K. Baker and G. Paternò: NUMERICAL CALCULATION OF THE ZERO BIAS CONDUCTIVITY FOR A SUPERCONDUCTING TUNNEL JUNCTION, IN THE PRESENCE OF "DEPAIRING".
K. Baker\textsuperscript{(x)} and G. Paternò: NUMERICAL CALCULATION OF THE ZERO BIAS CONDUCTIVITY FOR A SUPERCONDUCTING TUNNEL JUNCTION, IN THE PRESENCE OF "DEPAIRING".

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 $\sigma$. 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 $\sigma$ are calculated by Bermon\textsuperscript{(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 However, these values are no longer valid if the s.c. is in the presence of a factor which causes the breaking of superconducting pairs.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 $\sigma$, 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\textsuperscript{(1)}:

\textsuperscript{(x)} - fellowship CNEN.
\[ \frac{dI}{dV} = \left( \frac{dI}{dV} \right)_N \int_{-\infty}^{+\infty} G(\varepsilon) \left( \frac{1}{kT} \frac{e^{\frac{x}{2}}}{(1 + e^{\frac{x}{2}})^2} \right) d\varepsilon \]

with

\[ x = (\varepsilon - eV)/kT \quad G(\varepsilon) = \frac{N_s(\varepsilon)}{N(0)} \]

\( \varepsilon \) 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 Boltzmann 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:

\[ G(\varepsilon) = \begin{cases} 0 & |\varepsilon| < \Delta_0 \\ \frac{|\varepsilon|}{(\varepsilon^2 - \Delta_0^2)^{1/2}} & |\varepsilon| \geq \Delta_0 \end{cases} \]

where \( 2\Delta_0 \) 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 \( G(\varepsilon) \) 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 expressible 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 \( I \ll \xi_0/(1 = \text{mean free path}, \xi_0 = \text{coherence length}), \) Maki(4) has derived the expression:
\[ J = K \left( \frac{\pi}{2} - \frac{2}{3} Z^{3/2} \right) \quad \text{for } Z \leq 1 \]
\[ J = K \left( \text{arc} \sin Z^{-3/2} - \frac{2}{3} \left( Z^{3/2} - \sqrt{Z^{-3}} \right) + \frac{1}{3} \sqrt{1 - Z^{-3}} \right) \quad \text{for } Z > 1 \]

\( J \) 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:

\[ G(\varepsilon, Z) = \frac{\varepsilon}{\Delta} \frac{1}{Z^{1/2}} \text{Im} \frac{1}{(\bar{x} - Z)} \tag{3} \]

where \( \bar{x} \) is the complex solution of the fourth order polynomial:

\[ x^4 - 2Zx^3 + x^2 \left( \frac{1}{Z} \left( \frac{\varepsilon}{\Delta} \right)^2 - \frac{1}{Z} + Z^2 \right) + 2x - Z = 0 \tag{4} \]

For \( \varepsilon > \varepsilon_m \), this equation has two real roots and two roots which are complex conjugates. \( \varepsilon_m \) is given by the expression\(^{(4)}:\)

\[ \varepsilon_m = \Delta (1-Z)^{3/2} \quad \text{for } Z \leq 1 \]
\[ \varepsilon_m = 0 \quad \text{for } Z > 1 \tag{5} \]

\( \Delta \) is the gap in the presence of "depairing". It is related to the gap in the absence of "depairing", \( \Delta_o \), by the relation\(^{(4)}:\)

\[ \Delta = \Delta_o \exp\left(-\frac{\pi}{4} Z^{3/2}\right) \quad \text{for } Z \leq 1 \]
\[ \Delta = \Delta_o \exp\left(-\text{arc} \cosh Z^{3/2} - \frac{1}{2} \left( Z^{3/2} \text{arc} \sin Z^{-3/2} - (1-Z^{-3})^{1/2} \right) \right) \quad \text{for } Z > 1 \tag{6} \]

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 \( \beta = \frac{\Delta_0}{kT} \) 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 \( \sigma \) v. s. \( Z \) for three values of \( \beta \).

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

\[
\sigma(\beta, Z) = 2 \left( \frac{\Delta}{kT} \right) \int_{\frac{\epsilon_m}{\Delta}}^{\infty} G(E, Z) \frac{e^{E \cdot \Delta / kT}}{(1 + e^{E \cdot \Delta / kT})^2} \, dE
\]

where \( E = \frac{\epsilon}{\Delta} \) is the energy measured with respect to the gap in the presence of "depairing".

One passes from \( \Delta_0 / kT \) to \( \Delta / kT \) 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 \( 5 \times 10^{-8} \).

Since the integrand for \( Z < 1 \) or for large values of \( \beta \) has a pronounced peak at \( E \approx 1 \), the interval of integration is broken into smaller intervals.

The first interval goes from \( \frac{\epsilon_m}{\Delta} \) 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 \( x_0 \pm i \gamma_0 \), \( (2) \) becomes

\[
G(E, Z) = \frac{E}{Z^{1/2}} \frac{|\gamma_0|}{(x_0 - Z)^2 + \gamma_0^2}
\]

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:

\[
x^2 + \frac{a}{2} + \frac{1}{2} y = ex + f \quad \quad x^2 + \frac{a}{2} x + \frac{1}{2} y = -ex - f
\]

where
\[ e = \sqrt{\frac{a}{4} - b + y} \], \quad 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:

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

In our case the resolvent becomes:

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

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

\[ p = \frac{a}{3} + b \]
\[ q = 2\left(\frac{a}{3}\right)^3 - \frac{ab}{3} + c \]

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:

\[ y_1 = 2 \sqrt[3]{\frac{-q}{2} - \frac{a}{3}}, \quad y_2 = y_3 = -\sqrt[3]{\frac{-q}{2} - \frac{a}{3}} \]
3) \( Q < 0 \): The cubic has three real roots that are written in trigonometrical form:

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

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

where

\[
\varphi = -2 \frac{\sqrt{-Q}}{q}
\]

and

\[
\frac{\pi}{2} \leq \varphi \leq \pi \quad \text{if} \quad q > 0, \quad 0 \leq \varphi \leq \frac{\pi}{2} \quad \text{if} \quad q < 0
\]

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 \( \leq 1 \times 10^{-4} \).

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

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REFERENCES.

10.

MAINPG

REAL*8 NEWINT
DOUBLE PRECISION EO,APTEST,FINT,COM
DOUBLE PRECISION FOUR,H,CONV
DOUBLE PRECISION DENS,Z,FORG,FUNC,FUNL,FINC,EMIN,EMAX,PET,A
DOUBLE PRECISION TOTINT,ATEST,TEST,FUNMIN,FUNMAX,OMEGA,EXPO,PESO,TNO
DIMENSION TEST(30),ATST(30),FUNMIN(30),FUNMAX(30)
DIMENSION ZA(30),EINT(30),SIGZER(30)
DIMENSION BET(30),NEWINT(30),TOTINT(30,30),FINT(30)
DIMENSION FOUR(30),THD(30),IFLAG(30),KFLAG(30)
JMAX=17
IMAX=18
READ 91,(ZA(I),I=1,IMAX)
91 FORMAT(I13,6)
READ 90,(EINT(J),SIGZER(J),J=1,IMAX)
90 FORMAT(2F7.5)
EPSI=.5E-66
EPSEC=1.0E-03
PIGR=3.1415926535897932
DO 250 JB=1,JMAX
Z=ZA(JB)
CALL ZFUCN(Z,A,EO)
PRINT 600, Z, A, EO
600 FORMAT(1H0, Z=",E14.7,10X,A",",E14.7,10X,EO=",",E14.7)

C **************CALCULA LA FUNZIURF PER E=1
C E=1.
CALL DENSIT(Z,E,DENS,KFR)
FUNC=DENS
Fun=FUNC
FINC=1.
EMIN=EO
EMAX=1.
APTEST=0.
DO 5 10=1,IMAX
BETA(10)=EINT(10)=A
PRINT 601, BETAT(10)
601 FORMAT(1H0, BETAT(10)=",E14.7)
10=JP+1
TOTINT(IP,10)=0.
KFLAG(IB)=0.
ATST(IB)=0.
TEST(IB)=0.
FUNMIN(IB)=0.
C **************CALCULA LA FUNZIONE DI FERMI
OMEGA=BETAT(10)*E
EXPOM=EXP(OMEGA)
C0M=(EXP0N+1.)
C0M=C0M*C0M
PESO=EXP0N*C0M
5 FUNMAX(IB)=PESO*FUN1
9 DO 10 IB=1,IMAX
IFLAG(IB)=0.
TWG(IP)=0.
10 FOUR(IB)=0.
H=(FUNMAX-FINT)/2.
N=1.
EMIN+H
PRINT 602, E
602 FORMAT(1H0,'E=E,E14.7)  
CALL DENSIT(Z,E,DENS,KER)  
FUNC=DENS  
DO 11 ID=1,IBMAX  
IF(KFLAG(IB).EQ.1) GO TO 11  
OMEGA=BETA(IB)*E  
EXP0=DEXP(OMEGA)  
COM=(EXP0+1.)  
COM=COM*COM  
PESO=EXP0/COM  
FUN=PESO*FUNC  
FOUR(IB)=FOUR(IB)+FUN  
FINT(IB)=(H*Ffunmin(IB)+FUNMAX(IB)+4.*FOUR(IB))/3.  
FINT(IB)=2.*BETA(IB)*FINT(IB)  
11 CONTINUE  
C  
EVOLUTION LOGP  
25 H=H/2.  
N=2*N  
E=E+EIN  
DO 12 IB=1,IBMAX  
IF(KFLAG(IB).EQ.1 OR KFLAG(IB).EQ.1) GO TO 12  
TWO(IB)=TWO(IB)+FOUR(IB)  
FOUR(IB)=0.  
12 CONTINUE  
DO 26 IP=1,N  
CALL DENSIT(Z,E,DENS,KER)  
FUNC=DENS  
DO 13 IR=1,IBMAX  
IF(KFLAG(IR).EQ.1 OR KFLAG(IB).EQ.1) GO TO 13  
OMEGA=BETA(IR)*E  
EXP0=DEXP(OMEGA)  
COM=(EXP0+1.)  
COM=COM*COM  
PESO=EXP0/COM  
FUN=PESO*FUNC  
FOUR(IB)=FOUR(IB)+FUN  
13 CONTINUE  
26 E=E+E+H  
LFLAG=0  
DO 14 ID=1,IBMAX  
IF(KFLAG(IB).EQ.1) IFLAG(IB)=1  
IF(KFLAG(IB).EQ.1) GO TO 17  
NEWINT(IB)=4.*FUNMNX(IB)+FUNMAX(IB)+2.*TWO(IB)+4.*FURU(IB))/3.  
NEWINT(IB)=2.*BETA(IB)*NEWINT(IB)  
TEST(IB)=ABS(FINT(IB)-NEWINT(IB))  
ABTEST=ABTEST+ABS(NEWINT(IB))  
IF(NEWINT(IB)+L,F=~EPSI. AND. L,BTEST,LE,EPSEC) IFLAG(IB)=1  
17 LFLAG=LFLAG+IFLAG(IB)  
FINT(IB)=NEWINT(IB)  
14 CONTINUE  
IF(NGT,20000,OR,H,LE,EPIS) 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,EPIS. AND. EMIN,GT,1.) KFLAG(IB)=1  
15 NFLAG=NFLAG+KFLAG(IB)
16 CONTINUE
   IF(NFLAG-I MAX) 20,31,31
20 CONTINUE
   EMIN=E MAX
   F MAX=F MIN+E INC
   E=E MAX
   CALL DENSIT(Z,E,DENS,KER)
   FUNC=DENS
   DO 30 IB=1,IB MAX
   IF(KFLAG(IB),F .GE. 1) GO TO 30
   FUN MIN(IB)=FUN MAX(IB)
   OMEGA=BETA(IB)*E
   EXPO=EXP(OMEGA)
   CM=CM*CM
   P=SG=EXPO/CM
   FUN MAX(IB)=P*E SU+FUNC
30 CONTINUE
   GO TO 9
31 CONTINUE
   DO 10 G IB=1,IB MAX
   TEST(IB)=ATEST(IB)
   CONDU=TOT INT(IB,IBB)/SIG ZER(IB)
   PRINT 97, BETA(IB),Z,TOT INT(IB,IBB),N,TEST(IB),CONDU
97 FORMAT(3X,2F10.5,10X,DI 4.6,110,17X,DI 7.6,DI 5.6,/)  
100 CONTINUE
250 CONTINUE
   DO 6000 IB=1,IB MAX
6000 TOT INT(IB,1)=SIG ZER(IB)
   JBIG=JB MAX
   DO 7000 JB=1,JB MAX
   JBB=JBIG+1
   ZA(JBB)=ZA(JBIG)
7000 JBIG=J BIG-1
   ZA(1)=0.0000
   NN=0
   NN=1
9000 NN=NN+5
   ************
   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=-'),'I',120(I=-'),2(/,15X 2,'I'))
   DO 5000 IB=1,IB MAX
5000 PRINT 1000,BETA(IB),(TOT INT(IB,JB),JB=NN,NM)
1000 FORMAT(3X,F10.5,2X,'I',3X,5(D14.6,5X),/15X,'I')
   NN=NN+5
   IF(NN.LE.(JB MAX+1)) GO TO 9000
STOP
END
14.

**DENSIT**

SUBROUTINE DENSIT(Z,EN,DENS,IER)
DOUBLE PRECISION A,B,C,A3,P,Q,YCUB,DELTA,AA,BB,ARG,AA1,BB1,FI,CONTR
DOUBLE PRECISION E,F,B1,C1,DSC,X,Y,COEF4,CUB,Z,EN,ZZ,XZ,DENS,P1GR
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.
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(PR) 15,16,17
15 AA=(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
C' SONO TRE RADICI REALI DI CUI 2 COINCIDENTI
20 IF(Q) 21,4,22
C
SEGLIE LA RADICE POSITIVA
21 YCUB=2.5*DEXP(DLOG(-Q)/3.)
IER=5
GO TO 50
22 YCUB=DEXP(DLOG(Q)/3.)
IER=5
GO TO 50
C
C' SONO 3 RADICI REALI DISTINTE
30 DELTA=-DELTA
IER=5
ARG=DSQRT(DELTA)/Q
FI=DATAN(ARG)
IF(FI) 32,33,33
32.*PIGR+FI
33 YCUB=2.5*DSQRT(-P)*UCOS(FI/3.)
50 YCUB=YCUB-A3
C *******************************************************************************************************
CONTR=YCBU*YCBU*YCBU+AYCBU+YCBU+BYCBU+C
C*******************************************************************************************************
C RISOLUZIONE EUGALE, IV GRADO
A=YCBU-(EN*EN-1.)/Z
B=-2.*Z*YCBU
C=Z+YCBU*YCBU/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 SCELGIE QUella COMPLESSA
80 B1=GCF4/2.*E
C1=YCBU/2.*F
C CALCOLA IL DISCRIMINANTE
81 DISC=M1*B1-4.*C1
IF(DISC) 85,82,82
82 B1=GCF4/2.*E
C1=YCBU/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(IHO,'NON CI SONO RADICI COMPLESSE',15)
DEN=0.
GO TO 805
C E O F SONO COMPLESSI
91 IER=3
800 Z=DSQRT(Z)
XZ=X-Z
DEN=(EN/Z2)*(Y/(XZ*XZ+Y*Y))
805 CONTINUE
RETURN
END

ZFUNC

SUBROUTINE ZFUNC(Z,A,ED)
DOUBLE PRECISION PI9R,ALFA
DOUBLF PRECISION 7,U,A9OHU,ARGU,ASIN,A,ED
PI9R=3.1415926535897932
IF (Z-1) 608,608,607
608 ALFA=DEXP(3.*DLOG(Z)/Z2.)
A=DEXP((-PI9R/4.)*ALFA)
IF (Z-1) 609,610,610
609 ED=DEXP(3.*DLOG(1.-Z)/Z2.)
RETURN
610 ED=0.
RETURN
607 U=DEXP(3.*DLOG(Z)/Z2.)
A9OHU=DLOG(U+DSQRT(U*U-1))
ARGU=DSQRT(1./U*(U-1))
ASIN=CATAN(ARGU)
A=DEXP(-A9OHU-{U*ASIN-DSQRT(1.-1./U*U)})/2.)
ED=0.
RETURN
END
$\sigma(\beta, Z) \text{ V.S. } Z \text{ for } \beta=1, \beta=2.2, \beta=4.0$
<table>
<thead>
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<th>DELTA/κT</th>
<th>0.0</th>
<th>0.050</th>
<th>0.100</th>
<th>0.150</th>
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