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Bogoliubov Laboratory of Theoretical Physics

FINAL REPORT ON THE
SUMMER STUDENT PROGRAM

On pairing correlations and blocking effect in nuclei within the BCS theory

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Abstract

Pairing correlations in nuclei near ^{56}Fe are studied within the BCS theory. Pairing gap is calculated in spherical atomic nuclei with valence nucleons located on $1f_{7/2}$ and $2p_{3/2}$ shells. In systems consisting of odd number of nucleons, blocking effect is taken into account.

1 Introduction

Now it is well established that pairing correlations have a significant influence on nuclear structure and various properties of nuclei, including their form, decay parameters, etc [1, 2]. Of particular interest is the phenomenon taking place in systems with odd number of nucleons and known as the blocking effect. The blocking effect appears to be of great importance, as it may allow to account for the location of low-lying one- and two-quasiparticle states in heavy nuclei [3].

In this work, pairing correlations are studied for the set of sample nuclei, ^{51}Sc, ^{52}Ti, ^{53}V, ^{54}Cr, ^{55}Mn, ^{56}Fe, ^{57}Fe, ^{57}Co, and blocking effect is taken into account. It is assumed that all isotopes considered in this work are spherical. The proton and neutron mean fields are approximated by the Woods-Saxon potential. The BCS theory is applied to calculate the energy gap and to study the blocking effect. The parameters of the Woods-Saxon potential and the strength of pairing interaction are adjusted to reproduce nucleon separation energies.

2 Theoretical background

2.1 Model Hamiltonian

More than 50 years ago Bohr, Mottelson, Pines [4] and Belyaev [5] made a suggestion, according to which the observed pairing interaction in atomic nuclei may share properties similar to those in superconductors. First worked out by Bardeen, Cooper and Schrieffer [6], the theory of superconductivity can be adjusted to describe the low-energy excited states of medium and heavy nuclei.

To describe pairing correlations in atomic nuclei, we start from a simple Hamiltonian containing mean field for protons and neutrons and the pairing interaction:

$$H_0 = H_{av} + H_{pair} = \sum_{\tau=n,p}\sum_{j,m}(E_j - \lambda_\tau)a^\dagger_{jm}a_{jm} - \sum_{\tau=n,p}\frac{G_\tau}{4}\sum_{\substack{j_1,m_1\\ j_2,m_2}} a^\dagger_{j_1m_1}a^\dagger_{\overline{j_1m_1}}a_{\overline{j_2m_2}}a_{j_2m_2}, \qquad (1)$$

$$a_{\overline{jm}} = (-1)^{j-m}a_{j,-m}. \qquad (2)$$

Here, E_j is the single particle energies, λ_τ stands for chemical potential, and G_τ is the strength of pairing interactions.

In order to describe the mean field of spherical nuclei, Woods-Saxon potential is used. There are two terms contributing to the Woods-Saxon potential:

1. the central term

$$V(r) = -\frac{V_0^{N,Z}}{1+\exp[\alpha(r-R_0)]} \qquad (3)$$

2. and the spin-orbital term

$$V_{ls} = -\varkappa \frac{\mathrm{d}V(r)}{\mathrm{d}r}(\mathbf{ls}). \tag{4}$$

Here, $V_0^{N,Z}$ stands for the depth of neutron and proton potential wells; α is the diffusion parameter; $\varkappa$ is the constant of spin-orbital interaction; $R_0 = r_0 A^{1/3}$ is the nuclear radius. For protons, this potential should be further complemented with the term corresponding to Coulomb interaction. For a uniformly charged sphere it reads as:

$$V_c = \frac{(Z-1)e^2}{r} \begin{cases} (3/2)(r/R_0) - (1/2)(r/R_0)^3, & r \leqslant R_0; \\ 1, & r > R_0. \end{cases} \tag{5}$$

Parameters of the Woods-Saxon potential α, $\varkappa$ and r_0 are chosen according to parametrization suggested in [7]. The depth of the potential, $V_0^{N,Z}$, is adjusted to reproduce the neutron and proton separation energies (see the discussion below).

2.2 BCS method

To account for pairing correlations in the nuclear system described by the Hamiltonian (1) we apply the method suggested by N.N. Bogoliubov and further developed by V.G. Soloviev. Namely, we introduce quasiparticle creation and annihilation operators:

$$a^\dagger_{jm} = u_j \alpha^\dagger_{jm} + v_j \alpha_{\overline{jm}}, \tag{6}$$

$$a_{jm} = u_j \alpha_{jm} + v_j \alpha^\dagger_{\overline{jm}}. \tag{7}$$

Quasipartile creation and annihilation operators should satisfy the fermionic anticommutation relations. Therefore, the following relations between real functions u_j and v_j should be valid:

$$\eta_j = u_j^2 + v_j^2 - 1 = 0. \tag{8}$$

The vacuum of quasiparticles,

$$\alpha_{jm}|BCS\rangle = 0, \langle BCS|\alpha^\dagger_{jm} = 0, \tag{9}$$

is the ground state for a system with even number of particles.

To find the energy and the structure of Bogoliubov quasiparticles we should minimize the expectation value of the pairing Hamiltonian with respect to the BCS vacuum state

$$\langle BCS|H_0|BCS\rangle \equiv \langle H_0\rangle. \tag{10}$$

To compute $\langle H_0\rangle$ we need to know the matrix elements $\langle a^\dagger_{jm} a_{jm}\rangle$ and $\langle a^\dagger_{j_1 m_1} a^\dagger_{\overline{j_1 m_1}} a_{\overline{j_2 m_2}} a_{j_2 m_2}\rangle$. For $\langle a^\dagger_{jm} a_{jm}\rangle$ we have

$$\langle a^\dagger_{jm} a_{jm}\rangle = \langle v_j \alpha_{\overline{jm}} v_j \alpha^\dagger_{\overline{jm}}\rangle = v_j^2.$$

To compute $\langle a^\dagger_{j_1m_1} a^\dagger_{\overline{j_1m_1}} a_{\overline{j_2m_2}} a_{j_2m_2}\rangle$ we apply Wick's theorem. As a result we get

$$\begin{aligned}\langle a^\dagger_{j_1m_1} a^\dagger_{\overline{j_1m_1}} a_{\overline{j_2m_2}} a_{j_2m_2}\rangle &= \langle a^\dagger_{j_1m_1} a^\dagger_{\overline{j_1m_1}}\rangle\langle a_{\overline{j_2m_2}} a_{j_2m_2}\rangle \\ &- \langle a^\dagger_{j_1m_1} a_{\overline{j_2m_2}}\rangle\langle a^\dagger_{\overline{j_1m_1}} a_{j_2m_2}\rangle \\ &+ \langle a^\dagger_{j_1m_1} a_{j_2m_2}\rangle\langle a^\dagger_{\overline{j_1m_1}} a_{\overline{j_2m_2}}\rangle \\ &= u_{j_1}u_{j_2}v_{j_1}v_{j_2} + (\delta_{m_1m_2} - \delta_{m_1-m_2})\delta_{j_1j_2}v^2_{j_1}v^2_{j_2}(-1)^{j_1+j_2-m_1-m_2}.\end{aligned}$$

Then, taking into account the $(2j+1)$-degeneracy of the spherical nuclei levels, we obtain the following expression for $\langle H_0\rangle$:

$$\langle H_0\rangle = \sum_{\tau j} v^2_j(2j+1)[E_j - \lambda_\tau] - \sum_\tau \frac{G_\tau}{4}\left[\sum_j u_j v_j (2j+1)\right]^2. \tag{11}$$

To minimize $\langle H_0\rangle$ we vary it with respect to unknown u_j and v_j functions. Since these functions are not independent and Eq. (8) should be satisfied, we introduce additional Lagrange multipliers μ_j. Then, variations δu_j and δv_j can be treated as independent, and the extremum condition takes the form:

$$\delta\Big\{\langle BCS|H_0|BCS\rangle + \sum_j \mu_j\eta_j\Big\} = 0. \tag{12}$$

This condition can be applied to the proton and neutron systems separately. As a result, we get the following system of equations:

$$\begin{cases} 2(2j+1)(E_j-\lambda_\tau)v_j - \dfrac{G_\tau}{2}u_j(2j+1)\displaystyle\sum_{j'} u_{j'}v_{j'}(2j'+1) + 2\mu_j v_j = 0, \\ -\dfrac{G_\tau}{2}v_j(2j+1)\displaystyle\sum_{j'} u_{j'}v_{j'}(2j'+1) + 2\mu_j v_j = 0. \end{cases} \tag{13}$$

By excluding μ_j we obtain:

$$2(2j+1)v_ju_j(E_j-\lambda_\tau) - \frac{G_\tau}{2}(2j+1)(u^2_j - v^2_j)\sum_{j'} u_{j'}v_{j'}(2j'+1) = 0. \tag{14}$$

Now, we introduce the so-called correlation function (also referred to as the pairing gap):

$$\Delta_\tau = \frac{G_\tau}{2}\sum_j u_j v_j (2j+1). \tag{15}$$

With the help of the correlation function Eq. (14) can be rewritten as:

$$2(2j+1)v_ju_j(E_j-\lambda_\tau) - \frac{G_\tau}{2}(2j+1)(u^2_j - v^2_j)\Delta_\tau = 0. \tag{16}$$

This equation should be supplemented by the particle number equation:

$$N = \sum_j (2j+1)v^2_j, \tag{17}$$

where the value $(2j+1)v_j^2$ stands for particle density on the j shell.

The non-trivial solution of Egs. (16) and (17) is given by:

$$u_j^2 = \frac{1}{2}\left(1 + \frac{E_j - \lambda_\tau}{\varepsilon_j}\right), \tag{18}$$

$$v_j^2 = \frac{1}{2}\left(1 - \frac{E_j - \lambda_\tau}{\varepsilon_j}\right), \tag{19}$$

where $\varepsilon_j = \sqrt{(E_j - \lambda_\tau)^2 + \Delta_\tau^2}$ is the quasiparticle energy. By means of straightforward derivations, we can show that:

$$u_j v_j = \frac{1}{2}\frac{\Delta_\tau}{\varepsilon_j}. \tag{20}$$

This equation along with (15) gives:

$$1 = \frac{G_\tau}{4}\sum_j \frac{2j+1}{\sqrt{(E_j - \lambda_\tau)^2 + \Delta_\tau^2}}. \tag{21}$$

At the same time, from (17) and (19) we obtain:

$$N = \frac{1}{2}\sum_j (2j+1)\left(1 - \frac{E_j - \lambda_\tau}{\varepsilon_j}\right). \tag{22}$$

Equations (21) and (22) are well known BCS equations for spherical nuclei. The solution of these equations describes superfluid properties of the nuclear system with the Hamiltonian (1).

Within the BCS theory the Hamiltonian (1) describes the system of non-interacting Bogoliubov quasiparticles

$$H_0 \approx \sum_\tau \sum_{jm} \varepsilon_{jm} \alpha_{jm}^\dagger \alpha_{jm}. \tag{23}$$

Elementary excitations in such a system are given by two-quasiparticle states built on the top of the BCS vacuum, i.e., $\alpha_{j_1 m_1}^\dagger \alpha_{j_2 m_2}^\dagger |BCS\rangle$. The energy of these states is separated from the ground-state energy by the energy gap

$$\varepsilon_{j_1} + \varepsilon_{j_2} \geq 2\Delta. \tag{24}$$

2.3 Blocking effect

Equations (21) and (22) hold only for even systems. If we place an odd particle on a given single-particle level, this level becomes partially blocked due to Pauli principle. So it is clear that odd particle should affect the superfluid properties of the system.

Within the BCS theory the system containing odd number of nucleons is described as a one-quasiparticle state $\alpha_{jm}|BCS\rangle$. To describe pairing correlations in such a system we should minimize the expectation value of the Hamiltonian (1) with respect to one-quasiparticle state. For

the expectation value we have

$$\langle \alpha_{j'm'} H_\tau \alpha^\dagger_{j'm'} \rangle = E_{j'} - \lambda_\tau + (2j'-1)\left[E_{j'} - \lambda_\tau - \frac{G_\tau}{2} v^2_{j'}\right] v^2_{j'}$$

$$+ \sum_{j \neq j'} v^2_j (2j+1)\left[E_j - \lambda_\tau - \frac{G_\tau v^2_j}{2}\right] - G_\tau \left[\sum_{j \neq j'} (j+\frac{1}{2}) u_j v_j + (j'-\frac{1}{2}) u_{j'} v_{j'}\right]^2 . \quad (25)$$

Here, j' stands for the single-particle level containing the quasiparticle. To minimize (25), we apply the method described in the previous section. Then, after some algebra we derive:

$$2(2j+1) v_j u_j (E_j - \lambda_\tau) - \frac{G_\tau}{2}(2j+1)(u^2_j - v^2_j)\left\{\sum_{j'' \neq j'} (2j''+1) u_{j''} v_{j''} + (2j'-1) u_{j'} v_{j'}\right\}^2 = 0. \quad (26)$$

For the odd system the correlation function (i.e., the pairing gap) is defined as:

$$\Delta_\tau(j') = \frac{G_\tau}{2}\left\{\sum_{j \neq j'} (2j+1) u_j v_j + (2j'-1) u_{j'} v_{j'}\right\}. \quad (27)$$

Then the BCS equations for the odd system take the form:

$$1 = \frac{G_\tau}{4}\left\{\sum_{j \neq j'} \frac{2j+1}{\varepsilon(j|j')} + \frac{2j'-1}{\varepsilon(j'|j')}\right\}, \quad (28)$$

$$N = \sum_{j \neq j'} (2j+1) v^2_j(j') + (2j'-1) v^2_{j'}(j') + 1, \quad (29)$$

where

$$\varepsilon(j|j') = \sqrt{(E_j - \lambda_\tau(j'))^2 + \Delta^2_\tau(j')},$$

$$v^2_j(j') = \frac{1}{2}\left(1 - \frac{E_j - \lambda_\tau(j')}{\varepsilon(j|j')}\right), \;\; u^2_j(j') = 1 - v^2_j(j').$$

For the odd system, the ground state correspond to one-quasiparticle configuration with minimal energy. Then, the energies of excited one-quasiparticle configurations are

$$\varepsilon_{j_2} - \varepsilon^{min}_{j_1}. \quad (30)$$

So, it is seen that in the odd systems there is no an energy gap between the ground and excited states.

3 Results

To obtain the single-particle level scheme the parameters of Woods-Saxon potential are fitted for ^{56}Fe according to parametrizion from Ref. [7]. The numerical solution of the Schroedinger

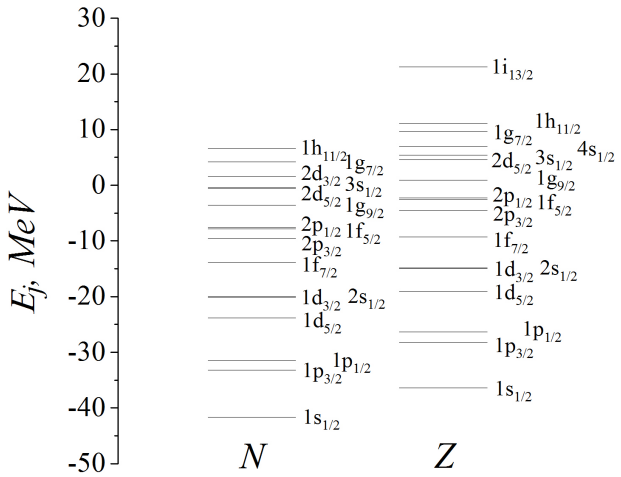

Figure 1: Neutron (to the left) and proton (to the right) single-particle energies in ^{56}Fe

equation is performed with the help of Fortran code described in Ref. [8]. The depth of the potential and the strength of pairing interaction are adjusted to reproduce experimental nucleon separation energies and odd-even mass difference:

$$S_\tau = \Delta_\tau - \lambda_\tau, \quad (\tau = n,\ p), \tag{31}$$

$$\Delta_p = \frac{1}{4}\{3M(Z-1,N) + M(Z+1,N) - 3M(Z,N) - M(Z-2,N)\}, \tag{32}$$

$$\Delta_n = \frac{1}{4}\{3M(Z,N-1) + M(Z,N+1) - 3M(Z,N) - M(Z,N-2)\}. \tag{33}$$

For ^{56}Fe we have $S_n = 11.197$ MeV, $S_p = 10.183$ MeV, $\Delta_n = 1.36$ MeV, $\Delta_p = 1.57$ MeV. The resulting values for $V_0^{N,Z}$ and $G_{n,p}$ are: $V_0^N = 51.90$ MeV, $V_0^Z = 57.19$ MeV, $G_n = 0.303$ MeV, $G_p = 0.335$ MeV. The obtained single-particle level scheme for protons and neutrons is shown in Fig. 1.

To solve the BCS equations with and without blocking effect the Fortran code was created (see Appendix). The code solves the nonlinear BSC equations by applying the Newton method. As an output, the code provides the pairing energy gaps $\Delta_{n,s}$, the chemical potentials $\lambda_{n,p}$, the coefficients u_j, v_j of the Bogoliubov transformation, and the energies ε_j for proton and neutron quasiparticles.

For ^{57}Fe and ^{57}Co we study the effect of unpaired odd particle on pairing correlations. To this aim we place an unpaired particle on different single-particle levels and solve the BCS equations taking into account the blocking effect. Note, that in the ground state of ^{57}Fe the odd neutron is located on $2p_{3/2}$ orbit, while in ^{57}Co the odd proton is located on $1f_{7/2}$ orbit. In Figs. 2 and 3 we show the value of pairing gap as a function of odd particle quantum numbers. As we can see, for considered nuclei the pairing gaps reaches their minimal values in the nuclear ground states. When we put an unpaired particle on single-particle levels far from the Fermi level, the pairing correlations gain strength and the pairing gap monotonically increases.

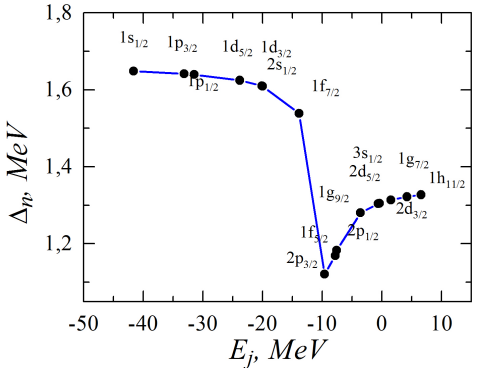

Figure 2: Energy gap in ^{57}Fe as a function of odd neutron single-particle energy.

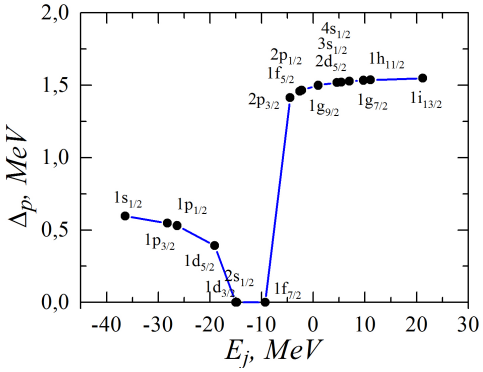

Figure 3: Energy gap in ^{57}Co as a function of odd proton single-particle energy.

Of particular interest is the behaviour of the proton energy gap in ^{57}Co. In the ground state of ^{57}Co, the proton pairing correlations completely vanish due to blocking effect. This is also true if we put an odd proton on $2s_{1/2}$ and $1d_{3/2}$ levels, both of which are quite close to Fermi level. However, the blocking effect diminishes with moving away from the Fermi level and, therefore, pairing correlations appear. This effect demonstrates that pairing correlations in nuclear excited states can differ significantly from those in the nuclear ground state.

We also study the proton pairing correlations in isotones with $N = 30$. In Fig. 4 we show the pairing gap as a function of the proton number Z. As seen from the figure, pairing correlations completely vanish for $Z = 20$ This corresponds to completely empty $1f_{7/2}$ orbit. Pairing correlations are most pronounced when the $1f_{7/2}$ level is half-filled. From the figure we also observe that the pairing gap in the odd systems is lesser than that in the neighbouring even systems. This clearly demonstrates the blocking effect.

4 Summary

Pairing gap behaviour and blocking effect in even-even and odd-A nuclei near ^{56}Fe were studied. It is shown that taking into account the blocking effect allows us to explain the reduction or vanishing of pairing correlations in the considered odd nuclei.

In the course of this work, I was aimed to study the BCS model describing pairing correlations responsible for superfluidity in atomic nuclei. Toward this end I learned the theoretical methods of nuclear many-body problem. Namely, the method of second quantization, the method of u, v Bogoliubov transformation, and the concept of quasiparticle. I derived BCS equations for even and odd nuclear systems. In the latter case, the blocking effect was taken into account. To perform numerical calculations, I improved my skills and abilities in writing Fortran codes. To solve the non-linear BCS equations, I got familiar with Newton's method.

During my summer practice I got acquainted with many scientists working in theoretical nuclear physics. Discussions with them broadened my scientific background and let me learn about

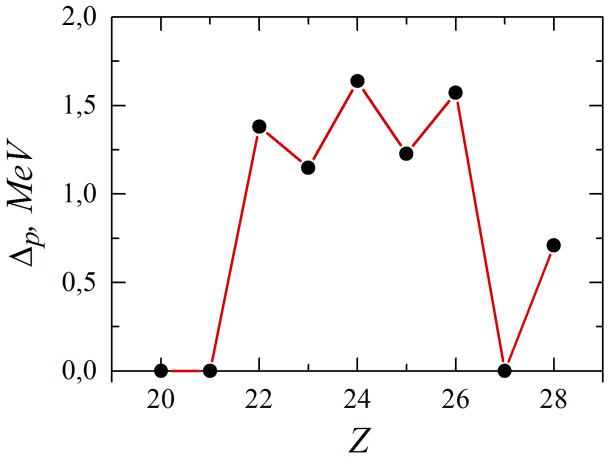

Figure 4: Δ_p as a function of Z in isotones with $N = 30$

actual problems of modern nuclear physics.

5 Acknowledgements

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References

[1] S. Frauendorf, A.O. Macchiavelli // Progress in Particle and Nuclear Physics 78 (2014) 2490

[2] F.Šimkovic, Ch.C. Moustakidis, L. Pacearescu, Amand Faessler // Proton-neutron pairing in the deformed BCS approach

[3] V. G. Soloviev // Theory of Complex Nuclei (Publishing house "Science", Home edition of Physical and Mathematical Literature, Moscow, 1976) [in Russian]

[4] A. Bohr, B.R. Mottelson, D. Pines // Phys. Rev. 110, 936 (1958)

[5] S.T. Belyaev // Mat. Fys. Medd. Dan. Vid. Selsk. 31, no 11, 1 (1957)

[6] J. Bardeen, L.N. Cooper, J.R. Schrieffer // Phys. Rev. 108, 1175 (1957)

[7] V.A. Chepurnov // Nuclear Physics, Vol. 5, 955 (1967)

[8] M.H. Gizatkulov, I.V. Puzynin, R.M. Yamaleev // JINR P11 - 10029 (1976) [in Russian]

[9] A. Bohr, B.R. Mottelson // Nuclear Structure. Vol. 1. N. Y., (1969)

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Fortran program for numerical solution of BCS equations

The following program was used in order to solve the BCS equations.

```
      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON/EINDE/E(100),INDE(100)
      COMMON/EPSUV/EPS(100),U(100),V(100)
      dimension rj(100)
      integer odd_n, odd_p
      logical flag_n, flag_p


 6017 FORMAT(/20X,'EVEN-EVEN NUCLEUS Z =',I3,'  A =',I3
     */1X,'GR. STATE N =',I4,5X,'GR. STATE Z =',I4,5X,'GN =',F10.3
     *,5X,'GP =',F10.3/1X,'CN =',F10.5,5X,'CP =',F10.5,5X,'LAMN =',
     *F10.5,5X,'LAMP =',F10.5)
 6019 FORMAT(/9X,'I',' INDE',9X,'E',7X,'EPS',9X,'U',9X,'V')
 6020 FORMAT(I10,I5,4F10.5,e12.3)
 6028 FORMAT(/2X,'*****INCORRECT GROUND STATE N =',I4,5X,'Z =',I4)
 6029 FORMAT(/2X,'*****INCORRECT ODD NEUTRON OR ODD PROTON STATE')



      OPEN(15,FILE='bcs.inp',FORM='FORMATTED',STATUS='OLD')
      OPEN(16,FILE='bcs.out',FORM='FORMATTED',STATUS='unknown')



C.....READ AND PRINT ENERGIES
      OPEN(71,FILE='sp.n',FORM='FORMATTED',STATUS='OLD')
      read(71,*)nen
      do  i=1,nen
      read(71,*)inde(i),e(i)
      enddo
      close(71)
      OPEN(71,FILE='sp.z',FORM='FORMATTED',STATUS='OLD')
      read(71,*)nep
      do  i=1,nep
      read(71,*)inde(i+nen),e(i+nen)
      enddo
      close(71)

      MIN=NEN+1
```

```
    MAX=NEN+NEP



    READ(15,*) IZ,IA                                    ! Z and A
    READ(15,*) GN,GP
    read(15,*) odd_n
    read(15,*)  odd_p


    IGRN=0
    IGRP=0
    flag_n=.FALSE.
    flag_p=.FALSE.

    DO 501 I=1,NEN                                      ! finding  the
    J=INDE(I)-(INDE(I)/10)*10                           ! last neutron
    IGRN=IGRN+2*(J+1)                                   ! occupied level
    IF(IGRN.LT.IA-IZ) GO TO 501
    IGRSTN=I
    IGRN=INDE(I)
    RLAMN = E(I)
    GO TO 502
501 CONTINUE
502 CONTINUE



    DO 511 I=MIN,MAX                                    ! finding  the
    J=INDE(I)-(INDE(I)/10)*10                           ! last proton
    IGRP=IGRP+2*(J+1)                                   ! occupied level
    IF(IGRP.LT.IZ) GO TO 511
    IGRSTP=I
    IGRP=INDE(I)
    RLAMP = E(I)
    GO TO 512
511 CONTINUE
512 CONTINUE

    IF (odd_n.EQ.0) THEN                                ! looking for
        flag_n=.TRUE.                                   ! the odd neutron
    ELSE                                                ! level
        DO 513 I=1,NEN
            IF (odd_n.EQ.INDE(I)) THEN
                flag_n=.TRUE.
                odd_n = I
```

```
                GO TO 514
              END IF
  513     CONTINUE
      END IF
  514 CONTINUE

      IF (odd_p.EQ.0) THEN                                ! looking for
          flag_p=.TRUE.                                   ! the odd proton
      ELSE                                                ! level
          DO 515 I=MIN,MAX
              IF (odd_p.EQ.INDE(I)) THEN
                  flag_p=.TRUE.
                  odd_p = I
                  GO TO 516
              END IF
  515     CONTINUE
      END IF
  516 CONTINUE

  144 IF(IGRSTN.NE.0.AND.IGRSTP.NE.0) GO TO 146
      WRITE(*, 6028)IGRN, IGRP
      stop
  146 CONTINUE
      IF(flag_n.AND.flag_p) GO TO 147
      WRITE(*, 6029)
      stop
  147 CONTINUE

c>>>>>>>>>>>>>>>>>>>>>>>>>>>>  BEGIN BCS <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<

   !     gap and lambda for neutrons
      CN = 0.0d0
      CALL CLAM(1,NEN, IA-IZ+0.d0,GN,0,0,CN,RLAMN,EGRN,odd_n)
!     gap and lambda for protons
      CP = 0.0d0
      CALL CLAM(NEN+1,NEN+NEP,IZ+0.D0,GP,0,0,CP,RLAMP,EGRP,odd_p)
!     eps, u, v
      CALL EPSUVS(CN,CP,RLAMN,RLAMP,NEN,NEP)

c>>>>>>>>>>>>>>>>>>>>>>>>>>>>  END BCS <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<




c     ***************** start printing BCS results ************************
```

```
      write(*,'(1x)')
write(*,'(A4,I3,A7,I3)')' A =',IA,'    Z =',IZ
write(*,'(1x)')
      write(*,'(A11,F6.3,A4,A11,F6.3,A4)')'      G_n =',GN,    ' MeV',
     *                                    '      G_p =',GP,    ' MeV'
      write(*,'(1x)')
write(*,'(A8,F5.2,A4,A12,F7.3,A4)')'   C_n =',CN,    ' MeV',
     *                              '  Lambda_n =',rlamn, ' MeV'
write(*,'(A8,F5.2,A4,A12,F7.3,A4)')'   C_p =',CP,    ' MeV',
     *                              '  Lambda_p =',rlamp, ' MeV'
      write(*,'(1x)')


      WRITE(16, 6017)IZ,IA,IGRN,IGRP,GN,GP,CN,CP,RLAMN,RLAMP

      WRITE(16, 6019)

      write(16,'(1x)')
      Zn=0.d0
      WRITE(16, '(A25)')'          N E U T R O N S'
      DO 3 I=1,NEN                                          ! control N
      RJ(i)=INDE(i)-(INDE(i)/10)*10+1.0D0
      RJ(i)=RJ(i)*0.5
Zn=Zn+2.0*rj(i)*(1-(E(i)-rlamn)/eps(i))
    3 WRITE(16, 6020)I,INDE(I),E(I),EPS(I),U(I),V(I)
      IF (odd_n.NE.0) Zn=Zn-(1-(E(odd_n)-rlamn)/eps(odd_n))+1
      print*,'Nn=',zn



      write(16,'(1x)')
      WRITE(16,'(A23)')'          P R O T O N S'
      Zp=0.d0
      DO 4 I=MIN,MAX
      RJ(i)=INDE(i)-(INDE(i)/10)*10+1.0D0
      RJ(i)=RJ(i)*0.5
Zp=Zp+2.0*rj(i)*(1-(E(i)-rlamp)/eps(i))                ! control P
    4 WRITE(16, 6020)I,INDE(I),E(I),EPS(I),U(I),V(I)
      IF (odd_p.NE.0) Zp=Zp-(1-(E(odd_p)-rlamp)/eps(odd_p))+1
      print*,'Np=',zp


c      *************************end printing BCS ************************


      CLOSE(15)
```

```
      CLOSE(16)
      pause
      END



C*********************************************************************
      SUBROUTINE CLAM(MIN,MAX,RN,G,IQP1,IQP2,C,RLAM,ENBCS,ODD)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/EINDE/E(100),INDE(100)
      CHARACTER IZZZ*1
      INTEGER ODD

 6000 FORMAT(5X,13H*****INITIAL ,A1,
     * 36H VALUE FOR GROUND STATE IS NOT FOUND)
 6001 FORMAT(5X,32H*****C AND LAM ARE NOT FOUND C =,E15.6,10X,5HLAM =,
     *E15.6)



      CINIT=C
      RLINIT=RLAM

  200 C1=0
      C2=0
      DO 1 J=MIN,MAX
      RJI=INDE(J)-(INDE(J)/10)*10+0.5D0
      C2=C2+(2.D0*RJI+1.D0)
    1 CONTINUE
      C2=C2*G/4.D0

      IF(ODD.EQ.0) THEN
          DO 3 IT=1,30
          C=(C1+C2)/2.D0
          IF(DABS(C1-C2).LE.0.1D0)GOTO100
  101     F=-4.D0/G
          CP2=C*C
          DO 2 J=MIN,MAX
          IF(J.EQ.IQP1.OR.J.EQ.IQP2)GOTO2
  150     CALL CLAMH(J,C,RLAM,RJI,EPSJ,EL,VJ2)
          F=F+(2.D0*RJI+1.D0)/EPSJ
    2     CONTINUE
  160     IF(F)102,102,103
  102     C2=C
          GO TO 3
  103     C1=C
```

```
  3     CONTINUE
    ELSE
        DO 203 IT=1,30
        C=(C1+C2)/2.D0
        IF(DABS(C1-C2).LE.0.1D0)GOTO100
301     F=-4.D0/G
        CP2=C*C
        DO 202 J=MIN,MAX
        IF(J.EQ.IQP1.OR.J.EQ.IQP2)GOTO202
350     CALL CLAMH(J,C,RLAM,RJI,EPSJ,EL,VJ2)
        F=F+(2.D0*RJI+1.D0)/EPSJ
202     CONTINUE
        CALL CLAMH(ODD,C,RLAM,RJI,EPSJ,EL,VJ2)
        F=F-(2.D0*RJI+1.D0)/EPSJ+(2.D0*RJI-1.D0)/EPSJ
360     IF(F)302,302,303
302     C2=C
        GO TO 203
303     C1=C
203     CONTINUE
    ENDIF


    IZZZ='C'
165 WRITE(16,6000)IZZZ
    ENBCS=7777.D0
    GO TO 120

100 DO 4 IT=1,30
    B1=-4.D0/G
    B2=-RN
    CP2=C*C
    ENBCS=-CP2/G
    A11T=0.D0
    A12=0.D0
    DO 5 J=MIN,MAX
    IF(J.EQ.IQP1.OR.J.EQ.IQP2)GOTO5
105 CALL CLAMH(J,C,RLAM,RJI,EPSJ,EL,VJ2)
    RJIS=2.D0*RJI+1.D0
    B1=B1+RJIS/EPSJ
    B2=B2+RJIS*VJ2
    A11T=A11T+RJIS/EPSJ**3
    A12=A12+RJIS*EL/EPSJ**3
    ENBCS=ENBCS+RJIS*E(J)*VJ2
  5 CONTINUE
    IF(ODD.NE.0) THEN
    CALL CLAMH(ODD,C,RLAM,RJI,EPSJ,EL,VJ2)
```

```
      B1=B1-2/EPSJ
      B2=B2+1-2*VJ2
      A11T=A11T-2/EPSJ**3
      A12=A12-2*EL/EPSJ**3
      ENDIF

  106 DET1=CP2*A11T*A11T+A12*A12
      DET=-0.5D0*C*DET1
      B1=-B1
      B2=-B2
      IF(DABS(B1)+DABS(B2).LE.1.D-07)GOTO120
  180 DELTAC=(0.5D0*CP2*B1*A11T-B2*A12)/DET
      DELTAL=-C*(A11T*B2+0.5D0*A12*B1)/DET
      C=C+DELTAC
      RLAM=RLAM+DELTAL
      IF(.NOT.(DABS(C).LE.0.001D0))GOTO4
  181 C=0.D0
      GO TO 120
    4 CONTINUE
      WRITE(16,6001)C,RLAM
      ENBCS=0.D0

  120 RETURN
      END
C*********************************************************************
      SUBROUTINE CLAMH(I,C,RLAM,RJI,EPSJ,EL,VJ2)
      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON/EINDE/E(100),INDE(100)

      RJI=INDE(I)-(INDE(I)/10)*10+0.5D0
      EL=E(I)-RLAM
      EPSJ=DSQRT(C*C+EL*EL)
      VJ2=0.5D0*(1.D0-EL/EPSJ)

      RETURN
      END
C*********************************************************************
      SUBROUTINE EPSUVS(CN,CP,RLAMN,RLAMP,KEN,KEP)
      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON/EINDE/E(100),INDE(100)
      COMMON/EPSUV/EPS(100),U(100),V(100)

      DO 1 K=1,2
      J=K-1
```

```
      C=CN*(1-J)+CP*J
      RLAM=RLAMN*(1-J)+RLAMP*J
      MIN=1+J*KEN
      MAX=KEP*J+KEN
      DO 1 I=MIN,MAX
      EL=E(I)-RLAM
      EPS(I)=DSQRT(C*C+EL*EL)
      V(I)=DSQRT((1.D0-EL/EPS(I))/2.D0)
      IF(.NOT.(V(I).LE.0.05D0))GOTO3
2     V(I)=0.D0
      U(I)=1.0D0
      GO TO 1
3     U(I)=DSQRT(1.D0-V(I)*V(I))
1     CONTINUE
      RETURN
      END
```