CALCULATION OF THE COMPLEX ELECTRICAL CONDUCTIVITY OF SUPERCONDUCTING LEAD AND TIN*

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The complex electrical conductivity is calculated by the strong-coupling theory for superconducting lead and tin. The theory is shown to be internally consistent and in agreement with Palmer and Tinkham's experiments. We demonstrate that the real part is simply related to the real part of the gap function for large frequencies.

Recently[1] the strong-coupling theory has been invoked to explain the anomalously steep electromagnetic absorption edge in superconducting lead and the anomalously large transmission through thin films at the gap frequency. Nam's published calculations[2] of the normalized real and imaginary conductivities, σ_{S1}/σ_N and σ_{S2}/σ_N, showed very little change in the region of the gap frequency compared with the weak-coupling theory of Mattis and Bardeen.[3] However, Palmer and Tinkham[1] noticed that the $\sigma_{S1}(\omega)$ of Nam[2] at high frequency required, by the Ferrell-Glover sum rule[4] and the Kramers-Kronig relations, that $\sigma_{S2}(\omega)$ should be considerably smaller than the Mattis-Bardeen result at low frequencies. Such a decrease in σ_{S2} in the gap region could explain the steep absorption edge and the large transmission. Nam has recalculated σ_{S2} and found the required decrease.[5]

However, the difference between Nam's new[5] σ_{S2} and the Mattis-Bardeen result is almost twice the change in σ_{S2} estimated by Palmer and Tinkham.[1] Thus there is a question as to whether the theoretical results are still inconsistent with the sum rule and the Kramers-Kronig relation. In order to check on this apparent inconsistency, and also to calculate more accurate values for the complex conductivity by using the better phonon spectra and electron-phonon interaction for Pb now available,[6] we give here the results of new calculations of $\sigma_{S1}(\omega)/\sigma_N$ for lead together with an accurate integration of the sum rule and the Kramers-Kronig relation. We find that there is a long tail in $[\sigma_{S1}{}^{SC}(\omega)-\sigma_{S1}{}^{MB}(\omega)]/\sigma_N$ at frequencies, where the first term refers to the strong-coupling (SC) expression and the second term is for the Mattis-Bardeen (MB) result. Thus it is difficult to make a graphical estimate of the area involved. We find by better numerical techniques that the change in $\sigma_{S2}(\omega)$ found by Nam[5] is consistent with that required by the sum rule and the Kramers-Kronig relation. The differences between our σ_{S2} via the Kramers-Kronig relation and the σ_{S2} directly calculated by Nam[5] can be understood in terms of the different models for the phonon spectrum for lead.

We also show that $\sigma_{S1}(\omega)/\sigma_N$ at large frequencies is directly related to $\Delta_1(\omega-\Delta_0)$, where Δ_1 is the real part of the energy-gap function. We suggest that accurate measurements of $\sigma_{S1}(\omega)$ at large frequencies (of the order of and larger than the Debye frequency) would be useful to determine directly $\Delta_1(\omega)$.

The real part of the conductivity of a superconductor at low temperatures and in the extreme anomalous limit (l and $\xi \gg \lambda$) can be calculated from the complex energy-gap function $\Delta(\omega)$ as follows[2]:

$$\frac{\sigma_{S1}(\omega)}{\sigma_N}=\frac{2}{\omega}\int_{\Delta_0}^{\omega/2} d\omega_1 \left[\mathrm{Re}\left\{\frac{\omega_1}{[\omega_1{}^2-\Delta(\omega_1)^2]^{1/2}}\right\}\mathrm{Re}\left\{\frac{\omega-\omega_1}{[(\omega-\omega_1)^2-\Delta(\omega-\omega_1)^2]^{1/2}}\right\}\right.$$
$$\left.-\mathrm{Re}\left\{\frac{\Delta(\omega_1)}{[\omega_1{}^2-\Delta(\omega_1)^2]^{1/2}}\right\}\mathrm{Re}\left\{\frac{\Delta(\omega-\omega_1)}{[(\omega-\omega_1)^2-\Delta(\omega-\omega_1)^2]^{1/2}}\right\}\right], \quad (1)$$

where σ_N is the conductivity in the normal state. This expression is also valid in the London limit (l and $\xi \ll \lambda$, where l is the mean free path, ξ the coherence distance, and λ the penetration depth). For both of these limits, the wave number dependence of σ drops out in the ratio σ_S/σ_N and only the frequency dependence remains.

Equation (1) can be interpreted in terms of a photon of frequency ω being absorbed with the excitation of two quasiparticles (breaking two Cooper pairs), one of energy ω_1 and the other of energy $\omega-\omega_1$, so that energy is conserved.

The energy-gap function $\Delta(\omega)$ at $T=0$ is obtained by solving the BCS complex gap equation from the strong-coupling theory.[7] We have done this for Pb using the $\alpha^2F(\omega)$, the square of the electron-phonon interaction times the phonon dendensity of states, as determined from tunneling experiments of McMillan and Rowell.[6] Figure 1 shows the result of this calculation.[8]

Using this $\Delta(\omega)$ in Eq. (1), we have calculated $\sigma_{S1}(\omega)/\sigma_N$ for Pb. For Sn we have carried out the same procedure, again using the McMillan-Rowell $\alpha^2F(\omega)$.[9] Figure 2 is a plot of the difference between the SC result for $\sigma_{S1}(\omega)/\sigma_N$ and the MB weak-coupling result for both lead and tin. For each superconductor, the gap $2\Delta_0$ was taken to be the same for the SC and the MB calculations. Note the similarity in the structure of Fig. 2 for Pb and of $-\Delta_1(\omega)$ of Fig. 1 for Pb. The same is true for tin although we do not plot $\Delta_1(\omega)$ for tin in this paper. Since lead is a stronger-coupling superconductor than tin, the structure occurs at smaller energies (in units of $2\Delta_0$) and is more pronounced.

The structure in Fig. 2 for $\omega \gg 2\Delta_0$ can be understood from Eq. (1). The first term of Eq. (1) approaches $1+O(\Delta^2/\omega^2)$ and does not depend very strongly on the structure of $\Delta(\omega)$. At values of ω for which $\Delta(\omega)$ has structure, this is swamped by $\omega^2 \gg \Delta(\omega)^2$ in $[\omega^2-\Delta(\omega)^2]^{1/2}$. However, in the second term this is not true, and for large ω this term becomes

$$\sim -\frac{2}{\omega}\int_{\Delta_0}^{\omega/2} d\omega_1 \frac{\Delta_1(\omega_1)}{[\omega_1^2-\Delta(\omega_1)^2]^{1/2}} \frac{\Delta_1(\omega-\omega_1)}{\omega-\omega_1}$$

$$\sim -\frac{2\Delta_0\Delta_1(\omega-\Delta_0)}{\omega^2}\ln\frac{2\omega}{\Delta_0}, \qquad (2)$$

where we have used the fact that $[\omega_1^2-\Delta(\omega_1)^2]^{-1/2}$ is sharply peaked about $\omega_1=\Delta(\omega_1)=\Delta_0$. Thus the second term in Eq. (1) is proportional to $-\Delta_1(\omega-\Delta_0)$ for $\omega \gg \Delta_0$ with the other factors smoothly varying functions of ω.

We see that the contribution from Eq. (2) in the MB case [for which $\Delta_1(\omega-\Delta_0)=\Delta_0>0$ independent of ω] to σ_{S1}/σ_N is negative, while the first term is slightly less than 1 for large ω. Thus $\sigma_{S1}{}^{MB}/\sigma_N$ approaches 1 from below. On the other hand, for the SC case, $\Delta_1(\omega-\Delta_0)\to \text{const}<0$ for large ω and thus the second term is positive. This term overcomes the difference of the first term from 1, and $\sigma_{S1}{}^{SC}/\sigma_N$ approaches 1 from above.

Because $\sigma_{S1}{}^{SC}/\sigma_N-1$ is proportional to $-\Delta_1(\omega-\Delta_0)$ for large ω, accurate measurements of $\sigma_{S1}{}^{SC}/\sigma_N$ for $\omega \gtrsim$ Debye energy should give directly $\Delta_1(\omega)$. The only other experiment that

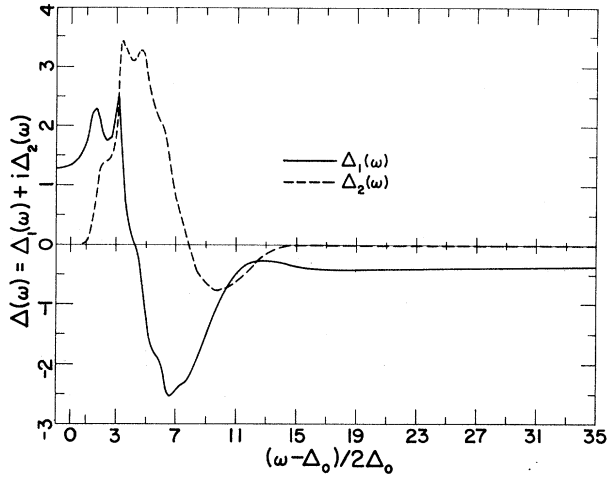

FIG. 1. The real and imaginary parts, Δ_1 and Δ_2, of the complex gap function as a function of energy ω for lead at $T=0$. For this calculation we have used $\alpha^2F(\omega)$ of McMillan and Rowell (Ref. 6), a Coulomb pseudopotential $U_C=0.127\,158$ for a cutoff $\omega_C=104$ meV. The $\alpha^2F(\omega)$ was multiplied by 1.105 to give a gap $2\Delta_0=2.681$ meV to agree with the tunneling experiments.

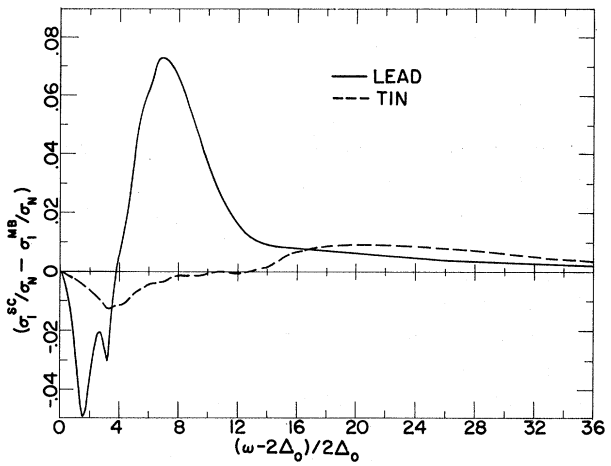

FIG. 2. The difference between $\sigma_{S1}{}^{SC}/\sigma_N$, the real part of the conductivity for the strong-coupling theory for lead and tin, and $\sigma_{S1}{}^{MB}/\sigma_N$, the Mattis-Bardeen weak-coupling expression (Ref. 3). These calculations are valid for either the extreme anomalous limit or the London limit.

gives information on $\Delta(\omega)$ for large energy is the anomalous tunneling, and this gives a mixed function of Δ_1 and Δ_2.

Using the result of numerical integration of Eq. (1) for $\sigma_{S1}{}^{SC}/\sigma_N$ (Fig. 2), we have found the change in the delta function contribution at $\omega = 0$ by the Ferrell-Glover sum rule[4]

$$\int_0^\infty \sigma_1(\omega)d\omega = \text{const.} \tag{3}$$

But

$$\sigma_{S1}(\omega)/\sigma_N = A_g\delta(\omega) + \sigma_{S1}'(\omega)/\sigma_N, \tag{4}$$

where $\sigma_{S1}'(\omega)$ is a smoothly varying function —namely equal to zero for $\omega \leq 2\Delta_0$ and given by Eq. (1) for $\omega > 2\Delta_0$. We find

$$\int_{2\Delta_0}^\infty d\omega(\sigma_{S1}{}^{SC} - \sigma_{S1}{}^{MB})/\sigma_N$$
$$= 0.502(2\Delta_0) \text{ for lead,}$$
$$= 0.209(2\Delta_0) \text{ for tin.}$$

The lead result is to be compared with $0.3(2\Delta_0)$ obtained by the rough integration of Nam's σ_{S1} by Palmer and Tinkham.[1] This means that A_g must decrease a corresponding amount so that Eq. (3) is satisfied. In carrying out the integral of $\delta\sigma_{S1}$, we have computed numerically from $\omega = 2\Delta_0$ to 20 or 50 times $2\Delta_0$. The remainder of the range was integrated analytically using the asymptotic expressions for $\sigma_{S1}{}^{SC}$ and $\sigma_{S1}{}^{MB}$.

The corresponding change in σ_{S2} is found from the Kramers-Kronig relation

$$\frac{\sigma_{S2}}{\sigma_N} = -\frac{2}{\pi}\frac{A_g}{\omega} - \frac{2\omega}{\pi}\int_{2\Delta_0}^\infty \frac{\sigma_{S1}(\omega_1)/\sigma_N}{\omega_1{}^2-\omega^2}d\omega_1, \tag{5}$$

where the first term on the right arises from the integration of the δ function in σ_{S1}. In the second term we can use either σ_{S1} or σ_{S1}' since they are equal except for the δ function. To emphasize that the δ function is not to be used in the second term, we start the integration from $2\Delta_0$ rather than from $\omega_1 = 0$.

The SC $\sigma_{S2}(\omega)/\sigma_N$ for $\omega \lesssim 2\Delta_0$ for Pb that we obtain from $\sigma_{S1}{}^{SC}$ by using the sum rule and Kramers-Kronig relations is plotted in Fig. 3, together with the experimental results of Palmer and Tinkham[1] and Nam's new direct calculation of σ_{S2}/σ_N. Of the difference between the present calculation and the MB result (BCS weak coupling), in this frequency range 99% is due to the change in A_g in Eq. (5), and only 1% is due to the change of σ_{S1} in the second term. The calculations are in good agreement with the experiments and with each other. The latter agreement demonstrates that the σ_{S1} and σ_{S2} calculated from the strong coupling theory are now consistent by the Kramers-Kronig relations.

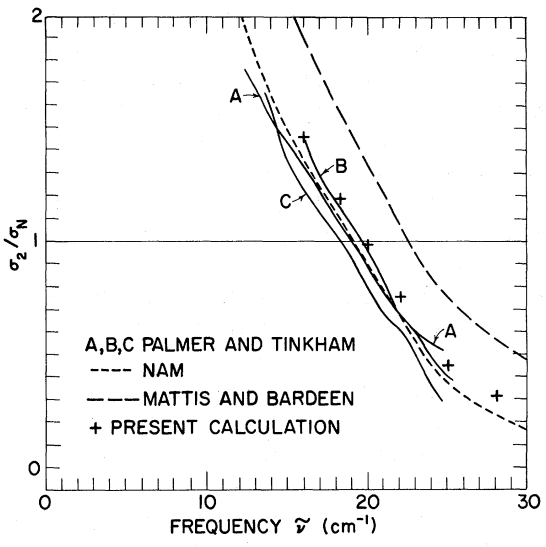

FIG. 3. The imaginary part, $\sigma_{S2}(\omega)/\sigma_N$, of the conductivity as a function of frequency (energy). The top curve is the Mattis-Bardeen weak coupling prediction from the BCS theory (Ref. 3). The curves *A*, *B*, and *C* are experimental results by Palmer and Tinkham (Ref. 1) on Pb. The result of Nam is his later result (Ref. 5) of a direct calculation of σ_{S2}/σ_N from $\Delta(\omega)$ as reported in Ref. 1. The present calculation is from $\sigma_{S1}(\omega)/\sigma_N$ via the sum rule and the Kramers-Kronig relation. Our calculation was for an interaction strength which gave a gap $2\Delta_0 = 2.681$ meV $= 21.63$ cm^{-1} (the gap from tunneling, Ref. 6), while the infrared experiments (those on this graph, Ref. 1) indicated a gap of $2\Delta_0 = 22.5$ cm^{-1}. In order to make a direct comparison we have shifted the frequencies of our calculated results by $22.5/21.63 = 1.04$ for this graph.

The difference that remains between the two calculations of σ_{S2} can be attributed to differences in the $\alpha^2F(\omega)$ used. Nam's calculation was based on the gap function of Scalapino, Schrieffer, and Wilkins,[7] which in turn used a two-Lorentzian approximation to α^2F. We have used the more accurate α^2F of McMillan and Rowell.[6]

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LINEAR-$\vec{k}$ VALENCE-BAND SPLITTING IN InSb

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In this Letter we report the observation of an interband magneto-optical transition in InSb caused by the linear-$\vec{k}$ term in the valence-band energy $E(\vec{k})$. An unambiguous assignment is made by a study of the anisotropy of the spectra [with the magnetic field $\vec{H}$ in the $(1\bar{1}0)$ crystal plane] using left- and right-circularly polarized light. From the relative strength and position of this transition we determine the size of the linear-$\vec{k}$ term. A similar procedure is used to measure the warping of the InSb valence band, a quantity over which there is currently some disagreement.

The theory of the inversion asymmetry terms in zinc-blende crystals has been known for some time.[1,2] These terms—the lowest order are k and k^3 terms—result from the antisymmetric potential or inversion asymmetry of the zinc-blende lattice. Combined with the spin-orbit interaction, they split the twofold energy degeneracy at a given $\vec{k}$ value. Because the splittings are small, they have been difficult to observe experimentally. Recently, it has been suggested that a beat frequency in the Shubnikov-de-Haas effect in n-type HgSe[3] gives the conduction-band inversion-asymmetry splitting,[4] and the same effect is apparently seen in n-type GaSb.[5] This has not been useful for determining the size of the linear-$\vec{k}$ term which splits the valence band.[6] Evidence of the linear-$\vec{k}$ splitting has been given recently by Robinson[7] from microwave cyclotron-resonance experiments in p-type InSb. However, difficulties in the interpretation of this type of experiment resulting from poor resolution of the lines ($\omega_c\tau \sim 0.9$) and the sensitivity to strain effects make it desirable to have independent determinations. We find the linear-$\vec{k}$ term to be about three times smaller than suggested in Ref. 7.

The physical explanation of "extra" transitions due to the linear-$\vec{k}$ and warping interactions is not difficult to understand and we discuss this before going into the theoretical formalism. The calculation of magnetic energy levels in InSb has been carried out by Pidgeon and Brown,[8] by an extension of the method used by Luttinger and Kohn for the Ge valence band.[9,10] Energy levels calculated by the method of Ref. 8 (to be discussed more fully below) are shown in Fig. 1 for the top of the valence band and the bottom of the conduction band. To diagonalize the magnetic Hamiltonian appropriate to this problem it is necessary to omit inversion-asymmetry terms and some of the valence-band warping.[11] The solid lines in Fig. 1 show the optical transitions which can take place in the Faraday configuration ($\vec{E} \perp \vec{H}$): Electrons can be excited from the two "a"-set valence-band ladders into the $m_J = \frac{1}{2}$ conduction sub-band, or from the two "b"-set ladders into the $m_J = -\frac{1}{2}$ conduction sub-band. Usually the inversion-asymmetry and warping terms omitted from the magnetic Hamiltonian cause negligible error. However, if two levels which interact through the omitted terms are nearly degenerate in energy, considerable admixing of wave functions can take place. This in turn can cause observable extra transitions. In