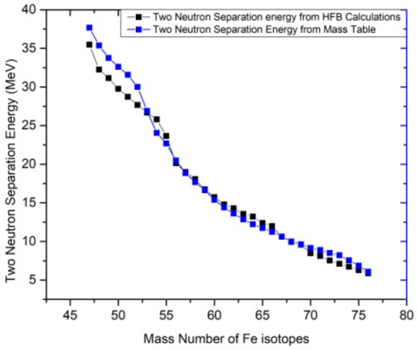

Fig.3 Plot of two-neutron separation energy against mass number of Fe isotopes.

References

[1] Tarasov et al., Bulletin of the Russian Academy of Sciences: Physics, 71, No. 6, 747–753 (2007) .

[2] M. V. Stoitsov et al., Computer Physics Communications 184,1592-1604 (2013) .

[3] P. Ring, P. Schuck, in: The Nuclear Many-Body Problem, Springer-Verlag, New York (1980).

[4] Chinese Physics C, 45, 030003 (2021).