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Optical conductivity of BCS superconductors with arbitrary purity

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An explicit expression for the complex optical and AC conductivity of a homogeneous BCS superconductor with arbitrary electron mean free path is given. This compact expression and a fast self-contained FORTAN program may be used to fit experimental data. For comparison, we give also the complex AC conductivity of high-T_c superconductors containing an elastically pinned, viscously moving flux-line lattice with flux creep.

1. Introduction

Even five years after their discovery [1,2], high-T_c superconductors (HTSCs) remain a fascinating object of experimental and theoretical research. One example are measurements of the infrared reflectivity $R=|\sqrt{\epsilon}-1|^2/|\sqrt{\epsilon}+1|^2$ from a planar surface, or of the transmission of HTSC films, which in principle allow the determination of the phonon structure and electronic excitations in these oxides. For an excellent review see Timusk and Tanner [3]. Usually the complex dielectric function $\epsilon(\omega)$ (ω=circular frequency of the light) is assumed to be a linear superposition (for a nonlinear superposition see, e.g. [4])

$$\epsilon(\omega)=\sum_{j=1}^{N}\frac{S_i\omega_i^2}{\omega_j^2-\omega^2-\mathrm{i}\omega\gamma_j}+\frac{\omega_{\mathrm{pl\,ib}}^2}{\omega_\mathrm{I}^2-\omega^2-\mathrm{i}\omega\gamma_{\mathrm{ib}}}+\epsilon_\infty+\frac{4\pi\mathrm{i}}{\omega}\sigma(\omega)$$

of N phonon lines with oscillator strengths S_j, a broad mid-infrared band with three fit parameters $\omega_{\mathrm{pl\,ib}}$, ω_I and γ_{ib} (electronic absorption caused by interband transitions), a high frequency part with a constant $\epsilon_\infty\approx 4$ (from core electrons), and the contribution of conduction electrons which we express in terms of a complex conductivity $\sigma(\omega)$.

For normal conductors this last term is well described by a Drude function, $\alpha_n(\omega)=\sigma_0/(1-\mathrm{i}\omega\tau)$, where $\sigma_0=\omega_\mathrm{p}^2\tau/4\pi=ne^2\tau/m^*$ is the DC conductivity of electrons with density n, charge e, mass m^*, plasma frequency $\omega_\mathrm{p}=(4\pi ne^2/m^*)^{1/2}$, and collision time τ. For superconductors, $\sigma_{\mathrm{sc}}(\omega)$ has been obtained from the BSC theory in the *impure limit* ($\tau\ll\hbar/2\Delta$) by Mattis and Bardeen [5]. Numerous reflection measurements on ceramics [6–8], monocrystals [9,10], and films [11,12] of HTSCs were fitted to this theory, usually by linearly superimposing the contributions to $\sigma_{\mathrm{sc}}(\omega)$ of various types of electrons with different gaps. However, since the coherence length ξ of HTSCs is smaller than the electron mean free path $l=v_\mathrm{F}\tau$, these superconductors possibly are closer to the pure limit ($\tau\gg\hbar/2\Delta$).

2. Complex conductivity of a BCS superconductor

In this section we present the complex conductivity $\sigma_{\mathrm{sc}}(\omega)$ of homogeneous isotropic BCS (=weak coupling) superconductors with arbitrary purity as calculated from microscopic expressions derived first by Zimmermann [13] using the quasi-classical for-

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malism of energy-integrated Green functions which was developed in this context by Rainer [14,15]. Similar expressions were derived from the usual BCS-formalism by Nam [16], Scharnberg [17], Bickers et al. [18], and Akis et al. [19]. Special cases were treated in the classical work [20] (clean limit) and in [21–23]. The optical conductivity was also calculated for strong coupling [15,19] and layered [24] superconductors or those with nodes in the energy gap [25,26], and from marginal Fermi liquid theory and bosonic mechanisms [27].

Our expression applies to isotropic BCS-superconductors with a spherical Fermi surface. Its extension to superconductors with anisotropic gap or to the presence of several gaps may be achieved by linear superposition. For HTSCs (and for all type-II superconductors) the "local" limit $q \to 0$ ($q=$ wave vector of the light) is appropriate, since the BCS coherence length ξ is much smaller than the magnetic penetration depth λ and the wavelength $2\pi/q$ of the light. The explicit expressions for $\sigma_{sc}(\omega)$ reads (with $\hbar=1$):

$$\sigma_{sc}(\omega)=\frac{\sigma_0 \mathrm{i}}{2\omega\tau}\times\left(J+\int_{\Delta}^{\infty} I_2\,\mathrm{d}E\right),$$

$$J(\omega\leq 2\Delta)=\int_{\Delta}^{\omega+\Delta} I_1\,\mathrm{d}E,$$

$$J(\omega\geq 2\Delta)=\int_{\Delta}^{\omega-\Delta} I_3\,\mathrm{d}E+\int_{\omega-\Delta}^{\omega+\Delta} I_1\,\mathrm{d}E,$$

$$I_1=\tanh\frac{E}{2kT}\left\{\left[1-\frac{\Delta^2+E(E-\omega)}{P_4P_2}\right]\frac{1}{P_4+P_2+\mathrm{i}/\tau}-\left[1+\frac{\Delta^2+E(E-\omega)}{P_4P_2}\right]\frac{1}{P_4-P_2+\mathrm{i}/\tau}\right\}$$

$$I_2=\tanh\frac{E+\omega}{2kT}\left\{\left[1+\frac{\Delta^2+E(E+\omega)}{P_1P_2}\right]\frac{1}{P_1-P_2+\mathrm{i}/\tau}-\left[1-\frac{\Delta^2+E(E+\omega)}{P_1P_2}\right]\frac{1}{-P_1-P_2+\mathrm{i}/\tau}\right\},$$

$$+\tanh\frac{E}{2kT}\left\{\left[1-\frac{\Delta^2+E(E+\omega)}{P_1P_2}\right]\frac{1}{P_1+P_2+\mathrm{i}/\tau}-\left[1+\frac{\Delta^2+E(E+\omega)}{P_1P_2}\right]\frac{1}{P_1-P_2+\mathrm{i}/\tau}\right\},$$

$$I_3=\tanh\frac{E}{2kT}\left\{\left[1-\frac{\Delta^2+E(E-\omega)}{P_3P_2}\right]\frac{1}{P_3+P_2+\mathrm{i}/\tau}-\left[1+\frac{\Delta^2+E(E-\omega)}{P_3P_2}\right]\frac{1}{P_3-P_2+\mathrm{i}/\tau}\right\},$$

$$P_1=\sqrt{(E+\omega)^2-\Delta^2},\quad P_2=\sqrt{E^2-\Delta^2},$$

$$P_3=\sqrt{(E-\omega)^2-\Delta^2},\quad P_4=\mathrm{i}\sqrt{\Delta^2-(E-\omega)^2}.$$

The real and imaginary parts of σ_{sc} are presented in figs. 1 and 2 in reduced units, $\sigma_{sc}=\sigma_0\times s(x, y, t_t)$

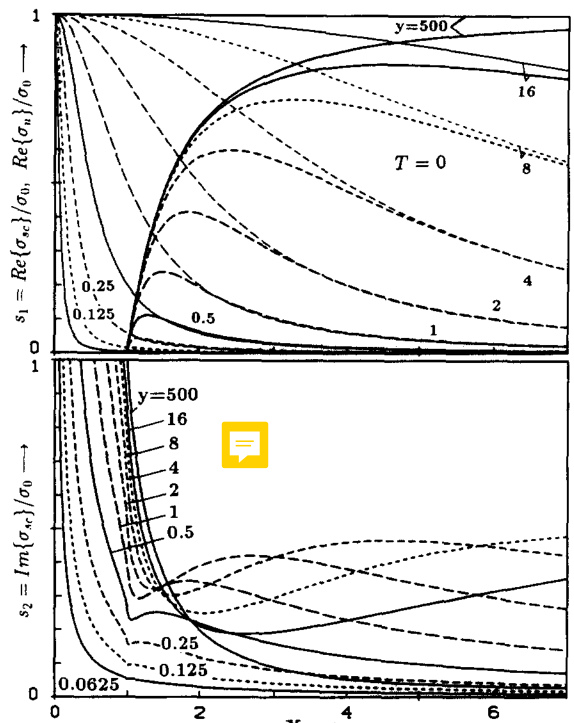

Fig. 1. Frequency dependent complex conductivity $\sigma_{sc}(\omega)$ of a BCS superconductor at temperature $T=0$ in reduced units $s=\sigma_{sc}(\omega)/\sigma_0$, $x=\hbar\omega/2\Delta$, and $y=\hbar/2\tau\Delta$ (impurity parameter) for $y=500$ ($\approx$impure limit), 16, 8, 4, 2, 1, 0.5, 0.25, 0.125 and 0.0625 ($\approx$pure limit). Top: real part $s_1=\mathrm{Re}\{\sigma_{sc}\}/\sigma_0$; also shown is the normal conductivity $\mathrm{Re}\{\sigma_n\}/\sigma_0=y^2/(x^2+y^2)$ (thin dashed Lorentzians). Note that $s_1=0$ for $\omega\leq 2\Delta/\hbar$. Bottom: imaginary part $s_2=\mathrm{Im}\{\sigma_{sc}\}/\sigma_0$.

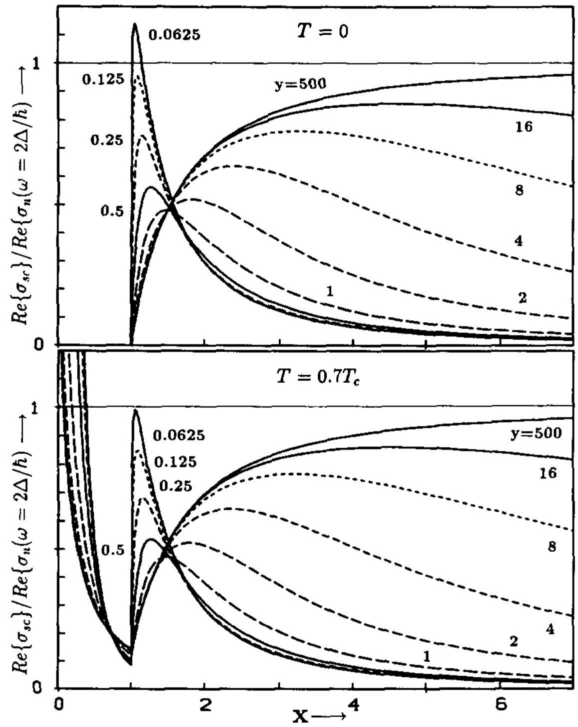

Fig. 2. Complex conductivity, real part, plotted with impurity-dependent magnification as $\mathrm{Re}\{\sigma_{sc}\}/\mathrm{Re}\{\sigma_n(\omega=2\Delta/\hbar)\}=(1+y^{-2})s_1(x)$, $x=\hbar\omega/2\Delta$, for impurity parameters $y=\hbar/2\tau\Delta=500$, 16, 8, 4, 2, 1, 0.5, 0.25, 0.125, 0.0625 as in fig. 1. Note the sharp cusp at $x=1$ in the pure case. Top: temperature $T=0$. Bottom: $T=0.7\,T_c$.

where $s=s_1+is_2$, $x=\omega\hbar/2\Delta$, and $y=\hbar/2\Delta\tau$. In the calculation it is convenient to introduce two reduced temperatures, $t_r=T/T_c$ and $t=kT/2\Delta$. We have used the approximate formula for the BCS gap $\Delta(T)$ of ref. [28].

In order to facilitate fitting of experimental data we give here a very fast, compact, and self-contained FORTRAN program (fig. 4) which computes the complex conductivity from our formula by a rapid integration procedure using the reduced units given above and in figs. 1 and 2. The above expression was presented in ref. [29] and used for the first time in ref. [30].

The formula for the complex conductivity given above yields also the exact AC conductivity of BCS superconductors at lower (non-optical) frequencies, where also other theoretical approaches or approximations have been used, e.g. a two-fluid model. For a recent overview on microwave absorption of HTSC see ref. [31], and for a recent ab-initio calculation within a low-frequency approximation see [32,33].

3. AC conductivity of HTSC in a magnetic field

Optical and microwave conductivities (or reflectivity, transmission, absorption, attenuation, surface impedance) are interesting material properties of superconductors also in the absence of an applied magnetic field B_a. At lower than optical frequencies, however, the complex conductivity of type-II superconductors is particularly interesting when a constant magnetic field generates Abrikosov vortices. Such experiments use, e.g. RF coils [34,35] or vibrating superconductors [36] in form of reeds from HTSC performing flexural vibrations at 300 to 3000 Hz [37], or HTSC platelets glued on a vibrating silicon tongue [38] or suspended on wires and oscillating at very low frequency <1 Hz [39]. Generally speaking, a superconductor performing tilt vibrations in a constant magnetic field B_a behaves as if an AC magnetic field were applied to it perpendicular to B_a.

In all these experiments the electromagnetic response of the type-II superconductor is determined by the behavior of the Abrikosov flux lines, in particular by their viscous motion with respect to the atomic lattice and by their pinning by inhomogeneities in the material. Flux lines have no inertial mass for frequencies $\omega \ll \Delta/\hbar$. If the flux lines were ideally pinned, a weak AC field with $\omega \ll \Delta/\hbar$ would penetrate to the usual magnetic penetration depth λ, i.e. the London depth at $T \ll T_c$ and Ginzburg–Landau penetration depth $\lambda(T) \propto (T_c - T)^{-1/2}$ at $T \approx T_c$. In the opposite limit, if the flux lines are not pinned at all, the superconductor with a constant magnetic field plus a small AC field applied, behaves almost as a normal conductor. The resistivity is now a "flux-flow resistivity" ρ_{FF}, due to the motion of flux lines driven by the Lorentz force.

The main two differences to normal conducting metals are (a) that this flux-flow resistivity ρ_{FF} is reduced from its normal value $\rho_n = 1/\sigma_0$ roughly by a factor $B/B_{c2}(T)$, where $B \approx B_a$ is the magnetic induction (flux density) and B_{c2} the upper critical field above which the bulk superconductor turns normal, and (b) that this resistivity is anisotropic (even in isotropic materials) because the flux lines (or B) define a direction along which the resistivity vanishes. A phenomenological theory of this flux flow, and of a modified flux flow caused a HTSC by thermally activated depinning, is given in [40]. For recent theories of the complex AC penetration depth into type-II superconductors and of the related AC resistivity and surface impedance, with complete consideration of elastic pinning, flux flow, and thermally activated depinning (creep) see [41,42].

For comparison with the above microscopic BCS conductivity $\sigma_{sc}(\omega)$ we give here the result of the phenomenological theory [42] for the complex AC resistivity caused by supercurrents and moving flux lines [we give this in the above notation where all fields are $\propto \exp(-i\omega t)$],

$$\rho_{AC}(\omega)=1/\sigma_{AC}=-\frac{4\pi\lambda^2}{c^2}i\omega+\rho_{TAFF}\frac{1-i\omega\tau}{1-i\omega\tau_0}$$

(fig. 3). Here $\rho_{TAFF}=\rho_{AC}(0)=(\tau_0/\tau)\rho_{FF}\ll\rho_{FF}\approx\rho_n B/B_{c2}(T)$ is the "thermally assisted flux-flow resistivity", $\tau=\rho_0\exp(U/kT)\gg\tau_0$ is the "creep time" with an activation energy U for flux jumps (thermally activated depinning), and $\tau_0=\eta/\alpha_L$ is the relaxation time of the flux-line lattice with $\eta=B^2/\rho_{FF}$ the flux-flow viscosity per unit volume and α_L (Labusch parameter) the restoring force per unit volume of an elastically pinned flux-line lattice.

One interesting difference to the complex optical conductivity ρ_{sc} is that here the conductivity σ_{sc}, and in the flux-line case the *resistivity* ρ_{AC}, yield the simpler expression, a sum in both cases. Physically, this is due to the additive contributions of all electrons to σ_{sc}, and of the losses caused by the viscous motion of flux lines to ρ_{AC}. However, if the pinning forces or viscous forces ($\propto\omega$) are sufficiently weak, the AC field penetrates much deeper than the magnetic penetration depth λ, namely to the Campbell depth $\lambda_C=(B^2/4\pi\alpha_L)^{1/2}$ [43] or to the skin depths $\delta=(2\rho_{FF}c^2/4\pi\omega)^{1/2}$, whatever is smaller; in both these cases the first term in $\rho_{AC}(\omega)$ (caused by the Meissner shielding currents) may be disregarded and one simply gets $\sigma_{AC}=\sigma_{TAFF}(1-i\omega\tau_0)/(1-i\omega\tau)$. At low frequencies this result formally coincides with a Drude conductivity, but with τ being a creep time (which is typically very large) rather than a collision time (which is typically very short).

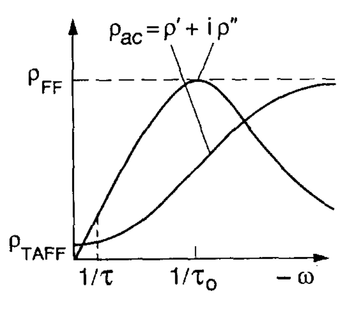

Fig. 3. Complex AC resistivity $\rho_{AC}=1/\sigma_{AC}$ of a high-T_c superconductor in which a constant magnetic field generates an equilibrium flux-line lattice. τ_0 is the relaxation time of the elastically pinned vortex lattice slowed down by viscous drag. $\tau\gg\tau_0$ is the creep time of the vortex lattice caused be thermally activated depinning.

Note that our expression for ρ_{AC} does not explicitly depend on the gap frequency since the order parameter was effectively assumed to be constant in space (London vortices) [42]. In contrast, the more complicated expression for $\rho_{AC}(\omega)=i\omega\lambda^2_{AC}(\omega)4\pi/c^2$ obtained from the complex penetration depth $\lambda_{AC}(\omega)$ of ref. [41] includes pair-breaking effects within the two-fluid model and thus depends on Δ or T_c when T comes close to T_c. Anyway, one may state that the two conductivities given in this paper describe essentially two different physical problems, the only common feature being the AC Meissner effect which follows, respectively, for $\omega\ll\Delta/\hbar$, where $\sigma_{sc}=ic^2/4\pi\lambda^2\omega$, and for rigid pinning ($\alpha_L\to\infty$, $\tau_0\to 0$, $\tau\to\infty$), where $\rho_{AC}=-i4\pi\lambda^2\omega/c^2=1/\sigma_{sc}$.

The theory [41,42] even as the above BCS expression for the optical conductivity, are *linear response* results. However, in the pressure of a flux-line lattice, *non-linear* dissipation may occur even at very small AC amplitudes. This non-linearity is mainly due to depinning processes [42] which occur, even at $T=0$, when the flux-lines vibrate. Due to the randomness of the pinning centers and the elasticity of the flux-line lattice [44], this non-linearity sets in at extremely small flux-line amplitudes of a fraction of an Å. Interestingly, the origin of the early onset of non-linear dissipation in HTSC is related to the origin of the late onset (at $\omega\approx 2\Delta/\hbar$) of structure in the optical conductivity as ω is increased: both ef-

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THESE 2 SUBROUTINES CALCULATE COMPLEX CONDUCTIVITY OF SUPERCONDUCTORS:
      SUBROUTINE BERS(x, y, tt, s)
c     Calculation of complex conductivity  sigma(q=0, omega) for
c     superconductors with arbitrary electron collision time tau
c     from BCS-theory; q=0 means local electrodynamics, London limit;
c       omega = circular frequency; normalization: sigma(omega=0) = 1.
c     Input:  x=omega/2Delta, y=1/(2*Delta*tau), tt=temperature/Tc
c       (Delta=gap, Tc=critical temp., one needs t=temperature/2Delta)
c     Output: s=sigma = sigma1 + i*sigma2    [E.H. Brandt, 18.12.1989]
c       Remark: Since the integrands (variable e=E/2Delta) diverge
c     at the boundaries, one substitutes e=e(u) with de/du=0 at the
c     integration boundaries. The new integration variable u goes from
c     0 to 1 with step width dx=1/integer (try: integer M =10...40).
              complex s, s1, s2, s3, GK
              parameter(M= 40  , d1=1./M )
              dx = 1./int(M*max(1.,sqrt(x)))
              t = tt/(3.528*sqrt(1-tt)*(0.9963 + 0.7733*tt))
                        s1=(0., 0.)
                        s2=(0., 0.)
                        s3=(0., 0.)
      do 2 u= dx*.5, 1., dx
    2    s2 = s2 +GK(.5 +(u/(1.-u))**2, x, y, t, 2)*u/(1.-u)**3
         s  = s2*dx*2.
                        if(x .lt. 1) then
      do 4 u= dx*.5, 1., dx
    4    s1 = s1 +GK(.5 +x*u*u*(3.-u-u), x, y, t, 1)*u*(1.-u)
         s  = s + s1*dx*6.*x
                        else
      do 6 u= dx*.5, 1., dx
    6    s3 = s3 +GK(.5 +(x-1.)*u*u*(3.-u-u), x, y, t, 3)*u*(1.-u)
      do 8 u= d1*.5, 1., d1
    8    s1 = s1 +GK(x-.5 +u*u*(3.-u-u), x, y, t, 1)*u*(1.-u)
         s  = s + (s3*dx*(x-1.) +s1*d1)*6.
                        end if
         s  = s *cmplx(0.,y)*.5/x
                        end
      COMPLEX FUNCTION GK(e, x, y, t, k)
c     Three different integrands  g1, g2, g3 (=gk, k=1,2,3)
                   complex  cy,p4,c42
      if(k.eq.2) p1=sqrt((e+x)**2 -.25)
                 p2=sqrt( e*e     -.25)
      if(k.eq.3) p3=sqrt((e-x)**2 -.25)
      if(k.eq.1) p4=cmplx(0., sqrt(.25 -(e-x)**2))
                 cy=cmplx(0., y)
      if(k.eq.1) c42=(.25 +e*(e-x))/(p4*p2 +1E-20)
      if(k.eq.2) c12=(.25 +e*(e+x))/(p1*p2 +1E-20)
      if(k.eq.3) c32=(.25 +e*(e-x))/(p3*p2 +1E-20)
                 th=tanh(e/(t+t+.001))
      if(k.eq.1) GK= th* ((1-c42)/(p4+p2+cy) -(1+c42)/( p4-p2+cy))
      if(k.eq.2) GK= tanh((e+x)/(t+t+.001))*
     &                   ((1+c12)/(p1-p2+cy) -(1-c12)/(-p1-p2+cy))
     &             + th* ((1-c12)/(p1+p2+cy) -(1+c12)/( p1-p2+cy))
      if(k.eq.3) GK= th* ((1-c32)/(p3+p2+cy) -(1+c32)/( p3-p2+cy))
                        end
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Fig. 4. FORTRAN program.

fects are due to the short BCS coherence length (or flux-line core radius) $\xi \approx 30$ Å which corresponds to a large BCS gap Δ.

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