

```

Program dwave
parameter(neps=180,nang=180,nfreq=100,nphys=1000)
double precision del0,alpha,scr,minfreq,maxfreq,trel,tc,wc
real e(nphys),sigma(nphys)
real pi,tc0,d0,ep,gam
* ,sigma0,sg,cut,w,wmin,wmax,rr,l,es,sum,sumn,epsinf
complex eps,epsx,cn
integer delflag,i,nw,it,nt
open(21,file='dwave.log')
pi=4.*atan(1.)
c   write(*,*) 'T, and Tc0 in units of Kelvin '
read(*,*) t,Tc0
trel=t/tc0
d0=tc0*0.695*1.73
del0=d0/(tc0 * 0.695)
c   write(*,*) 'give epsinfy, scattering cross section,
c   * and plasma frequency, decay rate in 1/cm '
read(*,*) epsinf,scr,ep,gam
alpha=gam/(2.* pi * tc0 * 0.695)
c   write(*,*) 'give lower and upper frequency
c   * in 1/cm and no of points'
read(*,*) wmin,wmax,nw
minfreq=0.05
maxfreq=8.05
wc=40.d0
delflag=1
nt=4
c   do 900 it=1,nt+1
c   trel=real(it)/real(nt)
***** calculate the real part of the conductivity using palumba's routines
call rcond(del0,alpha,scr,minfreq,maxfreq,nfreq,neps,nang,
* delflag,trel,tc,wc,e,sigma)
write(21,*) 'trel,tc0,tc,del0 ',trel,tc0,tc,del0
c   **convert t and tc to absolute units of K
c   t=trel*tc0
tc=tc*tc0
write(21,*) 'trel,tc0,tc,del0 ',trel,tc0,tc,del0
sigma0=ep**2 / (2. * gam )
***** convert back to absolut units: 1/cm for frequency and sigma.
***** and calculate the superfluid response part of epsilon using the
***** f-sum rule (integration using trapezium method, same was used in
***** the Kramers-Kronig transformation routine Hilber)
sum=0.0
do 100 i=1,nfreq
e(i)=real(e(i))*del0*tc0*0.695
sigma(i)=real(sigma(i))*sigma0
sum=sum+sigma(i)
100 continue
de=e(2)-e(1)
sum=(sum-sigma(1)/2.-sigma(nfreq/2.))*4.*de/pi
sumn=ep*ep*(2./pi)*atan(e(nfreq)/gam)
write(*,*) 'sums,sumn ',sum,sumn
if (sumn.gt.sum) then
es=sqrt(sumn-sum)
else
es=0.
endif
write(21,*) 'superfluid fraction = ', (es/ep)**2

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***** Make a Kramers-Kronig transform of the real part of sigma, assuming
***** that for  $w > e(\text{nfreq})$  the behaviour is purely Drude like. This part
***** of the Kramers-Kronig transform is calculated using an analytical
***** expression. Also the f-sum part is added.
      cut=e(nfreq)
      do 200 i=0,nw
      w=wmin+real(i)*(wmax-wmin)/real(nw)
      if (w.ne.cut) then
        CALL HILBER(sigma,e,nfreq,w,eps,l)
        call extrap(ep,gam,l,cut,w,epsx)
        eps=epsinf-(es/w)**2+eps+epsx
        write(*,*) w/8.0657,real(eps),aimag(eps)
      endif
200   continue
c900  continue
      close(21)
      end
*****
*****
      subroutine rcond(delo, alpha, sigma, wfreq0, maxfreq
* , Nfreq, Neps, Nang, delflag, T, tc, wc, xout, yout)
*****
c   **delo: Initial value for the gap amplitude in units of Tc0.
c   **alpha:  $1/2\pi\tau$  (tau=scattering rate) in units of Tc0.
c   **sigma: Scattering cross-section: 0.0 = Born limit; 1.0 = Unitarity
limit.
c   **wfreq: Initial frequency in units of gap amplitude (delo).
c   **maxfreq: Maximum frequency in units of gap amplitude (delo).
c   **Nfreq: Number of points at which to calculate the conductivity.
c   **Neps: Number of points used in the epsilon integral for the
conductivity.
c   **Nang: Number of points used in the angular integral for the
conductivity.
c   **delflag: If 0 -> Use the value given for "delo" as the gap amplitude.
c   **      If 1 -> Solve self-consistently for the gap amplitude.
c   **T: temperature in units of the "actual" Tc (only used if delflag=1).
c   **wc: Energy cutoff for the Matsubara sums in units of Tc0
c   **      (only used if delflag=1; 40 is a good number).
c   **
c   **Note: Tc0 = Transition temperature for the clean (alpha=0) system.
c   **      Tc = "Actual" transition temperature for the given alpha.
c   **
c   **Calculates the real part of the optical conductivity for a simple
c   **d-wave model.
c   **On output : xout = the Nfreq frequency values in units of Tc0
c   **      yout = the Nfreq conductivity values in units of sigma-0
c   **On output T is given in units of the actual tc
c   **on output delo is the new gap in units of Tc0
c   **on output Tc is given in units of tc0
c   **Original Version : 05-94
c   **Last revised : 23-09-94
c
c   **Written by:
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c   ** Universitaet Bayreuth
c   ** D-95440 Bayreuth, GERMANY
c   ** converted to subroutine format by D. van der Marel

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*****
implicit none
integer Nfreq, Neps, Nang, delflag, i, units
complex*16 csmall, cint1, cint2, cint3, cint4, cond, eps_int
double precision del0, alpha, sigma, T, wc
double precision wfreq0, maxfreq, delfreq, wfreq, Tc, pairbrk
double precision delta, epsilon, err, pi, range, llim, ulim, tmp
double precision zero, one, two, three, four, five
real xout(1000),yout(1000)
parameter (zero=0.0d0, one=1.0d0, two=2.0d0, three=3.0d0)
parameter (four=4.0d0, five=5.0d0)
c   ** Set some constants:
c   ** delta : Offset for the finite-differenced derivatives.
c   ** epsilon : Maximum residual for termination of the Newton iterations.
c   ** err : Integrate up to err from singularities.
c   ** csmall : +/- with epsilon to get retarded/advanced propagators.
c   ** pi : 3.14...
delta = 1.0d-6
epsilon = 1.0d-10
err = 1.0d-8
csmall = (zero,1.0d-8)
pi = acos(-one)
c   **Calculate the "actual" Tc
Tc = pairbrk(alpha)
c   **Calculate self-consistent gap if desired.
if (delflag .gt. 0) then
    call get_del0(del0,T*Tc,alpha,sigma,wc,delta,epsilon,1)
end if
c   **Determine the frequency (omega) step size in units of Tc0.
if (Nfreq .gt. 1) then
    delfreq = (maxfreq-wfreq0)*del0 / dble(Nfreq-1)
else
    delfreq = zero
end if
T = T*Tc
do 100 i = 1, Nfreq, 1
    wfreq = wfreq0*del0 + dble(i-1)*delfreq
    range = wfreq/two + 7.0d0*T
    cint1 = (zero,zero)
    cint2 = (zero,zero)
    cint3 = (zero,zero)
    cint4 = (zero,zero)
c   **For each frequency (wfreq) we must do an energy integral. This
c   **integral contains, in general, singularities (1/sqrt type). In
c   **fact we cannot locate them exactly since we integrate on epsilon
c   **while the singularities occur at:
c   ** Re( epsilon-tilde(epsilon) ) = (+/-) delta_0
c   ** Re( epsilon-tilde(epsilon+omega) ) = delta_0
c   **where epsilon-tilde is the renormalized or "dressed" energy. On
c   **the other hand the sigularities are only a problem when alpha->0,
c   **since here epsilon-tilde has almost no imaginary component; but
c   **as alpha->0, epsilon-tilde->epsilon so we can do a pretty good
c   **job of locating the sigularities in practice. The following if
c   **statement breaks the integral into pieces (around the "critcal"
c   **points) based on the following three cases repectively:
c   ** delta_0 < omega/2          (needs 3/4 regions)
c   ** delta_0 > omega           (needs 4 regions)
c   ** omega/2 < delta_0 < omega (needs 3/4 regions)

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c      **Note that epsilon=0 is always a special point since the integrand
c      **has a sharp jump there at low temperatures (coming from a tanh).
c      if ( del0 .le. (wfreq/two) ) then
c          **Do integral from -omega/2 to -del0 (if del0 != omega/2).
c          if ( (wfreq/two - del0) .gt. two*err ) then
c              llim = -(wfreq / two) + err
c              ulim = -del0 - err
c              cint1 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c              end if
c          **Do integral from -del0 to 0 (if del0 != omega/2).
c          llim = -del0 + err
c          ulim = -err
c          cint2 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c          **Do integral from 0 to (range-omega/2)
c          llim = err
c          ulim = range - (wfreq / two)
c          cint3 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c          else if ( del0 .gt. wfreq ) then
c              **Do integral from -omega/2 to 0.
c              llim = -(wfreq / two) + err
c              ulim = -err
c              cint1 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c              **Do integral from 0 to (range-omega/2)
c              llim = err
c              ulim = range - (wfreq / two)
c              cint2 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c          else
c              **Do integral from -omega/2 to del0-wfreq.
c              llim = -(wfreq / two) + err
c              ulim = (del0 - wfreq) - err
c              cint1 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c              **Do integral from del0-wfreq to 0 (if del0-omega != 0).
c              if ( (wfreq-del0) .gt. two*err ) then
c                  llim = (del0 - wfreq) + err
c                  ulim = -err
c                  cint2 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                      Nang,Neps,Nfreq)
c              end if
c              **Do integral from 0 to (range-omega/2)
c              llim = err
c              ulim = range - (wfreq / two)
c              cint3 = eps_int(llim,ulim,range,wfreq,del0,alpha,sigma,T,
#                  Nang,Neps,Nfreq)
c          end if
c          **In our units we multiply the resulting integral by alpha and
c          **divide by omega (plus a small imaginary piece to prevent an
c          **explosion as omega->0) to get the conductivity.
c          cond = -alpha*(cint1 + cint2 + cint3) / (wfreq + csmall)
c          xout(i) = wfreq/del0
c          yout(i) = real(cond)
100 write(21,*) 'rcond : ',xout(i),yout(i)
      continue

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return
end
*****
*****
SUBROUTINE HILBER(sigma,e,n,w,eps,l)
*****
*****HILBERT TRANSFORM of the imaginary part of epsilon to
*****the complex epsilon. The program takes on input only
*****positive values of frequency, but uses the fact that
*****Im(eps) is odd.
* An exact linear interpolation is performed in the intervals between the
* energies where the imaginary part of g is defined on input. The integration
* is 'smoothed' with an energy value l, also defined on input. This
* value must be made much smaller than the energy increments de of the input
* array. The output contains 'kinks' at the energies where Re sigma was
* defined on input.
* From input it reads
*(1) sigma: the real part of the dielectric conductivity function
*(2) E(i): the energy of the array element no i of the array sigma
*(3) n: the number of energy values contained in array sigma
*(4) w: The value of the energy for which epsilon is calculated
* To output it writes:
*(5) eps: The complex dielectric function.
* IT IS VERY IMPORTANT THAT BOTH REAL AND
* IMAGINARY PARTS OF THIS ARRAY ARE USED TOGETHER, because together
* they satisfy Kramers Kronig relations EXACTLY. Note that the imaginary
* part differs slightly from the input array, because of the broadening
* through l!!
*****
parameter(nphys=1000)
REAL sigma(nphys),sa,sb,e(nphys),A,B,l,w,rho,gam,pi,rcd,icd
COMPLEX eps,s,cw
INTEGER N,I,J
pi=4.*atan(1.)
*****l is the 'smoothing' parameter, chosen much smaller than delta-e
l=(e(2)-e(1))*1.e-5
cw=cplx(w,l)
S=(0.,0.)
DO 40 J=1,N-1
a=e(j)
b=e(j+1)
sa=sigma(J)
sb=sigma(J+1)
rho=(sa*b-sb*a)/(b-a)
gam=(sb-sa)/(b-a)
S=S+rho*(clog(b-cw)-clog(b+cw)+clog(a+cw)-clog(a-cw))/cw
* +gam*(clog(b**2-cw**2)-clog(a**2-cw**2))
40 CONTINUE
eps=S*2./pi
c write(*,*) i,w,eps
c WRITE(*,*) 'Hilberttransform ready.'
RETURN
END
*****
*****
subroutine extrap(ep,gam,l,cut,w,epsx)

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*****
      real g,ep,gam,l,cut,pi,w
      complex epsx,cw
      INTEGER I
      cw=cmplx(w,l)
      pi=4.*atan(1.)
      epsx=((ep**2)/(pi*(cw**2+gam**2))) *
*          ( (gam/cw)*(clog(cut+cw)-clog(cut-cw))
*            + 2*atan(cut/gam) - pi )
c      write(*,*) w,ep,gam,cut,epsx
      return
      end
*****

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c*****
c
c      complex*16 function eps_int(llim,ulim,range,wfreq,del0,alpha,
c      #                               sigma,T,Nang,Neps,iflag)
c
c      implicit none
c      double precision llim, ulim, range, wfreq
c      double precision del0, alpha, sigma, T
c      integer Nang, Neps, iflag
c
c      **This function uses Simpson's rule to do an energy integral from
c      **llim to ulim.  If iflag=1 then the integrand will be printed
c      **(in the file fort.20) showing which points were used.
c
c      integer j, Nc
c      complex*16 ct, cint, phi_int, phi_int2
c      double precision eps, deleps, pi, acos, delta, epsilon
c      double precision zero, one, two, three, four
c      parameter (zero=0.0d0, one=1.0d0, two=2.0d0, three=3.0d0)
c      parameter (four=4.0d0)
c
c      delta = 1.0d-6
c      epsilon = 1.0d-10
c      pi = acos(-one)
c
c      **Nc is calculated to keep the density of points roughly the same
c      **in each region.  However there is a lower bound put in by hand to
c      **be sure each region has enough points.  Since we use Simpson's rule,
c      **Nc MUST be positive.
c      Nc = 2*(( int((ulim-llim)*dble(Neps)/range) + 1 ) / 2)
c      if (Nc .lt. 20) Nc = 20
c      deleps = (ulim - llim) / dble(Nc)
c      eps = llim
c      cint = phi_int(eps,wfreq,del0,alpha,sigma,delta,epsilon,T,
c      #                               Nang,Neps)
c      if (iflag .eq. 1) write(20,*) eps, real(cint), dimag(cint)
c      do j = 1, Nc-1, 1
c          eps = eps + deleps
c          ct = phi_int(eps,wfreq,del0,alpha,sigma,delta,epsilon,T,
c      #                               Nang,Neps)
c          if (iflag .eq. 1) write(20,*) eps, real(ct), dimag(ct)
c          if (mod(j,2) .eq. 1) then

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        cint = cint + four*ct
    else
        cint = cint + two*ct
    end if
end do
eps = eps + deleps
ct = phi_int(eps,wfreq,del0,alpha,sigma,delta,epsilon,T,
#           Nang,Neps)
if (iflag .eq. 1) write(20,*) eps, real(ct), dimag(ct)
cint = cint + ct
cint = deleps*cint/three
c
    eps_int = cint
c
    return
end

c
c**File : integrals.f
c
c**A set of routines for doing the angular integrals in the conductivity.
c
c**Original Version : 05-94
c**Last revised : 11-10-94
c
c**Written by:
c** Mario Palumbo, Matthias Graf, and Dierk Rainer
c** Theoretische Physik III
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c** D-95440 Bayreuth, GERMANY
c

c    complex*16 function sqrt(x)
c    complex*16 x
c    sqrt=dcmplx(csqrt(cmplx(x)))
c    return
c    end
c
c    complex*16 function log(x)
c    complex*16 x
c    log=dcmplx(clog(cmplx(x)))
c    return
c    end
c
c    double precision function imag(x)
c    complex*16 x
c    imag=aimag(cmplx(x))
c    return
c    end
c-----
c
c    complex*16 function phi_int(eps,wfreq,del0,alpha,sigma,delta,
#                               epsilon,T,Nang,iflag)
c
c    double precision eps, wfreq, del0, alpha, sigma, delta, epsilon, T
c    integer Nang, iflag
c
c    **Performs the angular integration over the conductivity integrand,

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c  **and multiplies in the "tanh" factors at the end.
c
c  complex*16 csmall, ceps, cepst, cepsw, cepstw, get_cepst
c  complex*16 cint1, cint2, ctmp1, ctmp2
c  complex*16 ccepst, ctmpae, ctmpre, ctmprw, Dmr, Dmn, cg3bar
c  double precision err, epsw, tmp, phi0, phi0w
c  double precision zero, one, two, pi
c  parameter (zero=0.0d0, one=1.0d0, two=2.0d0)
c
c  pi = acos(-one)
c  err = 1.0d-6
c  csmall = (zero,1.0d-6)
c
c  epsw = eps + wfreq
c
c  **Calculate epsilon_tilde_retarded at epsilon and epsilon+omega.
c  ceps = eps + csmall
c  cepst = get_cepst(cepst,ceps,del0,alpha,sigma,delta,epsilon,0)
c  cepsw = epsw + csmall
c  cepstw = get_cepst(cepstw,cepsw,del0,alpha,sigma,delta,epsilon,0)
c
c  **Calculate the "D_minus" factors which appear in the conductivity
c  **integrand.
c  ccepst = conjg(cepst)
c  tmp = alpha*sqrt(sigma)*sqrt(one-sigma)
c  if (tmp .gt. 1.0d-8) then
c    ctmpae = one + (cg3bar(ccepst,del0,0)/pi)**2
c    ctmpre = one + (cg3bar(cepst,del0,0)/pi)**2
c    ctmprw = one + (cg3bar(cepstw,del0,0)/pi)**2
c    Dmr = ((tmp*ctmpre) / (one - sigma*ctmpre))
c    #   - ((tmp*ctmprw) / (one - sigma*ctmprw))
c    Dmn = ((tmp*ctmpae) / (one - sigma*ctmpae))
c    #   - ((tmp*ctmprw) / (one - sigma*ctmprw))
c  else
c    Dmr = zero
c    Dmn = zero
c  end if
c
c  **Determine how many sqrt-singularities our phi-integrand has.
c  phi0 = -one
c  phi0w = -one
c  tmp = real(cepst**2)
c  if (tmp .ge. zero) tmp = sqrt(tmp) / del0
c  if ((tmp .le. one) .and. (tmp .ge. zero)) phi0 = acos(tmp)
c  tmp = real(cepstw**2)
c  if (tmp .ge. zero) tmp = sqrt(tmp) / del0
c  if ((tmp .le. one) .and. (tmp .ge. zero)) phi0w = acos(tmp)
c
c  **Do the angular integral...
c  if ( (phi0 .lt. zero) .and. (phi0w .lt. zero) )then
c  **This is the case of no sqrt_singularities. Do a simple Simpson's
c  **rule from 0 to pi/2.
c    call simpson0(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
c  #   Dmr,Dmn,Nang,iflag)
c    if (iflag .eq. 1) write(21,*) eps, ' 0.0'
c  else if ( (phi0w .lt. zero) .and. (phi0 .gt. zero) )then
c  **This is the case of one sqrt_singularity at phi0. Here we do a
c  **Simpson's rule integral from 0 to phi0-err and from phi0+err to

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c    **pi/2 with the singular part of the integral subtracted out. The
c    **finite contribution of the sqrt-singularity is then added back
c    **by hand from an analytic expression.
      call simpson1(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
#           Dmr,Dmn,zero,phi0-err,phi0,1,Nang,iflag)
      call simpson1(cepst,cepstw,ctmp1,ctmp2,del0,alpha,sigma,T,
#           Dmr,Dmn,phi0+err,pi/two,phi0,1,Nang,iflag)
      cint1 = cint1 + ctmp1
      cint2 = cint2 + ctmp2
      if (iflag .eq. 1) write(21,*) eps, ' 1.0'
      else if ( (phi0w .gt. zero) .and. (phi0 .lt. zero) )then
c    **This is the case of one sqrt_singularity at phi0w. Here we do a
c    **Simpson's rule integral from 0 to phi0w-err and from phi0w+err to
c    **pi/2 with the singular part of the integral subtracted out. The
c    **finite contribution of the sqrt-singularity is then added back
c    **by hand from an analytic expression.
      call simpson1(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
#           Dmr,Dmn,zero,phi0w-err,phi0w,2,Nang,iflag)
      call simpson1(cepst,cepstw,ctmp1,ctmp2,del0,alpha,sigma,T,
#           Dmr,Dmn,phi0w+err,pi/two,phi0w,2,Nang,iflag)
      cint1 = cint1 + ctmp1
      cint2 = cint2 + ctmp2
      if (iflag .eq. 1) write(21,*) eps, ' 1.5'
      else
c    **This is the case of two sqrt_singularities at phi0 and phi0w.
c    **Here we divide the integration region (0 to pi/2) into 4 regions:
c    **0 to phi0w-err, phi0w+err to (phi0+phi0w)/2, (phi0+phi0w)/2 to
c    **phi0-err, and phi0+err to pi/2. Here we have assumed that phi0w
c    **will always be less than phi0! In the first 2 regions we subtract
c    **out the term which diverges at phi0w, while in the second 2 regions
c    **we subtract out the terms which diverges at phi0. The finite
c    **contributions of these 2 singular terms are added back by hand
c    **using an analytic expression.
      if (phi0 .lt. phi0w)
#       write(6,*) 'Warning: phi0 < phi0w! (eps,omega)= ', eps, wfreq
      call simpson1(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
#           Dmr,Dmn,zero,phi0w-err,phi0w,2,Nang,iflag)
      call simpson1(cepst,cepstw,ctmp1,ctmp2,del0,alpha,sigma,T,
#           Dmr,Dmn,phi0w+err,(phi0+phi0w)/two,phi0w,2,
#           Nang,iflag)
      cint1 = cint1 + ctmp1
      cint2 = cint2 + ctmp2
      call simpson1(cepst,cepstw,ctmp1,ctmp2,del0,alpha,sigma,T,
#           Dmr,Dmn,(phi0+phi0w)/two,phi0-err,phi0,1,
#           Nang,iflag)
      cint1 = cint1 + ctmp1
      cint2 = cint2 + ctmp2
      call simpson1(cepst,cepstw,ctmp1,ctmp2,del0,alpha,sigma,T,
#           Dmr,Dmn,phi0+err,pi/two,phi0,1,Nang,iflag)
      cint1 = cint1 + ctmp1
      cint2 = cint2 + ctmp2
      if (iflag .eq. 1) write(21,*) eps, ' 2.0'
      end if
c
c    **Multiply in the "tanh" factors and normalize.
      phi_int = tanh(eps/(two*T))*cint1
#           - tanh(epsw/(two*T))*conjg(cint1)
#           + (tanh(epsw/(two*T)) - tanh(eps/(two*T)))*cint2

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        phi_int = two*phi_int/pi
c
        return
        end
c
c*****
c
        subroutine cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,Dmr,Dmn,
#                               cterm1,cterm2,cterm3,cterm4,iflag)
c
        complex*16 cepst, cepstw, cterm1, cterm2, cterm3, cterm4, Dmr, Dmn
        double precision Gap2, del0, alpha, sigma
        integer iflag
c
        complex*16 Cpr, Cpn, ccepst, ctmpae, ctmpre, ctmprw
        double precision pi, acos, zero, one
        parameter (zero=0.0d0, one=1.0d0)
c
        pi = acos(-one)
        ccepst = conjg(cepst)
c
c **Calculate the "C_plus" factors.
        ctmpae = sqrt( Gap2 - ccepst**2 )
        ctmpre = sqrt( Gap2 - cepst**2 )
        ctmprw = sqrt( Gap2 - cepstw**2 )
        Cpr = -(ctmprw + ctmpre) / pi
        Cpn = -(ctmprw + ctmpae) / pi
c
c **Remove singular denominator if desired.
        if (iflag .eq. 1) then
            ctmpre = (one,zero)
            ctmpae = (one,zero)
        end if
        if (iflag .eq. 2) then
            ctmprw = (one,zero)
        end if
c
c **Calculate the four independent terms of the integrand.
        cterm1 = (pi**2)*Cpr / ((pi*Cpr)**2 + Dmr**2)
        cterm2 = cterm1*(cepst*cepstw + Gap2)/(ctmpre*ctmprw)
        cterm3 = (pi**2)*Cpn / ((pi*Cpn)**2 + Dmn**2)
        cterm4 = cterm3*(ccepst*cepstw + Gap2)/(ctmpae*ctmprw)
c
        return
        end
c
c*****
c
        subroutine simpson0(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
#                               Dmr,Dmn,Nang,iflag)
c
        complex*16 cepst, cepstw, cint1, cint2, Dmr, Dmn
        double precision del0, alpha, sigma, T
        integer Nang, iflag
c
        integer i
        complex*16 ct1, ct2, ct3, ct4
        double precision phi, dphi, Gap2

```

```

double precision zero, one, two, three, four, pi
parameter (zero=0.0d0, one=1.0d0, two=2.0d0, three=3.0d0)
parameter (four=4.0d0)
c
c
pi = acos(-one)
c
dphi = pi / dble(2*Nang)
phi = zero
Gap2 = (del0*cos(phi))**2
call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2,ct3,ct4,0)
if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
cint1 = ct1 + ct2
cint2 = ct3 + ct4
do i = 1, Nang-1, 1
  phi = phi + dphi
  Gap2 = (del0*cos(phi))**2
  call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2,ct3,ct4,0)
  if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
  if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
  if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
  if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
  if (mod(i,2) .eq. 1) then
    cint1 = cint1 + four*(ct1+ct2)
    cint2 = cint2 + four*(ct3+ct4)
  else
    cint1 = cint1 + two*(ct1+ct2)
    cint2 = cint2 + two*(ct3+ct4)
  end if
end do
phi = phi + dphi
Gap2 = (del0*cos(phi))**2
call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2,ct3,ct4,0)
if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
cint1 = cint1 + ct1 + ct2
cint2 = cint2 + ct3 + ct4
cint1 = cint1*dphi/three
cint2 = cint2*dphi/three
c
c
return
end
c
c*****
c
subroutine simpson1(cepst,cepstw,cint1,cint2,del0,alpha,sigma,T,
#           Dmr,Dmn,llim,ulim,phi0,sflag,Nang,iflag)
c
complex*16 cepst, cepstw, cint1, cint2, Dmr, Dmn
double precision del0, alpha, sigma, T
double precision llim, ulim, phi0

```

```

integer sflag, Nang, iflag
c
integer i, Nc
complex*16 ci, tmp1, tmp2, ctmp, carg, csum
complex*16 ct1, ct2, ct3, ct4
complex*16 ct2_0, ct4_0, ceps2, ceps4, sqrt
double precision phi, dphi, Gap2, diff
double precision reps2, ieps2, reps4, ieps4
double precision zero, one, two, three, four, pi
parameter (zero=0.0d0, one=1.0d0, two=2.0d0, three=3.0d0)
parameter (four=4.0d0)
c
pi = acos(-one)
ci = (zero,one)
c
if (sflag .eq. 1) then
    ceps2 = cepst
    ceps4 = conjg(cepst)
else if (sflag .eq. 2) then
    ceps2 = cepstw
    ceps4 = cepstw
else
    write(*,*) 'Bad value for sflag in simpson1: sflag = ', sflag
    stop
end if
reps2 = drealm(ceps2**2)
ieps2 = dimag(ceps2**2)
reps4 = drealm(ceps4**2)
ieps4 = dimag(ceps4**2)
tmp1 = del0**2 - two*reps2
tmp2 = sqrt(dcmplx(reps2))*sqrt(dcmplx(del0**2 - reps2))
call cond_terms(cepst,cepstw,reps2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2_0,ct3,ct4_0,sflag)
c
Nc = 2*((int(dble(2*Nang)*(ulim-llim)/pi) + 1) / 2)
if (Nc .lt. 10) Nc = 10
dphi = (ulim-llim) / dble(Nc)
phi = llim
diff = phi - phi0
Gap2 = (del0*cos(phi))**2
call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2,ct3,ct4,0)
ct2 = ct2 - ct2_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps2)
ct4 = ct4 - ct4_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps4)
if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
cint1 = ct1 + ct2
cint2 = ct3 + ct4
do i = 1, Nc-1, 1
    phi = phi + dphi
    diff = phi - phi0
    Gap2 = (del0*cos(phi))**2
    call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
#           Dmr,Dmn,ct1,ct2,ct3,ct4,0)
    ct2 = ct2 - ct2_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps2)
    ct4 = ct4 - ct4_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps4)

```

```

if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
if (mod(i,2) .eq. 1) then
  cint1 = cint1 + four*(ct1 + ct2)
  cint2 = cint2 + four*(ct3 + ct4)
else
  cint1 = cint1 + two*(ct1 + ct2)
  cint2 = cint2 + two*(ct3 + ct4)
end if
end do
phi = phi + dphi
diff = phi - phi0
Gap2 = (del0*cos(phi))**2
call cond_terms(cepst,cepstw,Gap2,del0,alpha,sigma,
# Dmr,Dmn,ct1,ct2,ct3,ct4,0)
ct2 = ct2 - ct2_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps2)
ct4 = ct4 - ct4_0 / sqrt(tmp1*(diff**2)-two*tmp2*diff-ci*ieps4)
if (iflag .eq. 1) write(44,*) phi, real(ct1), dimag(ct1)
if (iflag .eq. 1) write(45,*) phi, real(ct2), dimag(ct2)
if (iflag .eq. 1) write(46,*) phi, real(ct3), dimag(ct3)
if (iflag .eq. 1) write(47,*) phi, real(ct4), dimag(ct4)
cint1 = cint1 + ct1 + ct2
cint2 = cint2 + ct3 + ct4
cint1 = cint1*dphi/three
cint2 = cint2*dphi/three

```

c

```

if (dreal(tmp1) .lt. zero) then
  ctmp = ci*sqrt(ci*ieps2*tmp1 + tmp2**2)
  carg = (tmp1*(ulim-phi0) - tmp2) / ctmp
  csum = log(carg + sqrt(carg**2 + (one,zero)))
  carg = (tmp1*(llim-phi0) - tmp2) / ctmp
  csum = csum - log(carg + sqrt(carg**2 + (one,zero)))
  cint1 = cint1 + ct2_0*csum/sqrt(tmp1)
  ctmp = ci*sqrt(ci*ieps4*tmp1 + tmp2**2)
  carg = (tmp1*(ulim-phi0) - tmp2) / ctmp
  csum = log(carg + sqrt(carg**2 + (one,zero)))
  carg = (tmp1*(llim-phi0) - tmp2) / ctmp
  csum = csum - log(carg + sqrt(carg**2 + (one,zero)))
  cint2 = cint2 + ct4_0*csum/sqrt(tmp1)
else
  carg= two*sqrt(tmp1*(tmp1*(ulim-phi0)**2 - two*tmp2*(ulim-phi0)
# - ci*ieps2)) + two*tmp1*(ulim-phi0) - two*tmp2
  csum = log(carg)
  carg= two*sqrt(tmp1*(tmp1*(llim-phi0)**2 - two*tmp2*(llim-phi0)
# - ci*ieps2)) + two*tmp1*(llim-phi0) - two*tmp2
  csum = csum - log(carg)
  cint1 = cint1 + ct2_0*csum/sqrt(tmp1)
  carg= two*sqrt(tmp1*(tmp1*(ulim-phi0)**2 - two*tmp2*(ulim-phi0)
# - ci*ieps4)) + two*tmp1*(ulim-phi0) - two*tmp2
  csum = log(carg)
  carg= two*sqrt(tmp1*(tmp1*(llim-phi0)**2 - two*tmp2*(llim-phi0)
# - ci*ieps4)) + two*tmp1*(llim-phi0) - two*tmp2
  csum = csum - log(carg)
  cint2 = cint2 + ct4_0*csum/sqrt(tmp1)
end if

```

c

```
return
end
```

```
c
c**File : cepst_funcs.f
c
c**Routines for self-consistently calculating "epsilon_tilde" (the
c**renormalized quasiparticle excitation energy) for a given "bare"
c**excitation energy (ceps), gap amplitude (del0), scattering rate,
c**and scattering cross-section.
c
c**Original Version : 05-94
c**Last revised : 23-09-94
c
c**Written by:
c** Mario Palumbo, Matthias Graf, and Dierk Rainer
c** Theoretische Physik III
c** Universitaet Bayreuth
c** D-95440 Bayreuth, GERMANY
c
c-----
c
c      complex*16 function get_cepst(cepst,ceps,del0,alpha,sigma,
c      #                                delta,epsilon,iflag)
c
c      implicit none
c      complex*16 cepst, ceps
c      double precision del0, alpha, sigma, delta, epsilon
c      integer iflag
c
c      **Calculates the retarded epsilon_tilde (cepst) in the "real-energy"
c      **representation as a function of epsilon (ceps) using a simple Newton
c      **iteration technique.
c
c      integer i
c      complex*16 ci, cfunc, dfunc, cepst_func
c      double precision zero, one, pi
c      parameter (zero=0.0d0, one=1.0d0)
c
c      ci = (zero,one)
c      pi = acos(-one)
c
c      **If "iflag"=0 we use the normal state value for "cepst" as an initial,
c      **guess, otherwise we use the passed value.
c      if (iflag .eq. 0) cepst = ceps + ci*pi*alpha
c      cfunc = cepst_func(cepst,ceps,del0,alpha,sigma)
c      dfunc = cepst_func(cepst+delta,ceps,del0,alpha,sigma) - cfunc
c
c      do i = 1, 50, 1
c          cepst = cepst - delta*cfunc/dfunc
c          cfunc = cepst_func(cepst,ceps,del0,alpha,sigma)
c          if (abs(cfunc) .lt. epsilon) goto 10
c          dfunc = cepst_func(cepst+delta,ceps,del0,alpha,sigma) - cfunc
c      end do
c      write(*,*) 'Warning: cepst iteration did not converge at: '
c      write(*,*) '      ceps = ', ceps
```

```

        write(*,*) '      cepst = ', cepst
        write(*,*) '      cfunc = ', cfunc
10    continue
c
        get_cepst = cepst
c
        return
        end
c
c*****
c
        complex*16 function cepst_func(cepst,ceps,del0,alpha,sigma)
c
        implicit none
        complex*16 cepst, ceps
        double precision del0, alpha, sigma
c
c**Evaluates the "epsilon_tilde equation" in the real-energy rep.
c**for a given epsilon_tilde (cepst) and a given gap (del0).
c
        complex*16 cg3, cg3bar, ctmp
        double precision one, pi
        parameter (one=1.0d0)
c
        pi = acos(-one)
c
        cg3 = cg3bar(cepst,del0,0)
c
        ctmp = one - sigma*(one + (cg3/pi)**2)
        cepst_func = ceps - (alpha*cg3/ctmp) - cepst
c
        return
        end
c
c*****
c
        complex*16 function cg3bar(cepst,del0,flag)
c
        implicit none
        complex*16 cepst
        double precision del0
        integer flag
c
c**Calculates the retarded g3_bar in the "real-energy" representation
c**by doing a numerical integration from 0 to pi/2. First we determine
c**if the integrand is singular in the interval (0,pi/2), and then we
c**employ the appropriate integration technique.
c
        integer n, Nc0, Nc
        complex*16 ctmp, ctmp2, csum, csum2, cg1, cg2, ci
        double precision err, tmp, reps, ieps, phi0, phi, dphi
        double precision zero, one, two, three, four, pi
        parameter (zero=0.0d0, one=1.0d0, two=2.0d0, three=3.0d0)
        parameter (four=4.0d0)
c
        pi = acos(-one)
        ci = (zero,one)
c

```

```

err = 1.0d-4
Nc = 40
csum = (zero,zero)
csum2 = (zero,zero)
reps = dreal(cepst**2)
ieps = dimag(cepst**2)
tmp = reps
if (tmp .gt. zero) tmp = sqrt(tmp) / del0
c
if ( (tmp .gt. one) .or. (tmp .lt. zero) ) then
c
**This is the case of no singularities. Do a simple Simpson's rule
c
**from 0 to pi/2.
dphi = pi / (two*dbble(Nc))
phi = zero
csum = one / sqrt( (del0*cos(phi))**2 - cepst**2 )
if (flag .eq. 1) write(11,*) phi, real(csum), dimag(csum)
do n = 1, Nc-1, 1
phi = phi + dphi
ctmp = one / sqrt( (del0*cos(phi))**2 - cepst**2 )
if (flag .eq. 1) write(11,*) phi, real(ctmp), dimag(ctmp)
if (mod(n,2) .eq. 1) then
csum = csum + four*ctmp
else
csum = csum + two*ctmp
end if
end do
phi = phi + dphi
ctmp = one / sqrt( (del0*cos(phi))**2 - cepst**2 )
if (flag .eq. 1) write(11,*) phi, real(ctmp), dimag(ctmp)
csum = csum + ctmp
csum = dphi*csum/three
else
c
**This is the case of one sqrt-singularity located at the angle phi0.
c
**First evaluate phi0, then break the integral into two parts for
c
**phi less than and phi greater than phi0. The contribution due to
c
**the singularity (which is integrable!) will be removed from the
c
**numerical integral by a subtraction trick, and then added in
c
**analytically at the end.
phi0 = acos(tmp)
cg1 = del0**2 - reps
cg2 = cg1 / ( two*sqrt(reps)*sqrt(del0**2-reps) )
Nc0 = 100
c
c
**Do the first half of of the integral
if (phi0 .lt. err) goto 10
Nc = 2*((int((phi0-two*err)*dbble(2*Nc0)/pi) + 1) / 2)
if (Nc .lt. 20) Nc = 20
dphi = (phi0-two*err) / dbble(Nc)
phi = -phi0 + err
csum = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
# - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(csum), dimag(csum)
do n = 1, Nc-1, 1
phi = phi + dphi
ctmp = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
# - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(ctmp), dimag(ctmp)
if (mod(n,2) .eq. 1) then

```



```

        csum = csum + four*ctmp
    else
        csum = csum + two*ctmp
    end if
end do
phi = phi + dphi
ctmp = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
#   - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(ctmp), dimag(ctmp)
csum = csum + ctmp
csum = dphi*csum/three
c
10   continue
c
c   **Do the second half of of the integral
if (pi/two-phi0 .lt. err) goto 20
Nc = 2*((int((pi/two-phi0-two*err)*dble(2*Nc0)/pi) + 1) / 2)
if (Nc .lt. 20) Nc = 20
dphi = (pi/two-phi0-two*err) / dble(Nc)
phi = zero + err
ctmp = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
#   - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(ctmp), dimag(ctmp)
csum2 = csum2 + ctmp
do n = 1, Nc-1, 1
    phi = phi + dphi
    ctmp = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
#   - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(ctmp), dimag(ctmp)
if (mod(n,2) .eq. 1) then
    csum2 = csum2 + four*ctmp
else
    csum2 = csum2 + two*ctmp
end if
end do
phi = phi + dphi
ctmp = one / sqrt( (del0*cos(phi+phi0))**2 - cepst**2 )
#   - one / sqrt( cg1*(phi**2-(one/cg2)*phi - (ci/cg1)*ieps) )
if (flag .eq. 1) write(11,*) phi+phi0, real(ctmp), dimag(ctmp)
csum2 = csum2 + ctmp
csum2 = dphi*csum2/three
c
20   continue
c
c   **Add the contribution from the singular part.
ctmp = two*sqrt( (pi/two-phi0)**2 - (one/cg2)*(pi/two-phi0)
#   - (ci/cg1)*ieps )
#   + two*(pi/two-phi0) - (one/cg2)
ctmp2 = two*sqrt( phi0**2 + (one/cg2)*phi0 - (ci/cg1)*ieps )
#   - two*phi0 - (one/cg2)
ctmp = (one/sqrt(cg1))*(log(ctmp) - log(ctmp2))
csum = csum + csum2 + ctmp
end if
c
cg3bar = -two*cepst*csum
c
return
end

```

```

C-----
      Double Precision Function PAIRBRK(ALPHA)
C-----
C***BEGIN PROLOGUE  PAIRBRK
C***DATE WRITTEN   940419   (YYMMDD)
C***REVISION DATE  940425   (YYMMDD)
C***CATEGORY NO.
C***KEYWORDS  LIBRARY=PRIVATE, PAIRBREAKING PARAMTER ALPHA AND
C             TEMPERATURE T_C(ALPHA)/T_C(0) .
C             TYPE=DOUBLE PRECISION (PAIRBRK-D)
C***AUTHOR  M. J. GRAF, UNIVERSITY OF BAYREUTH
C***PURPOSE Store critical temperature for given pairbreaking
C             parameter ALPHA.
C
C On entry:
C   ALPHA -      Pairbreaking parameter (double precision)
C On Return:
C   PAIRBRK      -      Pairbreaking temperature (double precision)
C
C             Standard Fortran Subroutine
C***REFERENCES  (NONE)
C***ROUTINES CALLED  (NONE)
C
C***END PROLOGUE  PAIRBRK
C-----
      DOUBLE PRECISION ALPHA, ALFA(148), TC(148)
      INTEGER i
      DOUBLE PRECISION step
      DATA ALFA/
C          0.000000000000000D+00,  2.000000000000000D-03,
C          4.000000000000000D-03,  6.000000000000000D-03,
C          8.000000000000000D-03,  1.000000000000000D-02,
C          1.200000000000000D-02,  1.400000000000000D-02,
C          1.600000000000000D-02,  1.800000000000000D-02,
C          2.000000000000000D-02,  2.200000000000000D-02,
C          2.400000000000000D-02,  2.600000000000000D-02,
C          2.800000000000000D-02,  3.000000000000000D-02,
C          3.200000000000000D-02,  3.400000000000000D-02,
C          3.600000000000000D-02,  3.800000000000000D-02,
C          4.000000000000000D-02,  4.200000000000000D-02,
C          4.400000000000000D-02,  4.600000000000000D-02,
C          4.800000000000000D-02,  5.000000000000000D-02,
C          5.200000000000000D-02,  5.400000000000000D-02,
C          5.600000000000000D-02,  5.800000000000000D-02,
C          6.000000000000000D-02,  6.200000000000000D-02,
C          6.400000000000000D-02,  6.600000000000000D-02,
C          6.800000000000000D-02,  7.000000000000000D-02,
C          7.200000000000000D-02,  7.400000000000000D-02,
C          7.600000000000000D-02,  7.800000000000001D-02,
C          8.000000000000001D-02,  8.200000000000001D-02,
C          8.400000000000001D-02,  8.600000000000001D-02,
C          8.800000000000001D-02,  9.000000000000001D-02,
C          9.200000000000001D-02,  9.400000000000001D-02,
C          9.600000000000001D-02,  9.800000000000001D-02,
C          1.000000000000000D-01,  1.020000000000000D-01,
C          1.040000000000000D-01,  1.060000000000000D-01,
C          1.080000000000000D-01,  1.100000000000000D-01,

```

C	1.120000000000000D-01,	1.140000000000000D-01,
C	1.160000000000000D-01,	1.180000000000000D-01,
C	1.200000000000000D-01,	1.220000000000000D-01,
C	1.240000000000000D-01,	1.260000000000000D-01,
C	1.280000000000000D-01,	1.300000000000000D-01,
C	1.320000000000000D-01,	1.340000000000000D-01,
C	1.360000000000000D-01,	1.380000000000000D-01,
C	1.400000000000000D-01,	1.420000000000000D-01,
C	1.440000000000000D-01,	1.460000000000000D-01,
C	1.480000000000000D-01,	1.500000000000000D-01,
C	1.520000000000000D-01,	1.540000000000000D-01,
C	1.560000000000000D-01,	1.580000000000000D-01,
C	1.600000000000000D-01,	1.620000000000000D-01,
C	1.640000000000000D-01,	1.660000000000000D-01,
C	1.680000000000000D-01,	1.700000000000000D-01,
C	1.720000000000000D-01,	1.740000000000000D-01,
C	1.760000000000000D-01,	1.780000000000000D-01,
C	1.800000000000000D-01,	1.820000000000000D-01,
C	1.840000000000000D-01,	1.860000000000000D-01,
C	1.880000000000000D-01,	1.900000000000000D-01,
C	1.920000000000000D-01,	1.940000000000000D-01,
C	1.960000000000000D-01,	1.980000000000000D-01,
C	2.000000000000000D-01,	2.020000000000000D-01,
C	2.040000000000000D-01,	2.060000000000000D-01,
C	2.080000000000000D-01,	2.100000000000000D-01,
C	2.120000000000000D-01,	2.140000000000000D-01,
C	2.160000000000000D-01,	2.180000000000000D-01,
C	2.200000000000000D-01,	2.220000000000000D-01,
C	2.240000000000000D-01,	2.260000000000000D-01,
C	2.280000000000000D-01,	2.300000000000000D-01,
C	2.320000000000000D-01,	2.340000000000000D-01,
C	2.360000000000000D-01,	2.380000000000000D-01,
C	2.400000000000000D-01,	2.420000000000000D-01,
C	2.440000000000000D-01,	2.460000000000000D-01,
C	2.480000000000000D-01,	2.500000000000000D-01,
C	2.520000000000000D-01,	2.540000000000000D-01,
C	2.560000000000000D-01,	2.580000000000000D-01,
C	2.600000000000000D-01,	2.620000000000000D-01,
C	2.640000000000000D-01,	2.660000000000000D-01,
C	2.680000000000000D-01,	2.700000000000000D-01,
C	2.710000000000000D-01,	2.720000000000000D-01,
C	2.730000000000000D-01,	2.740000000000000D-01,
C	2.750000000000000D-01,	2.760000000000000D-01,
C	2.770000000000000D-01,	2.780000000000000D-01,
C	2.790000000000000D-01,	2.800000000000000D-01,
C	2.810000000000000D-01,	2.820000000000000D-01/

C

DATA	TC/	
C	1.000000000000000D+00,	9.94979985780569D-01,
C	9.90168211444149D-01,	9.85254826826387D-01,
C	9.80269824854986D-01,	9.75273290321524D-01,
C	9.70285176811678D-01,	9.65307020706046D-01,
C	9.60266689230268D-01,	9.55335334055061D-01,
C	9.50230656758989D-01,	9.45258666385887D-01,
C	9.40124878419510D-01,	9.35206234857973D-01,
C	9.30013743037869D-01,	9.24997229038698D-01,
C	9.19956199101609D-01,	9.14952268836332D-01,
C	9.09902595219130D-01,	9.04822495918116D-01,

C	8.99734266155204D-01,	8.94548354115810D-01,
C	8.89359501182762D-01,	8.84253369012316D-01,
C	8.79192325250694D-01,	8.74031693990246D-01,
C	8.68798856714218D-01,	8.63643441647420D-01,
C	8.58502452054537D-01,	8.53418908248721D-01,
C	8.48221321046611D-01,	8.42902405896712D-01,
C	8.37743834052559D-01,	8.32516860116987D-01,
C	8.27316377681085D-01,	8.21985741058676D-01,
C	8.16685376854979D-01,	8.11440692831239D-01,
C	8.06049828197337D-01,	8.00882381307412D-01,
C	7.95494556184380D-01,	7.90252180968870D-01,
C	7.84876573270205D-01,	7.79566288487801D-01,
C	7.74124290358790D-01,	7.68789008065455D-01,
C	7.63518570327797D-01,	7.58040750804586D-01,
C	7.52520135287419D-01,	7.47198991064242D-01,
C	7.41769455240884D-01,	7.36319086411256D-01,
C	7.30789145165074D-01,	7.2525453222533D-01,
C	7.19683568017091D-01,	7.14149685664602D-01,
C	7.08725228042168D-01,	7.03101828375263D-01,
C	6.97646455067538D-01,	6.91970931564599D-01,
C	6.86353417631351D-01,	6.80695172913838D-01,
C	6.75146034868489D-01,	6.69474029046236D-01,
C	6.63780153177413D-01,	6.58026030349122D-01,
C	6.52410657498903D-01,	6.46700337482505D-01,
C	6.40972677168680D-01,	6.35117953426164D-01,
C	6.29328930008711D-01,	6.23513875789632D-01,
C	6.17648313904561D-01,	6.11853896974146D-01,
C	6.05892188829178D-01,	6.00006359723133D-01,
C	5.94119111875201D-01,	5.88173537369706D-01,
C	5.82238615607424D-01,	5.76170013114152D-01,
C	5.70101015785300D-01,	5.64058797884797D-01,
C	5.58041546988724D-01,	5.51850865743404D-01,
C	5.45718626185905D-01,	5.39609150227492D-01,
C	5.33387951947750D-01,	5.27137801596926D-01,
C	5.20896896141043D-01,	5.14627762489749D-01,
C	5.08215757178552D-01,	5.01920351581060D-01,
C	4.95475666214391D-01,	4.89049034380746D-01,
C	4.82571580981771D-01,	4.76048611955350D-01,
C	4.69465271664764D-01,	4.62856162669029D-01,
C	4.56304114272036D-01,	4.49547022131376D-01,
C	4.42837420316735D-01,	4.36024140574640D-01,
C	4.29232665942347D-01,	4.22346204791249D-01,
C	4.15389083781882D-01,	4.08404788612145D-01,
C	4.01240326312244D-01,	3.94167742688480D-01,
C	3.86956483499255D-01,	3.79751416274201D-01,
C	3.72355145242825D-01,	3.64901791259141D-01,
C	3.57501548000570D-01,	3.49891880923231D-01,
C	3.42210542152577D-01,	3.34472586529999D-01,
C	3.26578870601291D-01,	3.18630173373065D-01,
C	3.10555789957023D-01,	3.02336141795134D-01,
C	2.94008192119330D-01,	2.85553607926441D-01,
C	2.77000508140849D-01,	2.68181677524817D-01,
C	2.59196124354300D-01,	2.49971067669985D-01,
C	2.40591452087387D-01,	2.31042331853926D-01,
C	2.21189970855487D-01,	2.10965309404162D-01,
C	2.00335369242877D-01,	1.89455118266312D-01,
C	1.78107339472908D-01,	1.66150851355199D-01,
C	1.53636815771606D-01,	1.40062226622720D-01,

```

C      1.33072394977902D-01,  1.25606591318740D-01,
C      1.17713159145716D-01,  1.09491290615641D-01,
C      1.00616735253519D-01,  9.10322435577660D-02,
C      8.08045506548403D-02,  6.87554249261647D-02,
C      5.46492128132853D-02,  3.59672322604878D-02,
C      3.87897322801049D-03,  0.00000000000000D+00/
C
C      SAVE ALFA, TC
C
C      If( ALPHA.LT.0d0 )Then
C          PAIRBRK=0d0
C          Return
C      EndIf
C-----
C          Locate TALPHA
C-----
C      If( ALPHA.LT.0.282d0)Then
C          If( ALPHA.LE.0.27d0 )Then
C              step=2d-03
C              i=1+int(ALPHA/step)
C          Else
C              step=1d-03
C              i=int(ALPHA/step)-134
C          EndIf
C          If( dabs(ALPHA-ALFA(i)).LE. 1d-04 )Then
C              PAIRBRK=TC(i)
C          Else
C              PAIRBRK=TC(i)+( (TC(i+1)-TC(i))/(ALFA(i+1)-ALFA(i))*
+              (ALPHA-ALFA(i)) )
C          EndIf
C          Else
C              PAIRBRK=0d0
C          EndIf
C
C      Write(*,*)'PAIRBRK=',PAIRBRK
C
C      Return
C      End

c
c**File : gap_funcs.f
c
c**Routines for self-consistently calculating the gap amplitude for a
c**given temperature, scattering rate, and scattering cross-section.
c
c**Original Version : 05-94
c**Last revised : 23-09-94
c
c**Written by:
c** Mario Palumbo, Matthias Graf, and Dierk Rainer
c** Theoretische Physik III
c** Universitaet Bayreuth
c** D-95440 Bayreuth, GERMANY
c
C-----
C
C      double precision function get_del0(del0,T,alpha,sigma,wc,delta,
#      epsilon,iflag)

```

```

c
    implicit none
    double precision del0, T, alpha, sigma, wc, delta, epsilon
    integer iflag
c
c  **Calculates self-consistently the gap amplitude (ie. the maximal
c  **value of the gap over the Fermi surface) using a simple Newton
c  **iteration method.
c
    integer i, N_cut
    double precision gfunc, gfunc1, gap_func
    double precision one, two, pi
    parameter(one=1.0d0, two=2.0d0)
c
    pi = acos(-one)
c
c  **Calculate the maximum N (N_cut) in the Matsubara sum from the
c  **cutoff energy "wc".
    N_cut = int((wc/(pi*T) - one) / two)
c
c  **Solve for del0 by means of Newton iteration.  If "iflag"=0 we set
c  **a default gap value for our starting guess, otherwise we use the
c  **passed value of "del0".
    if (iflag .eq. 0) del0 = two
    gfunc = gap_func(del0,T,alpha,sigma,delta,epsilon,N_cut)
    gfunc1 = gap_func(del0+delta,T,alpha,sigma,delta,epsilon,N_cut)
c
    do i = 1, 50, 1
        del0 = del0 - delta*gfunc/(gfunc1-gfunc)
        gfunc = gap_func(del0,T,alpha,sigma,delta,epsilon,N_cut)
        if (abs(gfunc) .lt. epsilon) goto 10
        gfunc1 = gap_func(del0+delta,T,alpha,sigma,delta,epsilon,N_cut)
    end do
    write(*,*) 'Warning: del0 iters did not converged at T = ', T
    write(*,*) '          del0, gfunc = ', del0, gfunc
10  continue
c
    get_del0 = del0
c
    return
end
c
c*****
c
    double precision function gap_func(del0,T,alpha,sigma,delta,
#                                     epsilon,N_cut)
c
    implicit none
    double precision del0, T, alpha, sigma, delta, epsilon
    integer N_cut
c
c  **Evaluates the gap-equation for a given "del0" and "T".  After
c  **the Matsubara sum is truncated (at N_cut), an asymptotic correction
c  **for the "high-epsilon" contribution is added.  The gap equation is
c  **written so that "gap_func=0" at the solution.
c
    integer i, j
    double precision epsn, epst, get_epst

```

```

double precision sum, g2, arg, K, E, delk, dele
double precision sterm1, sterm2, eps1, eps2, a, b
double precision zero, one, two, four, pi
parameter (zero=0.0d0, one=1.0d0, two=2.0d0, four=4.0d0)
c
c   pi = acos(-one)
c
c **Do the Matsubara sum. The "K" and "E" are elliptic integrals needed
c **in the calculation of "g2" (the Fermi surface average of the "tau_2"
c **component of the quasiclassical propagator "g").
c   sum = zero
c   epsn = dble(2*N_cut-1)*pi*T
c   epst = epsn + pi*alpha
c   do i = N_cut, 1, -1
c     epst = get_epst(epst,epsn,del0,alpha,sigma,delta,epsilon,1)
c     arg = one / sqrt(one + (epst/del0)**2)
c     K = delk(arg)
c     E = dele(arg)
c     g2 = two*((one/arg)*(E-K) + arg*K)
c     sum = sum + g2 - (pi*del0)/(two*epsn)
c     epsn = dble(2*i-3)*pi*T
c   end do
c
c **Add the asymptotic correction.
c   epsn = dble(2*N_cut-1)*pi*T
c   eps2 = get_epst(eps2,epsn,del0,alpha,sigma,delta,epsilon,0)
c   arg = one / sqrt(one + (eps2/del0)**2)
c   K = delk(arg)
c   E = dele(arg)
c   g2 = two*((one/arg)*(E-K) + arg*K)
c   sterm2 = g2 - (pi*del0)/(two*epsn)
c
c   epsn = dble(2*N_cut-7)*pi*T
c   eps1 = get_epst(eps1,epsn,del0,alpha,sigma,delta,epsilon,0)
c   arg = one / sqrt(one + (eps1/del0)**2)
c   K = delk(arg)
c   E = dele(arg)
c   g2 = two*((one/arg)*(E-K) + arg*K)
c   sterm1 = g2 - (pi*del0)/(two*epsn)
c
c   a = ((eps2**3)*sterm2 - (eps1**3)*sterm1) / (eps2 - eps1)
c   b = ((eps2**3)*eps1*sterm2 - (eps1**3)*eps2*sterm1)
c   # / (eps1 - eps2)
c   sum = sum + a / (two*pi*T*(eps2 + pi*T))
c   # + b / (four*pi*T*(eps2 + pi*T)**2)
c
c   gap_func = log(T)*del0 - four*T*sum
c
c   return
c   end
c
c *****
c
c   double precision function get_epst(epst,epsn,del0,alpha,sigma,
c   #                               delta,epsilon,iflag)
c
c   implicit none
c   double precision epst, epsn, del0, alpha, sigma, delta, epsilon

```

```

integer iflag
c
c **Calculates epsilon_tilde as a function of epsilon_sub_n (the
c **Masubara frequency), for a given value of the gap "del0",
c **using a simple Newton iteration technique.
c
integer i
double precision Fepst, dFepst, epst_func
double precision one, pi
parameter (one=1.0d0)
c
pi = acos(-one)
c
c **If "iflag"=0 we start with the normal state value for "epst",
c **otherwise we use the value passed in.
if (iflag .eq. 0) epst = epsn + pi*alpha
Fepst = epst_func(epst,epsn,del0,alpha,sigma)
dFepst = epst_func(epst+delta,epsn,del0,alpha,sigma) - Fepst
c
do i = 1, 50, 1
epst = epst - delta*Fepst/dFepst
Fepst = epst_func(epst,epsn,del0,alpha,sigma)
if (abs(Fepst) .lt. epsilon) goto 10
dFepst = epst_func(epst+delta,epsn,del0,alpha,sigma) - Fepst
end do
write(*,*) 'Warning: epst iters did not converge at epsn = ', epsn
write(*,*) '          epst, Fepst = ', epst, Fepst
10 continue
c
get_epst = epst
c
return
end
c
c*****
c
double precision function epst_func(epst,epsn,del0,alpha,sigma)
c
implicit none
double precision epst, epsn, del0, alpha, sigma
c
c **Evaluates the "epsilon_tilde equation" for a given "epsn" and "del0".
c **The equation is written such that "epst_func=0" at the solution.
c
double precision tmp1, tmp2, denom, g3bar, K, delk
double precision one, two, pi
parameter (one=1.0d0, two=2.0d0)
c
pi = acos(-one)
c
tmp1 = epst / del0
tmp2 = one / sqrt(one + tmp1**2)
K = delk(tmp2)
g3bar = two*tmp1*tmp2*K
c
denom = one - sigma*(one - (g3bar/pi)**2)
epst_func = epsn + (alpha*g3bar/denom) - epst
c

```



```
return
end
```

```
C -----
C      DOUBLE PRECISION FUNCTION DELE (XX)
C -----
C***BEGIN PROLOGUE
C***PURPOSE Evaluate the complete elliptic integral of the second
C      kind E(x).
C
C Usage:  DELE(X)
C
C***REMARK We use the Russian notation (see Gradshteyn/Ryzhik) !!!!
C
C***DESCRIPTION
C Arguments:
C   XX      - Argument for which the function value is desired.
C             (Input)
C             XX must be greater than or equal to 0 and less than or
C             equal to 1.
C   DELE    - Function value.  (Output)
C
C***ROUTINES CALLED  NONE
C***END PROLOGUE
C -----
C                                     SPECIFICATIONS FOR ARGUMENTS
C      DOUBLE PRECISION XX
C                                     SPECIFICATIONS FOR LOCAL VARIABLES
C      INTEGER          I
C      DOUBLE PRECISION X, CAYSQ, EPS, ETA, SUMA, SUMB
C                                     SPECIFICATIONS FOR SAVE VARIABLES
C      DOUBLE PRECISION A(10), B(10)
C      SAVE             A, B
C                                     SPECIFICATIONS FOR INTRINSICS
C      INTRINSIC  DLOG
C      DOUBLE PRECISION DLOG
C
C      DATA A(1)/0.1494662175718132D-03/
C      DATA A(2)/0.2468503330460722D-02/
C      DATA A(3)/0.8638442173604073D-02/
C      DATA A(4)/0.1077063503986645D-01/
C      DATA A(5)/0.7820404060959553D-02/
C      DATA A(6)/0.7595093422559432D-02/
C      DATA A(7)/0.115695957452954D-01/
C      DATA A(8)/0.2183181167613048D-01/
C      DATA A(9)/0.5680519456755915D-01/
C      DATA A(10)/0.4431471805608895D00/
C      DATA B(1)/0.3185919565550157D-04/
C      DATA B(2)/0.9898332846225384D-03/
C      DATA B(3)/0.6432146586438302D-02/
C      DATA B(4)/0.1680402334636338D-01/
C      DATA B(5)/0.2614501470031388D-01/
C      DATA B(6)/0.3347894366576162D-01/
C      DATA B(7)/0.4271789054738309D-01/
C      DATA B(8)/0.5859366125553149D-01/
C      DATA B(9)/0.9374999972120313D-01/
C      DATA B(10)/0.2499999999999017D00/
C -----
```

```

C
  X = XX*XX
  DELE = 1d+100
C
  IF (X.LT.0.0D0 .OR. X.GT.1.0D0)THEN
  Write(*,'(A18,D15.8,A18,A)')
+   'The argument, X = ',X,', must be greater ',
+   'than or equal to 0.0 and less than or equal to 1.0.'
  Return
  END IF
C
  EPS = 1d-14
  CAYSQ = X
C
  ETA = 1.0D0 - CAYSQ
C
  IF (ETA .GE. EPS) THEN
    SUMA = 0.0D0
    SUMB = 0.0D0
    DO 10 I=1, 10
      SUMA = (SUMA+A(I))*ETA
      SUMB = (SUMB+B(I))*ETA
10  CONTINUE
    DELE = SUMA - DLOG(ETA)*SUMB
    DELE = DELE + 1.0D0 + EPS
  ELSE
    DELE = 1.0D0
  END IF
C
  RETURN
  END

C -----
  DOUBLE PRECISION FUNCTION DELK (XX)
C -----
C***BEGIN PROLOGUE
C***PURPOSE Evaluate the complete elliptic integral of the second
C           kind K(x).
C
C Usage:   DELK(X)
C
C***REMARK We use the Russian notation (see Gradshteyn/Ryzhik) !!!!
C
C***DESCRIPTION
C Arguments:
C   XX      - Argument for which the function value is desired.
C            (Input)
C           XX must be greater than or equal to 0 and less than or
C            equal to 1.
C   DELK    - Function value. (Output)
C
C***ROUTINES CALLED  NONE
C***END PROLOGUE
C -----
C                                     SPECIFICATIONS FOR ARGUMENTS
C   DOUBLE PRECISION XX
C                                     SPECIFICATIONS FOR LOCAL VARIABLES
C   INTEGER      I

```

```
C      DOUBLE PRECISION X, CAYSQ, EPS, ETA, SUMA, SUMB
      SPECIFICATIONS FOR SAVE VARIABLES
DOUBLE PRECISION A(11), B(11)
SAVE      A, B
```

```
C      SPECIFICATIONS FOR INTRINSICS
C      INTRINSIC DLOG
C      DOUBLE PRECISION DLOG
C
```

```
DATA A(1)/0.1393087857006646D-03/
DATA A(2)/0.2296634898396958D-02/
DATA A(3)/0.8003003980649985D-02/
DATA A(4)/0.9848929322176892D-02/
DATA A(5)/0.6847909282624505D-02/
DATA A(6)/0.6179627446053317D-02/
DATA A(7)/0.8789801874555064D-02/
DATA A(8)/0.1493801353268716D-01/
DATA A(9)/0.3088514627130518D-01/
DATA A(10)/0.9657359028085625D-01/
DATA A(11)/0.138629436111989D01/
DATA B(1)/0.2970028096655561D-04/
DATA B(2)/0.9215546349632497D-03/
DATA B(3)/0.5973904299155429D-02/
DATA B(4)/0.155309416319772D-01/
DATA B(5)/0.2393191332311079D-01/
DATA B(6)/0.3012484901289892D-01/
DATA B(7)/0.373777397586236D-01/
DATA B(8)/0.4882804190686239D-01/
DATA B(9)/0.7031249973903835D-01/
DATA B(10)/0.124999999999908D00/
DATA B(11)/0.5D00/
```

```
C -----
```

```
X = XX*XX
```

```
C
DELK = 1d+100
```

```
C      IF (X.LT.0.0D0 .OR. X.GT.1.0D0)THEN
      Write(*,'(A18,D15.8,A18,A )')
+ 'The argument, X = ', X, ', must be greater ',
+ 'than or equal to 0.0 and less than or equal to 1.0.'
      Return
END IF
```

```
C      EPS = 1d-14
C      CAYSQ = X
```

```
C      ETA = 1.0D0 - CAYSQ
```

```
C      IF (ETA .GE. EPS) THEN
      SUMA = A(1)
      SUMB = B(1)
      DO 10 I=2, 11
      SUMA = SUMA*ETA + A(I)
      SUMB = SUMB*ETA + B(I)
10    CONTINUE
      DELK = SUMA - DLOG(ETA)*SUMB
ELSE
```

```
C      RETURN FOR SMALL ARGUMENT
      DELK = A(11) - DLOG(ETA)*B(11)
```

```
C      END IF
      RETURN
      END
```