J. Nucl. Phys. Mat. Sci. Rad. A. Vol. 9, No. 2 (2022), pp.203–207

CHITKARA

Journal of Nuclear Physics, Material Sciences, Radiation and Applications
Journal homepage: https://jnp.chitkara.edu.in/

A Hartree-Fock-Bogoliubov Study on the Pairing Correlations of the Isotopes of Cobalt

Nicemon Thomas*, Anjana A V and Antony Joseph

Department of Physics, University of Calicut, Kerala-673635, India

*nmtvattoth@gmail.com (Corresponding Author)

ARTICLE INFORMATION

Received: January 28, 2022
Accepted: May 09, 2022
Published Online: June 20, 2022

Keywords:
Pairing correlation, Hartree-Fock-Bogoliubov theory, Binding energy, Pairing gap, Neutron separation energy

DOI: 10.15415/jnp.2022.92030

ABSTRACT

Background: The phenomena of nucleon pairing could be outlined from the Bethe-Weizäcker semi-empirical formula, from which the nuclear properties, viz. the binding energy, stability, shape etc. could be clearly sketched. Though the pairing correlation seems to be a small correction to the binding energy term, it plays a determinative role in defining the structure of nuclear systems. The addition to the binding energy in turn affects the position of the isotope on the dripline and hence increases the stability.

Purpose: To study the effects of pairing in the ground state properties of the isotopes of Cobalt.

Methods: We use Hartree-Fock-Bogoliubov (HFB) theory for the study. The general wave functions for the HFB approach are determined by variational approach. The eigen functions for the Hamiltonian are connected with the particle operators through the Bogoliubov transformations. The Hartree-Fock energy is obtained through the minimization of the variational parameter and the HFB equation is solved by iterative diagonalization by restoring the particle number symmetry.

Results: The HFB analysis substantiates the effect of pairing correlation in the binding energies, neutron and proton pairing energies, neutron and proton pairing gaps and one- and two-neutron separation energies of the Cobalt isotopes. The binding energies and one and two-neutron separation energies match with the experimental values and for pairing energies and pairing gaps, the regions where pairing is significant and the effects of shell closure at the vicinity of magic configuration of neutrons could be recognized.

Conclusions: The Hartree-Fock-Bogoliubov calculations of the effects of pairing could be used as an efficient tool to study the nuclear structure effectively. It can be ascertained that the pairing plays an important role in determining the ground state properties of atomic nuclei.

1. Introduction

The nuclear structure and the properties of the nuclei are known to be a fascinating landscape for the researchers ever since the discovery of nucleus. The existence of nucleon pairing could be traced out from the Bethe-Weizäcker semi-empirical formula, which helps us understand the behavior of nuclear properties, viz. the binding energy, stability, shape etc. [1]. The possibility of nucleon pairing was studied by Bohr, Mottelson and Pines [2] as an analogy with Cooper pairs in BCS theory [3] of superconductors. Even though the correlation energy due to pairing appears to be a small correction to the binding energy, it has been proved to play a vital role in determining the structure of both finite and infinite nuclear systems. The additional binding that pairing offers provides increased stability and in turn affects the position of the dripline. Pairing correlations also influence reaction cross sections, neutrinoless double β decays, odd-even staggering, incompressibility, symmetry energy, moments of inertia, alignments, deformation etc.

For nuclei with N > Z, proton-proton (pp) and neutron-neutron (nn) pairs are known to exist with angular momentum $J = 0$ and isospin $T = 1$ and for those nuclei with N ≅ Z, apart from the above mentioned pairs, nucleons which are near the Fermi surface and tend to occupy identical orbitals leads to the formation of another type of pairs, namely the neutron-proton (*np*) pairs, having either $J = 0$ and $T = 1$ (isovector) or $J = 1$ and $T = 0$ (isoscalar) pairs. The charge independence of nuclear force leads us to the conclusion that the $J = 0$, $T = 1$ (*np*) pairs should have equal probability for existence as like $J = 0$, $T = 1$ (*nn*) and (*pp*) pairs in $N = Z$ nuclei. It is clear that in the isospin triplet channel, two nucleons near the Fermi level, with opposite spin states, couple to form isovector pairs, whereas the isospin singlet, ($T = 0$) is considered to be of less probability due to large spin- orbit coupling [1].

In the present study we aimed to investigate the effects of pairing correlation on various ground state properties of the isotopes of Cobalt, ranging from mass numbers 44 to 76.

ISSN No.: 2321-8649(Print) ISSN No.: 2321-9289(Online); Registration No. : CHAENG/2013/51628

The range of mass numbers include the magic configurations also and the effect of magicity on the properties could also be investigated in the light of pairing. The study was carried out using the HFBTHO code version 2.00d, employing SLy5 Skyrme force, with no reflection symmetry imposed. The results of numerical calculations are presented and are then compared with the available experimental values.

2. Materials and Methods

Hartree-Fock-Bogoliubov (HFB) theory is a mix of mean field and BCS theories. The general wave functions for the HFB approach incorporating the quasi-particles which move independently and as the possible correlations were determined by the variational principle. The HFB Hamiltonian in turn splits into two average potentials, viz. the self-consistent mean field Γ describing the shape of the nucleus and a pairing field Δ, originating from the BCS theory. In general, the HFB equations are a set of 2*M*-dimensional non-linear equations, where *M* represents the dimensionality of the quasi-particle space and possess 2*M* eigen values and eigen vectors [4].

The Hamiltonian used in the HFB approach can be written in occupation number representation as

$$H = \sum_{l_1 l_2} t_{l_1 l_2} c_{l_1} c_{l_2} + \frac{1}{4} \bar{v}_{l_1 l_2, l_3 l_4} c_{l_1} c_{l_2} c_{l_4} c_{l_3} \tag{1}$$

where $\bar{v}_{l_1 l_2, l_3 l_4} = v_{l_1 l_2 l_3 l_4} - v_{l_1 l_2 l_4 l_3}$, is the anti-symmetric two-body interaction matrix element. Here runs over all degrees of freedom of all available single particle states, here, up to M as stated before. We define eigen functions for the Hamiltonian as the ground state quasi-particle vacuum by using the Rayleigh-Ritz variational principle and are connected to the original particle operators through Bogoliubov transformation. The Hartree-Fock energy is obtained through the minimization of the variational parameter and thus the HFB equation is given by

$$\begin{bmatrix} e+\Gamma-\lambda & \Delta \\ -\Delta^* & (e+\Gamma)^* + \lambda \end{bmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix} \tag{2}$$

The HFB equation is solved by iterative diagonalization in the quasi-particle basis defined for protons and neutrons. In each iteration the particle number symmetry is restored by Lipkin-Nogami method, which acts the role of a Lagrange multiplier, by including an additional term λ in the HFB Hamiltonian [5].

The solution of HFB equation could be given by the expansion of quasi-particle wave function, which acts as the eigen function for the Hamiltonian, in a complete set of basis wave function, conserving axial symmetry and parity. After each iteration, with a given Fermi energy, we calculate the pairing gaps for both protons and neutrons given by

$$\Delta_k = 2E_k \sqrt{N_k (1 - N_k)} \tag{3}$$

where N_k is the norm of the single quasi-particle HFB wave functions and its sum over whole dimension would give the total particle number. The pairing interaction used here is given by

$$V_{pair}(r, r') = V_0 \left[1 - \eta \frac{\rho(r)}{\rho_0}\right] \delta(r - r') \tag{4}$$

where V_0 is the pairing strength, $\rho(r)$ is the isoscalar nucleonic density and $\rho_0 = 0.16\, fm^{-3}$. Setting the value of $\eta = 1$ gives us a pure pairing interaction, also known as surface interaction and $\eta = 0$ depicts a pairing interaction with no density dependence, known as volume interaction [4-8]. The value of $\eta = 0.5$, which is the average of the two interactions mentioned above, known as mixed pairing [9], is used in this program.

3. Results and Discussion

In tsection we present the results of our work, especially the effects of pairing on the binding energies, neutron and proton pairing energies, neutron and proton pairing gaps and one and two neutron separation energies.

The binding energies per nucleon of the isotopes of Cobalt, ranging from mass number 44 to 76, are calculated and could be seen that the binding energies of isotopes from our calculations with neutron numbers ranging from about 29, matches with the experimental values, till neutron number 37 Fig. 1 and the contribution due to the pairing is evident.

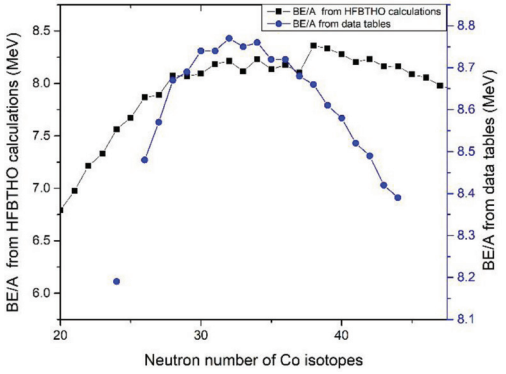

Figure 1: Graph showing BE/A from HFBTHO calculations plotted against neutron number of Co isotopes.

The pairing energies for the isotopes are calculated using the HFBTHO approach and is depicted in Fig. 2. The neutron pairing energy reaches its maximum at Z = 39 and Z = 22. For a particular range of isotopes, it can be seen that neutron pairing energy is zero, which means pair formation

is not obvious in those regions, which may be due to the shell closure effects in the vicinity of neutron magicity.

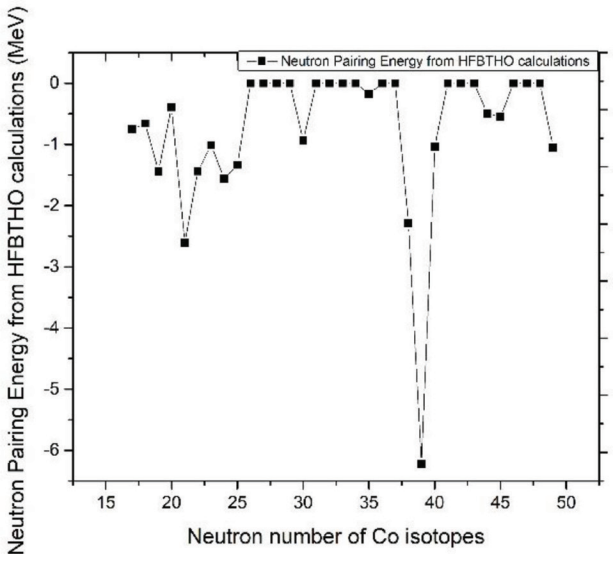

Figure 2: Graph showing neutron pairing energy from HFBTHO calculations plotted against neutron number of Co isotopes.

In the case of proton pairing energies Fig. 3, the pair formation is evident only in certain isotopes and around the regions of shell closure the pairing energy remains zero. Unlike the neutron pairing energies, the proton pairing energy remains zero for a continuous range of neutron numbers.

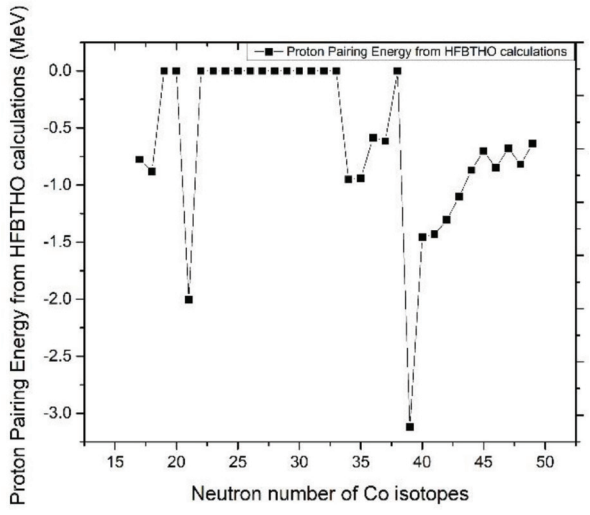

Figure 3: Graph showing proton pairing energy from HFBTHO calculations plotted against neutron number of Co isotopes.

The pairing gaps for both protons and neutrons (Fig. 4 and Fig. 5) exhibit a behavior quite opposite to that of the pairing energy. The proton pairing gaps for Z = 22 and Z = 39 are found to be the highest, which proves that the pairing is stronger in that region. Similarly, the neutron pairing gap (Fig. 5) is maximum for Z = 39 and for a majority of isotopes, the pairing gap is zero.

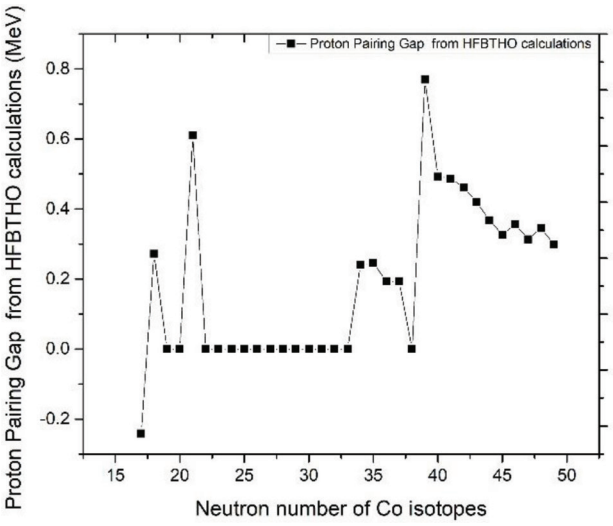

Figure 4: Graph showing proton pairing gap from HFBTHO calculations plotted against neutron number of Co isotopes.

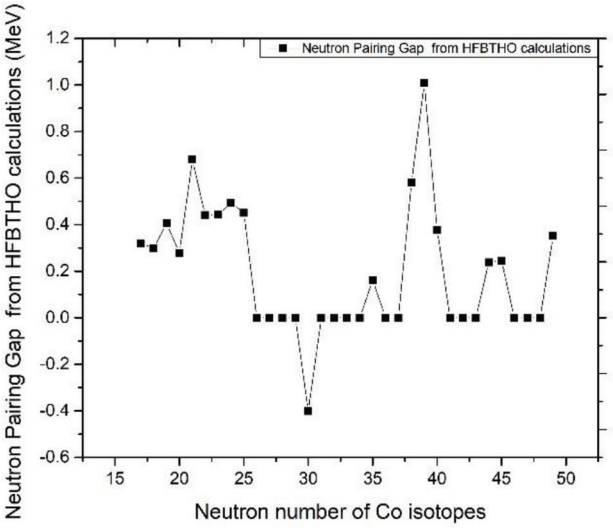

Figure 5: Graph showing neutron pairing gap from HFBTHO calculations plotted against neutron number of Co isotopes.

The one- and two-neutron separation energies are considered to be important parameters in describing the structure of nuclei. The one- $S_n(Z,N)$ and two- $S_{2n}(Z,N)$ neutron separation energies [7] could be defined as:

$$S_n(Z,N) = BE(Z,N) - BE(Z,N-1) \tag{5}$$

$$S_{2n}(Z,N) = BE(Z,N) - BE(Z,N-2) \tag{6}$$

where $BE(Z, N)$ represents binding energy of a nuclei with atomic number Z and neutron number N. The plots showing the variation of one- and two-neutron separation energies with respect to the neutron number are shown in Fig. 6 and Fig. 7 respectively.

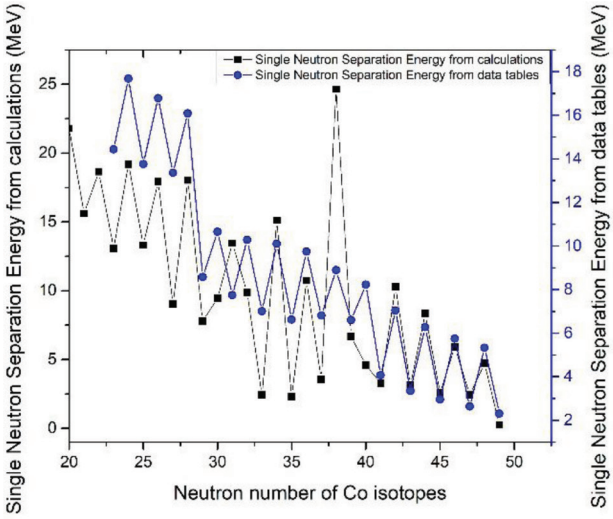

Figure 6: Graph showing single neutron separation energy from HFBTHO calculations plotted against neutron number of Co isotopes.

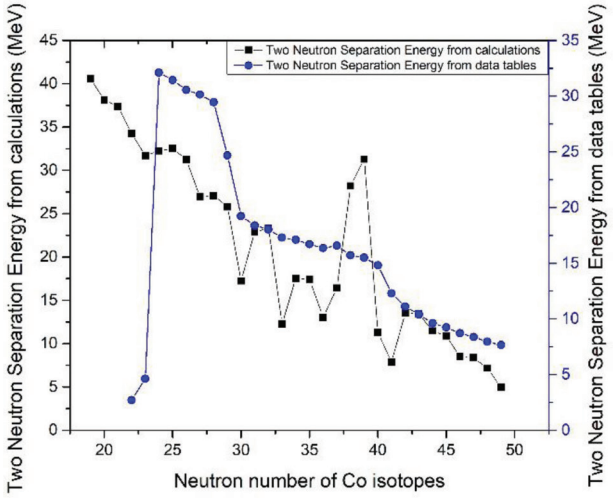

Figure 7: Graph showing two-neutron separation energy from HFBTHO calculations plotted against neutron number of Co isotopes.

It could be seen that the HFBTHO calculations of the one- and two-neutron separation energies agrees almost well with the theoretical results [10]. The sharp decreases which are clear around the magic configuration of neutrons are due to the shell closure effects. It could also be seen that as the neutron number approaches 50, both separation energies tend to approach zero and exhibits a trend to go negative.

Acknowledgements

One of the authors, Nicemon Thomas expresses his deep sense of gratitude to University Grants Commission, New Delhi, India, for the grant under Junior Research Fellowship (JRF) scheme (UGC-Ref. No.: 1386/ (CSIR-UGC NET JUNE 2017).

Authorship contribution

Nicemon Thomas: conception and design of the work, acquisition, analysis and interpretation of the data for the work, drafting and critical revision, review and editing. Anjana A V: technical editing and validation. Antony Joseph: overall supervision

Funding

No separate funding has been received by the authors for the research work mentioned in this article.

Conflict of Interest

The authors declare that there is no conflict of interest among the authors.

Declaration

The research work presented here is not published partially or fully, anywhere else, by me or someone else. It is declared that this is my original work.

References

[1] S. Frauendorf, A. O. Macchiavelli, Progress in Particle and Nuclear Physics, **78**, 24-90 (2014). https://doi.org/10.1016/j.ppnp.2014.07.001

[2] A. Bohr et al., Phys. Rev. **110**, 936 (1958). https://doi.org/10.1103/PhysRev.110.936

[3] R. A. Broglia and V. V. Zelevinsky, 50 years of Nuclear BCS Pairing in Finite Systems, (World Science Pub. 2012).

[4] P. Ring, P. Schuck, in: W. Beiglböck, et al. (Eds.), The Nuclear Many-Body Problem, (Springer-Verlag, New York, 1980).

[5] M. V. Stoitsov, J. Dobaczewski, et al., Comp. Phy. Comm. **167**(1), 43-63 (2005). https://doi.org/10.1016/j.cpc.2005.01.001

[6] J. Terasaki, et al., Nucl. Phys. A **600** 371–386 (1996). https://doi.org/10.1016/0375-9474(96)00036-X

[7] Y. El Bassem, M. Oulne, Nucl. Phys. A **957** 22-32 (2017). https://doi.org/10.1016/j.nuclphysa.2016.07.005

[8] M. V. Stoitsov et al., Computer Physics Communications **184,** 1592-1604 (2013). https://doi.org/10.1016/j.cpc.2013.01.013

[9] S. A.Changizi et al., Nuclear Physics A 940 210-226 (2015). http://dx.doi.org/10.1016/j.nuclphysa.2015.04.010

[10] X. Xia et al., At. Data Nucl. Data Tables, 121-122 1-215 (2018). http://dx.doi.org/10.1016/j.adt.2017.09.001

CHITKARA

Journal of Nuclear Physics, Material Sciences, Radiation and Applications

Chitkara University, Saraswati Kendra, SCO 160-161, Sector 9-C, Chandigarh, 160009, India

Volume 9, Issue 2 **February 2022** **ISSN 2321-8649**