COMITATO NAZIONALE PER L'ENERGIA NUCLEARE
Laboratori Nazionali di Frascati

LNF-72/10
8 Febbraio 1972

K. Baker and G. Paternò: NUMERICAL CALCULATION OF THE ZERO BIAS CONDUCTIVITY FOR A SUPERCONDUCTING TUNNEL JUNCTION, IN THE PRESENCE OF "DEPAIRING". -

Servizio Documentazione
dei Laboratori Nazionali di Frascati del CNEN
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1. - INTRODUCTION. -

In experimental work with a metal-insulator-superconductor tunnel junction, it is very important to know the theoretical values of the differential conductance σ. Knowing these values, it is possible to find the physical parameters of the superconductor (energy gap, etc.). For a superconductor in the pure state, the values of σ are calculated by Bermon[1]. However, these values are no longer valid if the s.c. is in the presence of a factor which causes the breaking of superconducting pairs.

In this work we present a numerical calculation for σ, when there is no voltage applied to the junction. The calculation is made for different values of temperature and of Z (parameter of "pair breaking") where Z can be less than or greater than one.

2. - NUMERICAL CALCULATION OF THE ZERO BIAS CONDUCTIVITY FOR A SUPERCONDUCTING TUNNEL JUNCTION, IN THE PRESENCE OF "DEPAIRING". -

For a metal-insulator-metal tunnel junction, in which one of the two metals is in the superconducting state, the differential conductance is given by the expression[1]:

(x) - fellowship CNEN.

$$(1) \qquad \left(\frac{dI}{dV}\right)_S = \left(\frac{dI}{dV}\right)_N \int_{-\infty}^{+\infty} G(\varepsilon)\left(\frac{1}{KT}\,\frac{e^x}{(1+e^x)^2}\right) d\varepsilon$$

with

$$x = (\varepsilon - eV)/KT \qquad G(\varepsilon) = N_S(\varepsilon)/N(0)$$

ε is the energy measured from the Fermi level; V is the voltage applied; $N_S(\varepsilon)$ is the density of states for the s.c. metal; N(0) is the density of states at the Fermi level when the metal is in the normal state. K is the Boltzman constant, and T is the temperature in degrees Kelvin.

In the absence of depairing factors, $G(\varepsilon)$ is calculated by the B.C.S. theory. It has the simple analytic form:

$$(2) \qquad G(\varepsilon) = \begin{cases} 0 & |\varepsilon| < \Delta_o \\ \dfrac{|\varepsilon|}{(\varepsilon^2 - \Delta_o^2)^{1/2}} & |\varepsilon| \geq \Delta_o \end{cases}$$

where $2\Delta_o$ is the energy gap in the excitation spectrum for the quasi particles in the superconductor.

A depairing factor, such as a current which passes through the s.c. or an applied magnetic field, etc., destroys the invariance of time reversal symmetry of the superconducting pairs. Therefore, the density of states in the s.c. becomes modified so that it can no longer be expressed by the simple expression (2) of the B.C.S. theory.

However, by using the Green function formalism, it is possible to calculate $G(\dot{\varepsilon})$ for a large number of mechanisms which cause the breaking of superconducting pairs. As Fulde[3] has shown, it is possible to calculate $G(\varepsilon)$ in terms of an adimensional parameter Z which is related to the strength of "depairing".

The parameter Z is also expressable in a different manner. It can be written as a function of the physical factors which cause the "depairing". For a s.c. crossed by a current in the case $1 \ll \xi_o$ (1 = = mean free path, ξ_o = coherence length), Maki[4] has derived the expression:

$$J = K\left(\frac{\pi}{2} - \frac{2}{3} Z^{3/2}\right) \qquad \text{for } Z \leq 1$$

$$J = K\left(\arcsin Z^{-3/2} - \frac{2}{3}\left(Z^{3/2} - \sqrt{Z^3 - 1}\right) + \frac{1}{3}\sqrt{1 - Z^{-3}}\right) \qquad \text{for } Z > 1$$

J is the current density in the superconductor. The constant K is related to the physical parameters of the s.c.

As Fulde[5] has shown, $G(\varepsilon, Z) = N_s(\varepsilon, Z)/N(0)$ is given by the expression:

$$(3) \qquad G(\varepsilon, Z) = \frac{\varepsilon}{\Delta} \frac{1}{Z^{1/2}} \operatorname{Im} \frac{1}{(\bar{x} - Z)}$$

where $\bar{x}$ is the complex solution of the fourth order plynomial:

$$(4) \qquad x^4 - 2Z x^3 + x^2\left(\frac{1}{Z}\left(\frac{\varepsilon}{\Delta}\right)^2 - \frac{1}{Z} + Z^2\right) + 2x - Z = 0$$

For $\varepsilon > \varepsilon_m$ this equation has two real roots and two roots which are complex conjugates. ε_m is given by the expression[4]:

$$(5) \qquad \varepsilon_m = \Delta (1 - Z)^{3/2} \qquad \text{for } Z \leq 1$$

$$\varepsilon_m = 0 \qquad Z > 1$$

Δ is the gap in the presence of "depairing". It is related to the gap in the absence of "depairing", Δ_o, by the relation[4]:

$$(6) \qquad \Delta = \Delta_o \exp\left(-\frac{\pi}{4} Z^{3/2}\right) \qquad Z \leq 1$$

$$\Delta = \Delta_o \exp\left(-\operatorname{arc\,cosh} Z^{3/2} - \frac{1}{2}\left(Z^{3/2} \arcsin Z^{-3/2} - (1 - Z^{-3})^{1/2}\right)\right) \qquad \text{for } Z > 1$$

The case of $Z > 1$ corresponds to the region of gapless superconductivity.

In this paper we present the numerical calculation of

$$\left(\frac{dI}{dV}\right)_s / \left(\frac{dI}{dV}\right)_N = \sigma\left(\frac{\Delta_o}{KT}, Z\right)$$

for different values of Z and for different values of $\beta = \Delta_o/KT$ when $V = 0$. The Fortran program used to make the calculations is given as well as a table of values calculated with the program. Also included is a graph of σ v.s. Z for three values of β.

In our case, $V = 0$, (1) becomes

$$\sigma(\beta, Z) = 2\left(\frac{\Delta}{KT}\right) \int_{\varepsilon_m/\Delta}^{\infty} G(E, Z) \frac{e^{E \cdot \Delta/KT}}{(1+e^{E \cdot \Delta/KT})^2} \, dE$$

where $E = \varepsilon/\Delta$ is the energy measured with respect to the gap in the presence of "depairing".

One passes from Δ_o/KT to Δ/KT by using (6). The integral is calculated by the Simpson method which doubles the number of points used to calculate the function until the difference between two successive calculations is less than 5×10^{-6}.

Since the integrand for $Z < 1$ or for large values of β has a pronounced peak at $E \simeq 1$, the interval of integration is broken into smaller intervals.

The first interval goes from ε_m/Δ to 1. The successive intervals have a width $\delta E = 1$.

The integral is calculated in the first interval, the second, and so one. Since for $E > 1$ the integrand is decreasing monotonically, the integration stops at the n^{th} interval in which the value of the integral is $< 0.5 \times 10^{-6}$.

G(E, Z) is calculated by solving analytically equation (4) to find the complex roots. If these solutions are indicated by $x_o \pm i\, Y_o$, (2) becomes

$$G(E, Z) = \frac{E}{Z^{1/2}} \frac{|Y_o|}{(x_o - Z)^2 + Y_o^2}$$

The roots of equation (4) are found using the method of Ferrari[6]. He has shown that when $x^4 + ax^3 + bx^2 + cx + d = 0$ is an equation of the fourth order with real coefficients, the four roots are given by the roots of the two quadratic equations:

$$x^2 + \frac{a}{2} + \frac{1}{2} y = ex + f \qquad x^2 + \frac{a}{2} x + \frac{1}{2} y = -ex - f$$

where

$$e = \sqrt{\frac{a^2}{4} - b + y}\,, \qquad f = \frac{-c + \frac{1}{2}ay}{2e}$$

and y is a real root of the following cubic equation which is called the resolvent of our fourth order polynomial:

$$y^3 - by^2 + (ac - 4d)y + 4bd - a^2 d - c^2 = 0$$

In our case the resolvent becomes:

$$(7) \qquad y^3 - y^2\left(\frac{1}{Z}(E^2 - 1) + Z^2\right) + 4E^2 = 0$$

where $E = \varepsilon / \Delta$. One finds a real root of (7) using the method of Cardan for resolving a third order polynomial. Given the equation

$$y^3 + ay^2 + by + c = 0\,,$$

one considers the discriminant

$$Q = \left(\frac{p}{3}\right)^3 + \left(\frac{q}{2}\right)^2$$

with

$$p = -\frac{a^2}{3} + b$$

$$q = 2\left(\frac{a}{3}\right)^3 - \frac{ab}{3} + c$$

There are three cases to consider.

1) $Q > 0$: The cubic has one real root and two complex conjugate roots. The real root is given by:

$$y_1 = \sqrt[3]{-\frac{q}{2} + \sqrt{Q}} + \sqrt[3]{-\frac{q}{2} - \sqrt{Q}} - \frac{a}{3}$$

2) $Q = 0$: The cubic has three real roots of which two are equal:

$$y_1 = 2\sqrt[3]{-\frac{q}{2}} - \frac{a}{3}, \qquad y_2 = y_3 = -\sqrt[3]{\frac{q}{2}} - \frac{a}{3}$$

3) $Q<0$: The cubic has three real roots that are written in trigonometrical form:

$$y_1 = 2\sqrt{-\frac{p}{3}}\cos\frac{\varphi}{3} - \frac{a}{3}, \qquad y_2 = -2\sqrt{\frac{p}{3}}\cos\left(\frac{\varphi}{3}+60^{\circ}\right) - \frac{a}{3}$$

$$y_3 = -2\sqrt{-\frac{p}{3}}\cos\left(\frac{\varphi}{3}-60^{\circ}\right) - \frac{a}{3}$$

where

$$\varphi = -2\,\frac{\sqrt{-Q}}{q}$$

and

$$\frac{\pi}{2} \le \varphi \le \pi \quad \text{if } q>0, \qquad 0 \le \varphi \le \frac{\pi}{2} \quad \text{if } q<0$$

The calculation of G(E, Z) is done by the subroutine DENSIT included at the end of this paper.

Originally, we solved the fourth order polynomial numerically using the iterative method of Newton-Rapson. Because G(E, Z) has to be calculated for a large number of points to produce the integral, the analytical method was substituted for the numerical method. The analytical method was found to be superior since it used less machine time and produced more accurate results.

Both the integral and the calculation of G(E, Z) are executed using double precision. This was found to be indispensable especially for values of $Z \ll 1$.

Taking into account the error in the calculation G(E, Z), the error in $\sigma(\beta, Z)$ can be estimated to be $\le 1 \times 10^{-4}$.

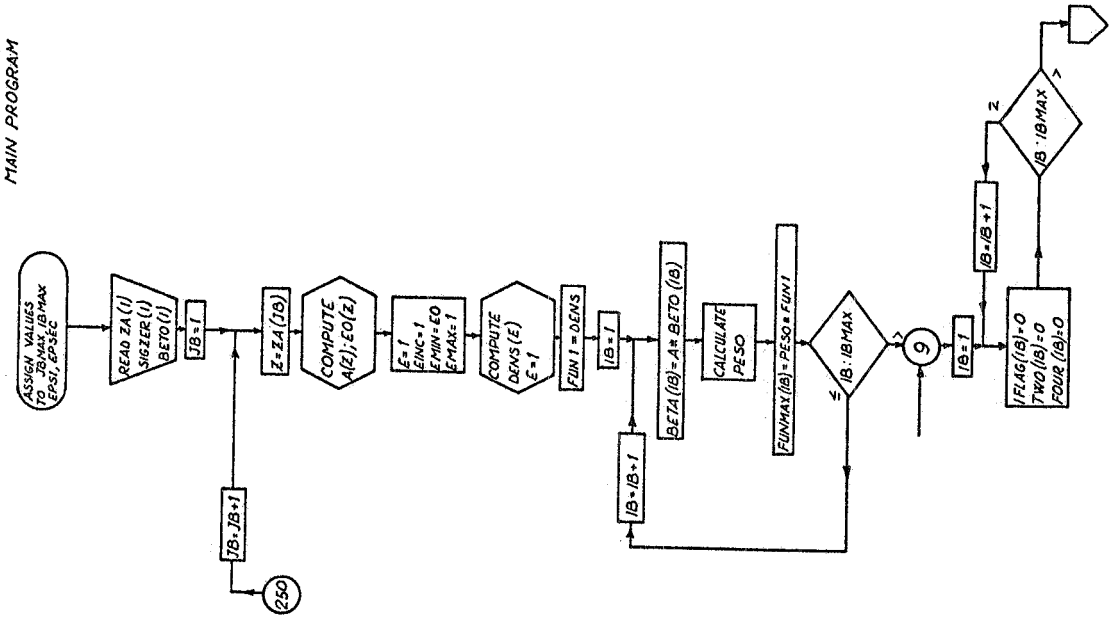
The values of G(E, Z) for $Z = 0$ are taken from ref. (1).

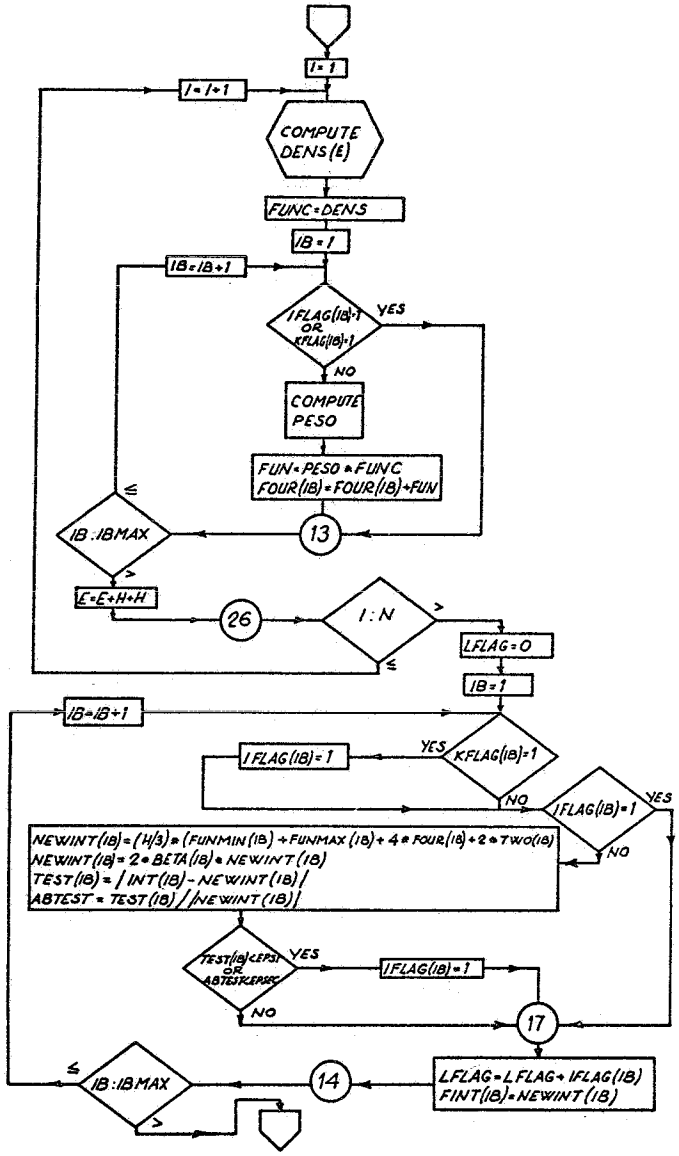
ACKNOWLEDGEMENTS. -

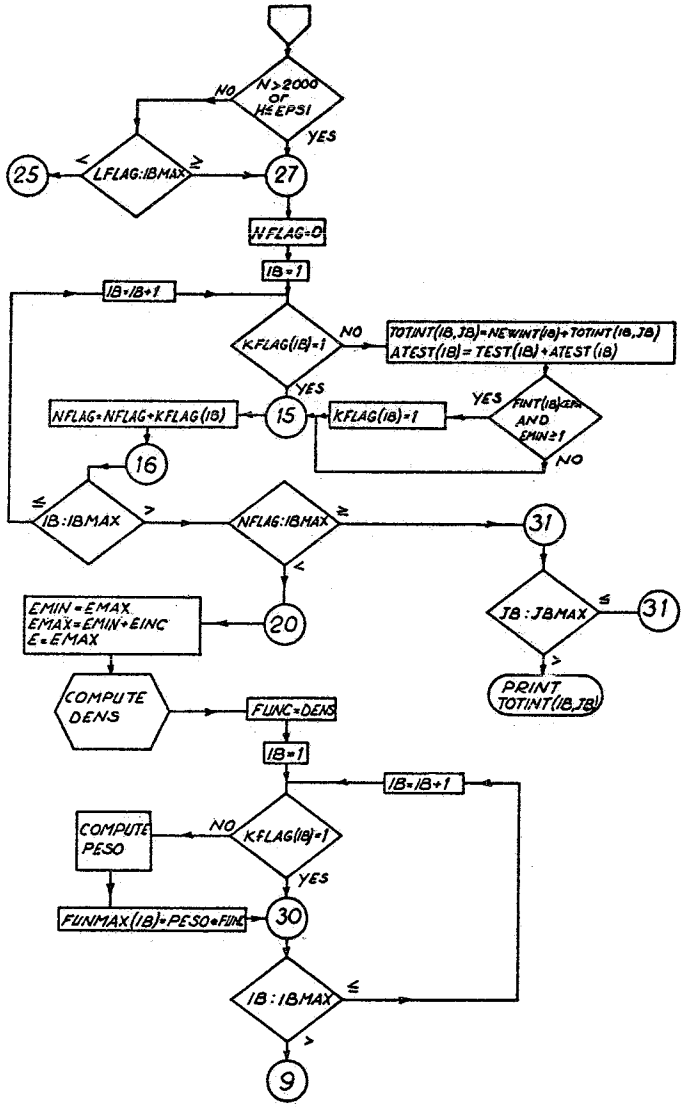
We are very grateful to our collegues of the Numerical Calculation Group, especially to Mrs. M. A. Spano-Mencuccini, for the helpful discussions.

REFERENCES. -

(1) - S. Bermon, Technical Report N. 1, Dept. of Phys., Univ. of Illinois, Urbana I-11, (1964).
(2) - J. Bardeen, L.N. Cooper and I.R. Schriffer, Phys. Rev. 108, 1175 (1957).
(3) - P. Fulde, Proc. Intern. Summer School on Electron Tunneling Phenomena in Solids, 1967, pag. 427 Plenum Press, 1969.
(4) - K. Maki, Progr. Theoret. Phys. 29, 333 (1963).
(5) - P. Fulde, Phys. Rev. 137, A 783 (1965).
(6) - J. V. Uspensky, Theory of Equations, McGraw-Hill Book Company (1948), pag. 94.


MAIN PROGRAM
ASSIGN VALUES TO JB,MAX,IB,MAX EPSI, EPSEC
READ ZA(I) SIGZER(I) BETO(I)
JB=JB+1
250
IB=1
Z=ZA(IB)
COMPUTE A(Z); EO(Z)
E=1 EINC=1 EMIN=EO EMAX=1
COMPUTE DENS(E) E=E
FUN1=DENS
IB=1
IB=IB+1
BETA(IB)=A*BETO(IB)
CALCULATE PESO
FUNMAX(IB)=PESO*FUN1
IB:IBMAX
9
IB=1
IB=IB+1
IFLAG(IB)=0 TWO(IB)=0 FOUR(IB)=0
IB:IBMAX
H=(EMAX-EMIN)/2
N=1
E=EMIN+H
COMPUTE DENS(E)
FUNC=DENS
IB=1
KFLAG(IB)=1
YES
NO
COMPUTE PESO
FUN=PESO*FUNC
FOUR(IB)=FOUR(IB)+FUN
FINT(IB)=(1/3)*(FUNMIN(IB)+FUNMAX(IB)+4*FOUR(IB))
FINT(IB)=2*BETA(IB)*FINT(IB)
11
IB:IBMAX
IB=IB+1
25
H=H/2
N=2*N
E=H+EMIN
IB=1
IFLAG(IB)=1
KFLAG(IB)=1
YES
NO
TWO(IB)=TWO(IB)+FOUR(IB)
FOUR(IB)=0
12
IB:IBMAX


I=1
I=I+1
COMPUTE DENS(E)
FUNC=DENS
IB=1
IB=IB+1
IFLAG(IB)=1 OR KFLAG(IB)=1
YES
NO
COMPUTE PESO
FUN=PESO*FUNC
FOUR(IB)=FOUR(IB)+FUN
13
IB:IBMAX
E=E+H+H
26
I:N
LFLAG=0
IB=1
IB=IB+1
KFLAG(IB)=1
IFLAG(IB)=1
IFLAG(IB)=1
NEWINT(IB)=(H/3)*(FUNMIN(IB)+FUNMAX(IB)+4*FOUR(IB)+2*TWO(IB))
NEWINT(IB)=2*BETA(IB)*NEWINT(IB)
TEST(IB)=|INT(IB)-NEWINT(IB)|
ABTEST=TEST(IB)/|NEWINT(IB)|
TEST(IB)<EPSI OR ABTEST<EPSI
IFLAG(IB)=1
17
14
IB:IBMAX
LFLAG=LFLAG+IFLAG(IB)
FINT(IB)=NEWINT(IB)


N>2000 OR H≤EPSI
NO
YES
LFLAG:IBMAX
25
27
NFLAG=0
IB=1
IB=IB+1
KFLAG(IB)=1
NO
TOTINT(IB,JB)=NEWINT(IB)+TOTINT(IB,JB)
ATEST(IB)=TEST(IB)+ATEST(IB)
YES
NFLAG=NFLAG+KFLAG(IB)
15
KFLAG(IB)=1
FINT(IB)≠ZERO AND EMIN≥1
16
IB:IBMAX
NFLAG:IBMAX
31
EMIN=EMAX
EMAX=EMIN+EINC
E=EMAX
20
JB:JBMAX
31
COMPUTE DENS
FUNC=DENS
PRINT TOTINT(IB,JB)
IB=1
IB=IB+1
COMPUTE PESO
KFLAG(IB)=1
FUNMAX(IB)=PESO*FUNC
30
IB:IBMAX
9

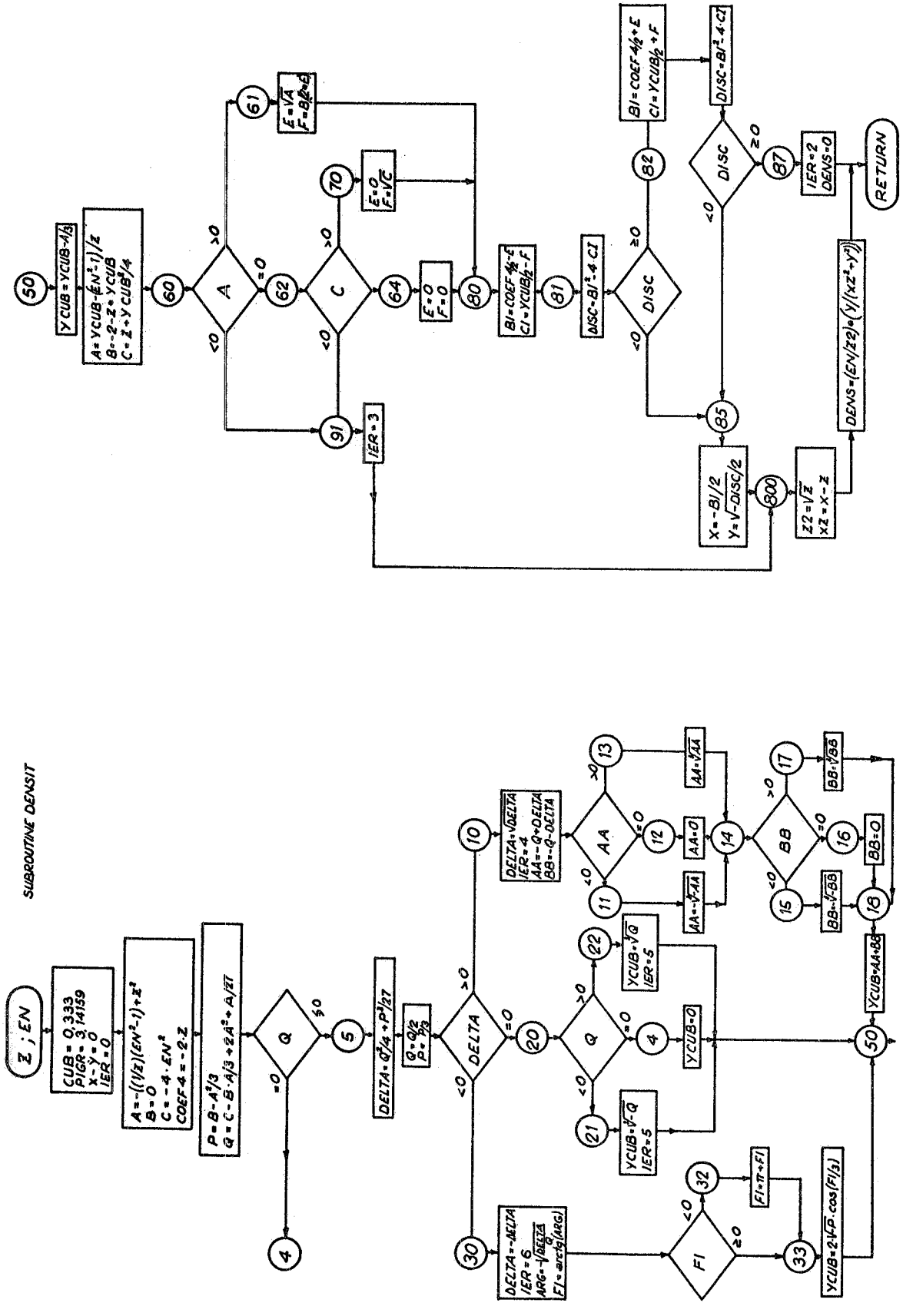
10.

MAINPGM

```
      REAL*8 NEWINT
      DOUBLE PRECISION E0,ABTEST,FINT,COM
      DOUBLE PRECISION FOUR,H,CONDU
      DOUBLE PRECISION DENS,Z,E,PIGR,FUNC,FUN1,EINC,EMIN,EMAX,BETA,A
      DOUBLE PRECISION TOTINT,ATEST,TEST,FUNMIN,FUNMAX,OMEGA,EXPO,PESO,TWO
      DIMENSION TEST(30),ATEST(30),FUNMIN(30),FUNMAX(30)
      DIMENSION ZA(30),BETO(30),SIGZER(30)
      DIMENSION BETA(30),NEWINT(30),TOTINT(30,30),FINT(30)
      DIMENSION FOUR(30),TWO(30),IFLAG(30),KFLAG(30)
      JBMAX=17
      IBMAX=18
      READ 91,(ZA(I),I=1,JBMAX)
   91 FORMAT(F13.6)
      READ 90,(BETO(J),SIGZER(J),J=1,IBMAX)
   90 FORMAT(2F7.5)
C*******************************************************************************
      EPSI=.5E-06
      EPSEC=1.0E-03
C*******************************************************************************
      PIGR=3.14159265358979 32
      DO 250 JB=1,JBMAX
      Z=ZA(JB)
      CALL ZFUNC(Z,A,E0)
      PRINT 600, Z, A, E0
  600 FORMAT(1H0,'Z=',E14.7,10X,'A=',E14.7,10X,'E0=',E14.7)
C                    CALCOLA LA FUNZIONE PER E=1
      E=1.
      CALL DENSIT(Z,E,DENS,KER)
      FUNC=DENS
      FUN1=FUNC
      EINC=1.
      EMIN=E0
      EMAX=1.
      ABTEST=0.
      DO 5 IB=1,IBMAX
      BETA(IB)=BETO(IB)*A
      PRINT 601, BETA(IB)
  601 FORMAT(1H0,'BETA(IB)=',E14.7)
      IBB=JB+1
      TOTINT(IB,IBB)=0.
      KFLAG(IB)=0
      ATEST(IB)=0.
      TEST(IB)=0.
      FUNMIN(IB)=0.
C                    CALCOLA LA FUNZIONE DI FERMI
      OMEGA=BETA(IB)*E
      EXPO=DEXP(OMEGA)
      COM=(EXPO+1.)
      COM=COM*COM
      PESO=EXPO/COM
    5 FUNMAX(IB)=PESO*FUN1
    9 DO 10 IB=1,IBMAX
      IFLAG(IB)=0.
      TWO(IB)=0.
   10 FOUR(IB)=0.
      H=(EMAX-EMIN)/2.
      N=1
      E=EMIN+H
      PRINT 602, E
```

```
  602 FORMAT(1HO,'E=',E14.7)
      CALL DENSIT(Z,E,DENS,KER)
      FUNC=DENS
      DO 11 IB=1,IBMAX
      IF(KFLAG(IB).EQ.1) GO TO 11
      OMEGA=BETA(IB)*E
      EXPO=DEXP(OMEGA)
      COM=(EXPO+1.)
      COM=COM*COM
      PESO=EXPO/COM
      FUN=PESO*FUNC
      FOUR(IB)=FOUR(IB)+FUN
      FINT(IB)=(H*(FUNMIN(IB)+FUNMAX(IB)+4.*FOUR(IB)))/3.
      FINT(IB)=2.*BETA(IB)*FINT(IB)
   11 CONTINUE
C                       EVALUATION LOOP
   25 H=H/2.
      N=2*N
      E=H+EMIN
      DO 12 IB=1,IBMAX
      IF(IFLAG(IB).EQ.1.OR.KFLAG(IB).EQ.1) GO TO 12
      TWO(IB)=TWO(IB)+FOUR(IB)
      FOUR(IB)=0.
   12 CONTINUE
      DO 26 I=1,N
      CALL DENSIT(Z,E,DENS,KER)
      FUNC=DENS
      DO 13 IB=1,IBMAX
      IF(IFLAG(IB).EQ.1.OR.KFLAG(IB).EQ.1) GO TO 13
      OMEGA=BETA(IB)*E
      EXPO=DEXP(OMEGA)
      COM=(EXPO+1.)
      COM=COM*COM
      PESO=EXPO/COM
      FUN=PESO*FUNC
      FOUR(IB)=FOUR(IB)+FUN
   13 CONTINUE
   26 E=E+H+H
      LFLAG=0
      DO 14 IB=1,IBMAX
      IF(KFLAG(IB).EQ.1) IFLAG(IB)=1
      IF(IFLAG(IB).EQ.1)   GO TO 17
      NEWINT(IB)=(H*(FUNMIN(IB)+FUNMAX(IB)+2.*TWO(IB)+4.*FOUR(IB)))/3.
      NEWINT(IB)=2.*BETA(IB)*NEWINT(IB)
      TEST(IB)=DABS(FINT(IB)-NEWINT(IB))
      ABTEST=TEST(IB)/DABS(NEWINT(IB))
      IF(TEST(IB).LT.EPSI.AND.ABTEST.LE.EPSEC) IFLAG(IB)=1
   17 LFLAG=LFLAG+IFLAG(IB)
      FINT(IB)=NEWINT(IB)
   14 CONTINUE
      IF(N.GT.2000.OR.H.LE.EPSI) GO TO 27
      IF(LFLAG-IBMAX) 25,27,27
   27 CONTINUE
      NFLAG=0
      DO 16 IB=1,IBMAX
      IF(KFLAG(IB).EQ.1) GO TO 15
      TOTINT(IB,IBB)=NEWINT(IB)+TOTINT(IB,IBB)
      ATEST(IB)=TEST(IB)+ATEST(IB)
      IF(FINT(IB).LE.EPSI.AND.EMIN.GT.1.) KFLAG(IB)=1
   15 NFLAG=NFLAG+KFLAG(IB)
```

```
   16 CONTINUE
      IF(NFLAG-IBMAX) 20,31,31
   20 CONTINUE
      EMIN=EMAX
      EMAX=EMIN+EINC
      E=EMAX
      CALL DENSIT(Z,E,DENS,KER)
      FUNC=DENS
      DO 30 IB=1,IBMAX
      IF(KFLAG(IB).EQ.1) GO TO 30
      FUNMIN(IB)=FUNMAX(IB)
      OMEGA=BETA(IB)*E
      EXPO=DEXP(OMEGA)
      COM=(EXPO+1.)
      COM=COM*COM
      PESO=EXPO/COM
      FUNMAX(IB)=PESO*FUNC
   30 CONTINUE
      GO TO 9
   31 CONTINUE
      DO 100 IB=1,IBMAX
      TEST(IB)=ATEST(IB)
      CONDU=TOTINT(IB,IBB)/SIGZER(IB)
      PRINT 97, BETO(IB),Z,TOTINT(IB,IBB),N,TEST(IB),CONDU
   97 FORMAT(3X,2F10.5,10X,D14.6,I10,17X,D17.6,D15.6,/)
  100 CONTINUE
  250 CONTINUE
      DO 6000 IB=1,IBMAX
 6000 TOTINT(IB,1)=SIGZER(IB)
      JBIG=JBMAX
      DO 7000 JB=1,JBMAX
      JBB=JBIG+1
      ZA(JBB)=ZA(JBIG)
 7000 JBIG=JBIG-1
      ZA(1)=0.000
      NM=0
      NN=1
 9000 NM=NM+5
C     ************************************
      PRINT 1005
 1005 FORMAT(1H1)
      PRINT 4000,(ZA(I),I=NN,NM)
 4000 FORMAT(5(15X,'I',/),12X,'Z',2X,'I',7X,4(F6.3,14X),F6.3,/,15X,'I',/
     1,3X,'DELTA/KT',4X,'I',/,15X,'I',/,' ',14('-'),'I',120('-'),2(/,15X
     2,'I'))
      DO 5000 IB=1,IBMAX
 5000 PRINT 1000,BETO(IB),(TOTINT(IB,JB),JB=NN,NM)
 1000 FORMAT(3X,F10.5,2X,'I',3X,5(D14.6,6X),/,15X,'I')
      NN=NN+5
      IF(NM.LE.(JBMAX+1)) GO TO 9000
      STOP
      END
```


SUBROUTINE DENSIT
Z ; EN
CUB = 0.333
PIGR = 3.14159
X-Y = 0
IER = 0
A=-((1/E)(EN²-1)+Z²
B=0
C=-4·EN²
COEF4=-2·Z
P=B-A²/3
Q=C-B·A/3+2A³+A/ZT
Q
=0
≠0
4
5
DELTA=Q²/4+P³/27
Q=Q/2
P=P/3
DELTA
<0
=0
>0
30
DELTA=-DELTA
IER=6
ARG=√(DELTA/Q)
FI=arctg(ARG)
FI
<0
≥0
32
FI=π+FI
33
YCUB=2·√(-P)·cos(FI/3)
10
DELTA=√DELTA
IER=4
AA=-Q+DELTA
BB=-Q-DELTA
AA
<0
=0
>0
11
AA=-√-AA
12
AA=0
13
AA=√AA
14
BB
<0
=0
>0
15
BB=-√-BB
16
BB=0
17
BB=√BB
18
YCUB=AA+BB
20
Q
<0
=0
>0
21
YCUB=∛-Q
IER=5
4
YCUB=0
22
YCUB=∛Q
IER=5
50
YCUB=YCUB-A/3
60
A
<0
=0
>0
91
IER=3
62
C
<0
=0
>0
64
E=0
F=0
70
E=0
F=√C
61
E=√A
F=B/2+Q
80
BI=COEF·A/2+E
CI=YCUB/2-F
81
DISC=BI²-4·CI
DISC
<0
≥0
85
X=-BI/2
Y=√-DISC/2
800
Z2=√Z
X2=X-Z
82
BI=COEF·A/2+E
CI=YCUB/2+F
DISC=BI²-4·CI
DISC
<0
≥0
87
IER=2
DENS=0
DENS=(EN/Z2)^(1/3)·(Y/(X·Z²-Y²))
RETURN

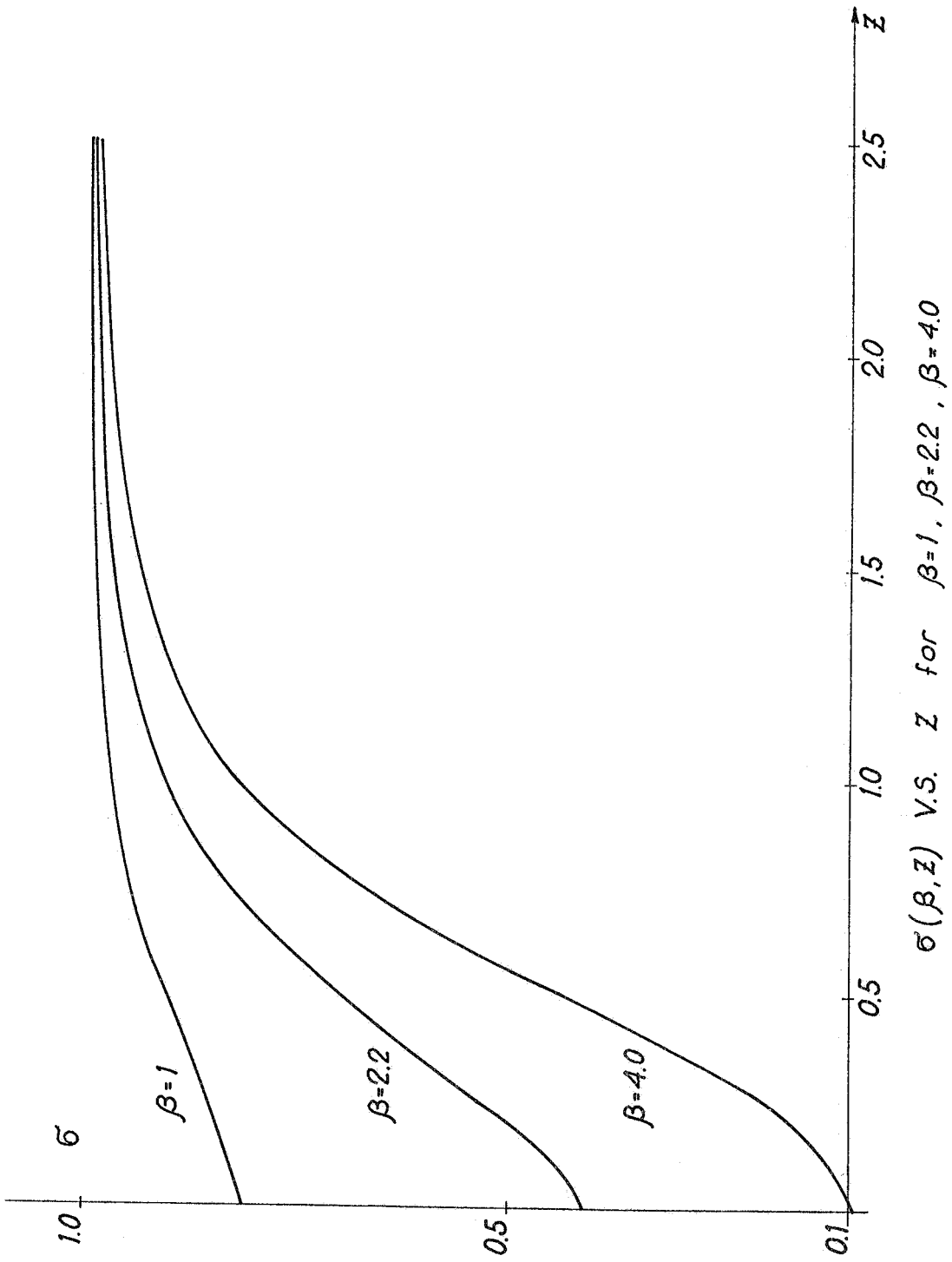
DENSIT

```
      SUBROUTINE DENSIT(Z,EN,DENS,IER)
      DOUBLE PRECISIONA,B,C,A3,P,Q,YCUB,DELTA,AA,BB,ARG,AA1,BB1,FI,CONTR
      DOUBLE PRECISION E,F,B1,C1,DISC,X,Y,COEF4,CUB,Z,EN,Z2,XZ,DENS,PIGR
      CUB=0.3333333333333333
      PIGR=3.1415926535897932
      X=0.0
      Y=0.0
      IER=0
C                    CALCOLA I COEFF. DELLA CUBICA RISOLVENTE
      A=-((1./Z)*(EN*EN-1.)+Z*Z)
      B=0.
      C=-4.*EN*EN
      COEF4=-2.*Z
      A3=A/3.
      P=B-A*A/3.
      Q=C-B*A/3.+2.*A*A*A/27.
      IF(Q) 5,4,5
    4 YCUB=0.
      GO TO 50
C     CALCOLA  IL  DISCRIMINANTE
    5 DELTA=Q*Q/4.+P*P*P/27.
      Q=Q/2
      P=P/3.
      IF(DELTA) 30,20,10
C     C'E'  UNA  SOLA  RADICE  REALE
   10 DELTA=DSQRT(DELTA)
      IER=4
      AA=-Q+DELTA
      BB=-Q-DELTA
      IF(AA) 11,12,13
   11 AA=-(DEXP(DLOG(-AA)/3.))
      GO TO 14
   12 AA=0.
      GO TO 14
   13 AA=DEXP(DLOG(AA)/3.)
   14 IF(BB) 15,16,17
   15 BB=-(DEXP(DLOG(-BB)/3.))
      GO TO 18
   16 BB=0.
      GO TO 18
   17 BB=DEXP(DLOG(BB)/3.)
   18 YCUB=AA+BB
      GO TO 50
C    CI  SONO  TRE  RADICI  REALI  DI  CUI  2  COINCIDENTI
   20 IF(Q) 21,4,22
C    SCEGLIE  LA  RADICE  POSITIVA
   21 YCUB=2.*DEXP(DLOG(-Q)/3.)
      IER=5
      GO TO 50
   22 YCUB=DEXP(DLOG(Q)/3.)
      IER=5
      GO TO 50
C    CI SONO  3  RADICI  REALI  DISTINTE
   30 DELTA=-DELTA
      IER=6
      ARG=-DSQRT(DELTA)/Q
      FI=DATAN(ARG)
      IF(FI) 32,33,33
   32 FI=PIGR+FI
   33 YCUB=2.*DSQRT(-P)*DCOS(FI/3.)
   50 YCUB=YCUB-A3
```

```
C*******************************************************************************
      CONTR=YCUB*YCUB*YCUB+A*YCUB*YCUB+B*YCUB+C
C*******************************************************************************
C    RISOLUZIONE  EQUAZ.    IV  GRADO
      A=YCUB-(EN*EN-1.)/Z
      B=-2.-Z*YCUB
      C=Z+YCUB*YCUB/4.
   60 IF(A) 91,62,61
   61 E=DSQRT(A)
      F=B/(2.*E)
      GO TO 80
   62 IF(C) 91,64,65
   64 E=0.
      F=0.
      GO TO 80
   65 E=0.
      F=DSQRT(C)
C      CALCOLA  LE  RADICI  E  SCEGLIE  QUELLA  COMPLESSA
   80 B1=COEF4/2.-E
      C1=YCUB/2.-F
C    CALCOLA  IL   DISCRIMINANTE
   81 DISC=B1*B1-4.*C1
      IF(DISC) 85,82,82
   82 B1=COEF4/2.+E
      C1=YCUB/2.+F
      DISC=B1*B1-4.*C1
      IF(DISC) 85,87,87
   85 X=-B1/2.
      Y=DSQRT(-DISC)/2.
      GO TO 800
C    NON  CI  SONO  RADICI   COMPLESSE
   87 IER=2
      PRINT 806,IER
  806 FORMAT(1H0,'NON CI SONO RADICI COMPLESSE',I5)
      DENS=0.
      GO TO 805
C    E  O  F   SONO  COMPLESSI
   91 IER=3
  800 Z2=DSQRT(Z)
      XZ=X-Z
      DENS=(EN/Z2)*(Y/(XZ*XZ+Y*Y))
  805 CONTINUE
      RETURN
      END
```

ZFUNC

```
      SUBROUTINE ZFUNC(Z,A,EO)
      DOUBLE PRECISION PIGR,ALFA
      DOUBLE PRECISION Z,U,ACOHU,ARGU,ASIN,A,EO
      PIGR=3.1415926535897932
      IF (Z-1) 608,608,607
  608 ALFA=DEXP(3.*DLOG(Z)/2.)
      A=DEXP((-PIGR/4.)*ALFA)
      IF (Z-1) 609,610,610
  609 EO=DEXP(3.*DLOG(1.-Z)/2.)
      RETURN
  610 EO=0.
      RETURN
  607 U=DEXP(3.*DLOG(Z)/2.)
      ACOHU=DLOG(U+DSQRT(U*U-1))
      ARGU=DSQRT(1./(U*U-1))
      ASIN=DATAN(ARGU)
      A=DEXP(-ACOHU-(U*ASIN-DSQRT(1.-1./(U*U)))/2.)
      EO=0.
      RETURN
      END
```



σ(β,z) V.S. z for β=1, β=2.2, β=4.0

Z / DELTA/KT	0.0	0.050	0.100	0.150	0.200
0.80000	0.8753000 00	0.8781850 00	0.8832430 00	0.8894330 00	0.8962760 00
1.00000	0.8143000 00	0.9186790 00	0.8263700 00	0.8357810 00	0.8461770 00
1.20000	0.7473000 00	0.7532540 00	0.7637800 00	0.7766820 00	0.7909560 00
1.40000	0.6772000 00	0.6848170 00	0.6981520 00	0.7145510 00	0.7327570 00
1.60000	0.6069000 00	0.6159270 00	0.6318380 00	0.6515030 00	0.6734500 00
1.80000	0.5385000 00	0.5486660 00	0.5667680 00	0.5892810 00	0.6145790 00
2.00000	0.4735000 00	0.4846160 00	0.5044210 00	0.5292400 00	0.5573600 00
2.20000	0.4132000 00	0.4246580 00	0.4458410 00	0.4723620 00	0.5026930 00
2.40000	0.3581000 00	0.3700490 00	0.3916890 00	0.4192970 00	0.4512010 00
2.60000	0.3085000 00	0.3204880 00	0.3423940 00	0.3704180 00	0.4032700 00
2.80000	0.2645000 00	0.2762040 00	0.2977790 00	0.3258750 00	0.3590970 00
3.00000	0.2257000 00	0.2370300 00	0.2580180 00	0.2856500 00	0.3187290 00
3.20000	0.1919000 00	0.2026660 00	0.2228000 00	0.2496030 00	0.2821000 00
3.40000	0.1626000 00	0.1727370 00	0.1918170 00	0.2175100 00	0.2490670 00
3.60000	0.1374000 00	0.1468250 00	0.1647190 00	0.1890940 00	0.2194310 00
3.80000	0.1158000 00	0.1245060 00	0.1411350 00	0.1640540 00	0.1929620 00
4.00000	0.9740000-01	0.1053630 00	0.1206960 00	0.1420770 00	0.1694110 00
4.20000	0.8180000-01	0.8900920-01	0.1030450 00	0.1228550 00	0.1485250 00

Z / DELTA/KT	0.250	0.400	0.500	0.600	0.800
0.80000	0.9034480 00	0.9248820 00	0.9378950 00	0.9493510 00	0.9673420 00
1.00000	0.8570620 00	0.8894770 00	0.9090270 00	0.9261210 00	0.9526840 00
1.20000	0.8059180 00	0.8505000 00	0.8773310 00	0.9007020 00	0.9367480 00
1.40000	0.7519020 00	0.8091990 00	0.8437560 00	0.8738200 00	0.9199690 00
1.60000	0.6966450 00	0.7666190 00	0.8090750 00	0.8460540 00	0.9026850 00
1.80000	0.6414970 00	0.7236130 00	0.7739090 00	0.8178600 00	0.8851540 00
2.00000	0.5879260 00	0.6808560 00	0.7387430 00	0.7895910 00	0.8675730 00
2.20000	0.5359400 00	0.6388720 00	0.7039520 00	0.7615150 00	0.8500900 00
2.40000	0.4861170 00	0.5980540 00	0.6698200 00	0.7338340 00	0.8328140 00
2.60000	0.4396360 00	0.5586890 00	0.6365550 00	0.7066980 00	0.8158230 00
2.80000	0.3963240 00	0.5209750 00	0.6043060 00	0.6802110 00	0.7991740 00
3.00000	0.3562710 00	0.4850410 00	0.5731770 00	0.6544480 00	0.7829050 00
3.20000	0.3194740 00	0.4509610 00	0.5432340 00	0.6294580 00	0.7670390 00
3.40000	0.2858580 00	0.4187650 00	0.5145150 00	0.6052690 00	0.7515910 00
3.60000	0.2552950 00	0.3884490 00	0.4870350 00	0.5818960 00	0.7365670 00
3.80000	0.2276220 00	0.3599850 00	0.4607730 00	0.5593420 00	0.7219670 00
4.00000	0.2026560 00	0.3333230 00	0.4357780 00	0.5376010 00	0.7077880 00
4.20000	0.1801790 00	0.3084060 00	0.4119580 00	0.5166620 00	0.6940220 00

Z / DELTA/KT	0.900	1.000	1.200	1.500	1.800
0.80000	0.974097D 00	0.979599D 00	0.987262D 00	0.993163D 00	0.995961D 00
1.00000	0.962552D 00	0.970541D 00	0.981622D 00	0.990139D 00	0.994176D 00
1.20000	0.950027D 00	0.960726D 00	0.975511D 00	0.986863D 00	0.992241D 00
1.40000	0.936862D 00	0.950418D 00	0.969094D 00	0.983420D 00	0.990208D 00
1.60000	0.923317D 00	0.939816D 00	0.962493D 00	0.979878D 00	0.988116D 00
1.80000	0.909592D 00	0.929083D 00	0.955807D 00	0.976289D 00	0.985995D 00
2.00000	0.895837D 00	0.918328D 00	0.949109D 00	0.972692D 00	0.983870D 00
2.20000	0.882166D 00	0.907642D 00	0.942452D 00	0.969119D 00	0.981759D 00
2.40000	0.868661D 00	0.897090D 00	0.935880D 00	0.965590D 00	0.979674D 00
2.60000	0.855383D 00	0.886718D 00	0.929423D 00	0.962125D 00	0.977627D 00
2.80000	0.842374D 00	0.876561D 00	0.923101D 00	0.958734D 00	0.975625D 00
3.00000	0.829663D 00	0.866640D 00	0.916931D 00	0.955427D 00	0.973673D 00
3.20000	0.817269D 00	0.856972D 00	0.910923D 00	0.952210D 00	0.971776D 00
3.40000	0.805202D 00	0.847563D 00	0.905082D 00	0.949086D 00	0.969934D 00
3.60000	0.793467D 00	0.838419D 00	0.899412D 00	0.946057D 00	0.968150D 00
3.80000	0.782063D 00	0.829538D 00	0.893913D 00	0.943125D 00	0.966424D 00
4.00000	0.770987D 00	0.820920D 00	0.888584D 00	0.940288D 00	0.964757D 00
4.20000	0.760234D 00	0.812558D 00	0.883423D 00	0.937547D 00	0.963147D 00

Z / DELTA/KT	2.000	2.200	2.500
0.80000	0.997032D 00	0.997757D 00	0.998461D 00
1.00000	0.995721D 00	0.996768D 00	0.997784D 00
1.20000	0.994300D 00	0.995695D 00	0.997050D 00
1.40000	0.992807D 00	0.994567D 00	0.996278D 00
1.60000	0.991270D 00	0.993407D 00	0.995483D 00
1.80000	0.989712D 00	0.992230D 00	0.994678D 00
2.00000	0.988151D 00	0.991051D 00	0.993870D 00
2.20000	0.986600D 00	0.989879D 00	0.993067D 00
2.40000	0.985068D 00	0.988723D 00	0.992275D 00
2.60000	0.983565D 00	0.987588D 00	0.991498D 00
2.80000	0.982094D 00	0.986477D 00	0.990737D 00
3.00000	0.980661D 00	0.985395D 00	0.989997D 00
3.20000	0.979268D 00	0.984344D 00	0.989277D 00
3.40000	0.977916D 00	0.983323D 00	0.988578D 00
3.60000	0.976607D 00	0.982336D 00	0.987903D 00
3.80000	0.975342D 00	0.981381D 00	0.987249D 00
4.00000	0.974119D 00	0.980459D 00	0.986619D 00
4.20000	0.972939D 00	0.979569D 00	0.986011D 00