A Study on Nuclear Pairing using BCS Theory

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Abstract. Pairing correlation in nuclei is recognized as the dominant many-body correlation beyond the nuclear mean-field. It was suggested by the occurrence of nuclear phenomena like the odd-even mass staggering (OES) and an energy gap of 1-2 MeV between the ground state and the lowest single-particle excitation. In this work, we have studied the temperature dependence of the pairing gap in ⁹⁴Sr & ¹²⁰Sn^{1,2}. The single-particle energies are calculated using the Nilsson Model and the pairing strength ($G_{p,n}$) by equating the pairing gap to the empirical pairing gap. The average pairing gap is found to vanish after the critical temperature. In the case of ¹²⁰Sn the proton pairing is found to be exactly zero at all temperatures (magic nuclei). The empirical pairing gap over the entire nuclear landscape, with the binding energy data taken from the Atomic Mass Evaluation 2020⁴. The empirical pairing gap data is grouped into four categories; even-even, odd-neutron, odd-proton and odd-odd. Each group is fitted with a power function aZ^b and aN^b for proton and neutron pairing respectively and the parameters are found. The overall fit in mass number (A) shows the power (b) to be $-\frac{1}{3}$ rather than the $-\frac{1}{2}$ from the accepted $12/\sqrt{A}$ law.

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1. INTRODUCTION

Pairing plays a crucial role in superconducting solids where it was first introduced by Bardeen, Cooper and Schrieffer [5]. This same theory was developed in the case of nuclei by Bohr, Mottelson and Pines [6] and Belyaev [7]. Bardeen, Cooper and Schrieffer (BCS) theory gives an approximate wave function for the pairing Hamiltonian and can be used to explain well-bound nuclei. In BCS theory two nucleons with the same quantum numbers except for the projection of their spin on the same axis interact attractively leading to a lower energy state. In section 2 we derive the FTBCS gap equation from the grand potential [1,2]. This gap equation along with particle number equation can be solved numerically and study the change in pairing gap with temperature. The empirical pairing gap can be calculated from odd-even mass staggering (OES) [3,8]. In section 3.1, the proton and neutron pairing gap of 94 Sr & 120 Sn are calculated using the finite temperature BCS equation

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(FTBCS). In section 3.2, we present the neutron and proton pairing gaps at zero temperature, these data are fitted with a power function aZ^b and aN^b for proton and neutron pairing respectively. The fitted parameters are given in Tables 1 & 2.

2. THEORETICAL FRAMEWORK

BCS theory was the first microscopic theory of superconductivity developed in 1957 [5]. It explained superconductivity in metals as the effect of condensation of Cooper pairs, which is the pairing of electrons near the Fermi level through the interaction with the crystal lattice. This coupling interaction is mediated by phonons. In BCS theory pairing takes place between electrons with opposite momenta and opposite spin (+k up,-k down). The pairs overlap strongly and form a condensate.

Similar phase transition behaviour is observed in atomic nuclei. In the case of nuclei, compared to a superconducting metal, it is finite and small. Secondly, there is not yet a reliable microscopic nuclear many-body theory where one can derive the pairing interaction and its strength. So to write the Hamiltonian of a nuclear system, we consider a single-particle model of non-degenerate orbitals ν (n, l, j, m_j). The pairing Hamiltonian of a system of nucleons interacting with the pairing force and having zero total angular momentum is written as follows [1,2].

$$\hat{H} = \sum_{\nu>0} (e_{\nu} - \lambda - E_{\nu}) + 2\sum_{\nu>0} E_{\nu} f_{\nu} + \frac{\Delta^2}{G}$$
(1)

Where G is the constant pairing strength, Δ is the pairing gap, λ is the Lagrange multiplier and also the chemical potential, e_{ν} is the single-particle energy, E_{ν} is the quasi-particle energy and f_{ν} is the Fermi-Dirac distribution function for quasi-particles.

$$E_{\nu} = \sqrt{\left(e_{\nu} - \lambda\right)^2 + \Delta^2} \tag{2}$$

$$f_{\nu} = \frac{1}{1 + e^{\beta E_{\nu}}} \tag{3}$$

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The grand potential is defined as

$$\Omega = \ln\left(Tr\left\{\exp(-\beta\hat{H})\right\}\right) \tag{4}$$

By substituting Eq. (1) in Eq. (4) we get.

$$\Omega = -\beta \sum_{\nu > 0} (e_{\nu} - \lambda - E_{\nu}) + 2 \sum_{\nu > 0} \ln\left[1 + \exp(-\beta E_{\nu})\right] - \beta \frac{\Delta^2}{G}$$
(5)

The standard choice for the gap parameter (Δ) is the value that minimizes the grand potential (Ω), so by minimizing Ω we get the finite temperature BCS gap equation.

$$\frac{\partial\Omega}{\partial\Delta} = \beta \sum_{\nu>0} \frac{\Delta}{E_{\nu}} - 2 \sum_{\nu>0} \frac{\exp(-\beta E_{\nu})}{1 + \exp(-\beta E_{\nu})} \frac{\beta\Delta}{E_{\nu}} - 2\beta \frac{\Delta}{G} = 0$$
(6)

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$$\sum_{\nu>0} \frac{1}{E_{\nu}} \left(1 - 2 \frac{\exp(-\beta E_{\nu})}{1 + \exp(-\beta E_{\nu})} \right) = \frac{2}{G}$$
(7)

The expression inside the bracket of Eq. (7) can be simplified as $\tanh\left(\frac{\beta E_{\nu}}{2}\right)$

$$\frac{2}{G} = \sum_{\nu>0} \frac{1}{E_{\nu}} \tanh\left(\frac{\beta E_{\nu}}{2}\right) \tag{8}$$

Similarly, the particle number expression can be derived from grand potential Ω .

$$N = \frac{\partial \Omega}{\partial \alpha} \tag{9}$$

Where $\alpha = \beta \lambda$

$$N = \sum_{\nu>0} \left[1 - \frac{(e_{\nu} - \lambda)}{E_{\nu}} \tanh\left(\frac{\beta E_{\nu}}{2}\right) \right]$$
(10)

Eq. (8) & Eq. (10) can be solved numerically. The dependence of Δ on T can be found. For a particular temperature, Δ becomes zero and is called critical temperature T_c . So Δ varies from $\Delta_0 \rightarrow 0$ as T varies from $0 \rightarrow T_c$.

3. RESULTS

3.1 FTBCS pairing gap

The pairing gap is calculated for 94 Sr & 120 Sn. We have found the single-particle energies of the nuclei from the Nilsson model. The maximum effect of pairing happens at T = 0 MeV, this is found by OES. The energy levels which are affected by the pairing are taken in summation which is close to the Fermi level. The levels are fixed and the pairing strength is adjusted so that the pairing gap matches the empirical odd-even staggering at T = 0 MeV.

3.1.1 Strontium - 94Sr

The proton pairing strength (G_p) of ⁹⁴Sr can be found by adjusting the proton pairing gap at zero temperature $(\Delta_p(0))$ to OES, which gives $G_p = 0.2803$ MeV and $\Delta_p(0) = 1.4961$ MeV. Similarly, we get $G_n = 0.18604$ MeV and $\Delta_n(0) = 1.0059$ MeV. The energy levels taken are $N_1 = 4$, $N_2 = 35$ and $N_1 = 14$, $N_2 = 45$ respectively. Where $N_1 \& N_2$ are lower and upper limits of the energy levels taken in the FTBCS equations.

3.1.2 Tin - ¹²⁰Sn

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In the case of ¹²⁰Sn, Z = 50 is a magic number (closed shell), there is no proton pairing due to the shell closure. Where as the neutron pairing is present as N = 70, the G_n value of ¹²⁰Sn can be

found by adjusting $\Delta_n(0)$ to OES, which gives $G_n = 0.2019$ MeV and $\Delta_n(0) = 1.3918$ MeV. The energy levels taken are $N_1 = 10, N_2 = 41$ and $N_1 = 18, N_2 = 52$ respectively.



Figure 1. The variation of proton and neutron pairing gaps in 94 Sr nucleus with the temperature is presented. The critical temperature, $T_c = 0.8282$ MeV for proton pairing and $T_c = 0.5455$ MeV for neutron pairing.



Figure 2. Same as Fig. 1, but for the nucleus ¹²⁰Sn. The critical temperature, $T_c = 0.7273$ MeV for neutron pairing and no proton pairing.

3.2 Empirical pairing gap

The empirical pairing gap is found using the five-point formula given in [3,8]. The binding energy data is taken from Atomic Mass Evaluation 2020 [4]. Neutron and proton pairing gaps are evaluated separately and fitted with function aX^b where X=N,Z respectively. Then the average pairing gap

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is found and fitted with function aA^b . Where a & b are fitting parameters. We exclude nuclei with a mass number (A) less than 16. In Figures 3 & 4 pairing gaps are fitted to neutron and proton numbers respectively. The numerical values of the fitting parameters are included in Tables 1 & 2.



Figure 3. The neutron pairing gap of the following nuclei are calculated and fitted. (a) Even-even nuclei (Δ_n^{e-e}) . (b) Odd-neutron nuclei (Δ_n^{o-n}) . (c) Odd-proton nuclei (Δ_n^{o-p}) . (d) Odd-odd nuclei (Δ_n^{o-o}) . The black dash-dotted line is determined by fitting to the data using the function aN^b .



Figure 4. The proton pairing gap of the following nuclei are calculated and fitted. (a) Even-even nuclei (Δ_p^{e-e}) . (b) Odd-neutron nuclei (Δ_p^{o-n}) . (c) Odd-proton nuclei (Δ_p^{o-p}) . (d) Odd-odd nuclei (Δ_p^{o-o}) . The black dash-dotted line is determined by fitting to the data using the function aZ^b .

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Table 1. The fittings of empirical neutron pairing gaps in even-even, odd-N, odd-Z and odd-odd nuclei from five point formula as functions of N and the corresponding root-mean-square deviation and coefficient of determination R^2 (with 95% confidence bounds).

Group of	Number of	parameter of the pairing		RMS	R square
Nuclei	Nuclei	gap function aN^b		Deviation (σ)	
		$a \pm \Delta a$	$b \pm \Delta b$		
Even-even	424	5.682 ± 0.221	-0.373 ± 0.011	0.341	0.741
Odd-Neutron	384	22.124 ± 1.584	-0.713 ± 0.018	0.317	0.830
Odd-Proton	445	2.377 ± 0.024	-0.224 ± 0.002	0.236	0.935
Odd-odd	410	6.764 ± 0.473	-0.496 ± 0.011	0.234	0.640

Table 2. The fittings of empirical proton pairing gaps in even-even, odd-N, odd-Z and odd-odd nuclei from five point formula as functions of Z and the corresponding root-mean-square deviation and coefficient of determination R^2 (with 95% confidence bounds).

Group of	Number of	parameter of the pairing		RMS	R square
Nuclei	Nuclei	gap function aZ^b		Deviation (σ)	
		a $\pm \Delta$ a	$b \pm \Delta b$		
Even-even	378	5.211 ± 0.195	-0.362 ± 0.011	0.340	0.737
Odd-Neutron	378	1.886 ± 0.108	-0.175 ± 0.017	0.265	0.233
Odd-Proton	339	8.223 ± 0.482	-0.476 ± 0.016	0.309	0.743
Odd-odd	346	1.293 ± 0.063	-0.027 ± 0.014	0.219	0.010

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4. CONCLUSION

The dependence of temperature on the pairing is studied using the finite-temperature BCS theory. We have plotted the average pairing gap with temperature for ⁹⁴Sr & ¹²⁰Sn. The G value (Pairing strength) for protons is found to be greater than neutrons as expected. The proton pairing is larger than neutron pairing as it is equated to OES. The proton pairing of ¹²⁰Sn is found to be zero which is exact for low pairing strength as Tin is a magic nucleus in proton number. The critical temperature on average is also related to Δ_0 as $T_c = 0.53\Delta_0$ for neutron and proton pairing. Above these critical temperature we found that the pairing to be zero.

We have calculated empirical nuclear pairing using the five-point formula and fitted it with a power function. The five-point formula reduces most of the effects from the persisting mean-field than the previously used three-point formula. A global calculation for both proton and neutron pairing gap over the entire nuclear landscape has been performed with the binding energy data from Atomic Mass Evaluation 2020 [4]. From these fits, we found that except for the proton pairing of odd-neutron nuclei (Fig. 4 (b)) and odd-odd nuclei (Fig. 4 (d)), the power function is giving a very good fit. The poor fit for these cases may indicate the presence of a constant term in the fitted function. We haven't checked the dependence of neutron excess (N – Z) in pairing. An overall fit corresponding to all nuclei groups to a function of mass number (A) is fitted. The result is $(4.609 \pm 0.014)A^{-0.33}$ which is a $-\frac{1}{3}$ dependence rather than the $-\frac{1}{2}$ from the accepted $12/\sqrt{A}$ law. This implies a weaker dependence on pairing gap than the usual [9], and The current result supports a $-\frac{1}{3}$ law [10].

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