Theory of Optical Conductivity in BCS Superconductors

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The optical conductivity is obtained *exactly* within BCS theory as a function of frequency, temperature, and disorder parameter, by simplifying the general impurity scattering mechanism to backward scattering. The familiar features of infrared measurements are recovered. In the dirty limit, the ratio of superconducting to normal absorption rate approaches the Mattis-Bardeen result.

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Infrared optical measurements on superconductors are known to play an important role in revealing the excitation spectrum and other properties of the superconducting state, since the energy scale here is about a few times the energy gap. The first calculation of optical (microwave) conductivity within the BCS theory was performed by Mattis and Bardeen [1] in the dirty limit. They assumed that the mean free path of carriers is much shorter than the superconducting coherent length. The Mattis-Bardeen result agrees with experiments very well. Its extensions [2] into the strong coupling regime revealed no major modifications. However, recent experimental measurements on the new high-T_c superconductors, which are believed to be in the clean limit, have tested the microscopic calculations [3]. In the Eliashberg formalism [3], the scattering mechanism is parametrized by finite mean free path or impurity scattering rates. Because agreement with experiments on the high-T_c materials is not completely satisfactory, it seems that new calculations are required to improve the quantitative fit of theory to experiment over the full range of temperature and frequencies.

In this Letter, rather than propose a model fit to any specific material, we provide the first *exact* evaluation of the Kubo formula in the superconducting state, combining BCS theory with an exactly soluble, simplified model of impurity scattering, in which it is assumed that singular backward scattering dominates the impurity collision kernel. The backward-scattering model cannot be derived in any simple way from random impurities or phonon scattering. It is, however, a mathematical construct which does allow the current in a many-electron system to decay and does provide a finite lifetime to quasiparticles in a many-body system. Its use here allows us to evaluate the Kubo formulas without the usual decoupling or other ill-characterized approximations. In treating impurity scattering in the usual way, one often uses a long-time limit with which to conserve energy ("Born approximation"), in which phase coherence between initial and final states is lost. By contrast in the present model the scattering mechanism is simple enough to be treated exactly, so that the necessary degree of phase coherence between the incoming and scattered waves is retained. This should prove especially valuable in applications to low-dimensional systems.

The backward-scattering model has already had several successful applications. In transport studies using the time-dependent Boltzmann equation [4], this model yielded the decay of the Boltzmann distribution almost indistinguishable from what was obtained with the more structured scattering mechanisms studied by Palmeri [4], and it did so with far less computational effort. In calculating the effects of scattering on T_c (the original hypothesis by Anderson that T_c should be unaffected by elastic scatterers holds, in fact, only in the lowest approximation) it has successfully distinguished between thin films and bulk superconductors [5,6]. In the optical absorption problem, this model will be seen to explain with great simplicity a number of features for which generally much more sophisticated theories are required.

In the model, it is assumed that electrons with wave vector $\mathbf{k}$ are scattered to $-\mathbf{k}$ only, via a random matrix element $v(k)$. The scattering potential $v(k)$, a real function, is distributed at random according to a probability function $P(v(k))$. Consider a BCS Hamiltonian [7] with such a backscattering interaction:

$$H = H_{\rm BCS} + H_{\rm BS} = \sum_{p_z>0} H_p \tag{1}$$

denoting $1 = p\uparrow$, $2 = -p\uparrow$, $3 = p\downarrow$, $4 = -p\downarrow$, for the momentum and spin. Then,

$$\begin{aligned} H_p = {} & \epsilon(p)(c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3 + c_4^\dagger c_4) \\ & +\Delta(p)(c_1^\dagger c_4^\dagger + c_4 c_1 + c_2^\dagger c_3^\dagger + c_3 c_2) \\ & +v(p)(c_1^\dagger c_2 + c_2^\dagger c_1 + c_3^\dagger c_4 + c_4^\dagger c_3). \end{aligned} \tag{2}$$

The gap function [7] Δ is determined self-consistently by the generalized gap equation [6]. H_p is readily diagonalized by a Bogoliubov transformation:

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3^\dagger \\ c_4^\dagger \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_1 & u_2 & v_1 & v_2 \\ u_1 & -u_2 & v_1 & -v_2 \\ -v_1 & -v_2 & u_1 & u_2 \\ -v_1 & v_2 & u_1 & -u_2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3^\dagger \\ a_4^\dagger \end{pmatrix}, \tag{3}$$

where

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$$u_i^2 - v_i^2 = \frac{\epsilon(p) \pm v(p)}{E_i}, \quad 2u_i v_i = \mp\frac{\Delta(p)}{E_i}, \quad E_i = \sqrt{[\epsilon(p) \pm v(p)]^2 + \Delta(p)^2} \qquad (i = 1, 2) \tag{4}$$

which leads to

$$H_p = E_1(a_1^\dagger a_1 + a_3^\dagger a_3) + E_2(a_2^\dagger a_2 + a_4^\dagger a_4) + c\text{-number}. \tag{5}$$

As we have previously demonstrated [6], the current operator keeps its conventional form $J_z = \sum_{p\sigma}(ep_z/m)c_{p\sigma}^\dagger c_{p\sigma}$ in the z direction, even in the presence of backward scatterings. When c's are expressed in terms of a's, we found

$$\begin{aligned} J_z(t) =& \sum_{p>0} \frac{ep_z}{m}(u_1u_2 - v_1v_2)[e^{i(E_1-E_2)t}(a_1^\dagger a_2 + a_3^\dagger a_4) + \text{H.c.}] \\ &+ \sum_{p>0} \frac{ep_z}{m}(u_1v_2 + v_1u_2)[e^{i(E_1+E_2)t}(a_1^\dagger a_4^\dagger + a_2^\dagger a_3^\dagger) + \text{H.c.}]. \end{aligned} \tag{6}$$

According to Kubo formula [8], the conductivity is given by

$$i\omega\sigma_{\alpha\beta}(\omega, T) = \left\langle -\frac{ne^2}{m}\delta_{\alpha\beta} + i\int_0^\infty dt\, e^{i\omega t}\langle[J_\alpha(t), J_\beta(0)]\rangle \right\rangle, \tag{7}$$

where $\langle\cdots\rangle$ denotes thermal average, and $\langle\,\cdots\,\rangle$ the average over random variables. The current-current correlation function can be evaluated exactly for arbitrary configuration of $v(p)$'s. By symmetry, $\sigma_{\alpha\beta}(\omega, T) = \sigma(\omega, T)\delta_{\alpha\beta}$, we have

$$\begin{aligned} \sigma(\omega, T) = A(T)\delta(\omega) &+ \frac{ne^2}{m\omega}\left\langle \frac{2\pi}{3N_e}\sum_p \left(\frac{p^2}{2m}\right)[\delta(\omega + E_1 - E_2) - \delta(\omega - E_1 + E_2)](u_1u_2 - v_1v_2)^2[f_1 - f_2] \right. \\ &\left. + \frac{2\pi}{3N_e}\sum_p \left(\frac{p^2}{2m}\right)[\delta(\omega + E_1 + E_2) - \delta(\omega - E_1 - E_2)](u_1v_2 + v_1u_2)^2[f_1 + f_2 - 1] \right\rangle \\ &+ i\frac{ne^2}{m\omega}\left\langle 1 - \frac{4}{3N_e}\sum_p \left(\frac{p^2}{2m}\right) P_C \frac{(E_1 - E_2)}{\omega^2 - (E_1 - E_2)^2}(u_1u_2 - v_1v_2)^2[f_1 - f_2] \right. \\ &\left. - \frac{4}{3N_e}\sum_p \left(\frac{p^2}{2m}\right) P_C \frac{(E_1 + E_2)}{\omega^2 - (E_1 + E_2)^2}(u_1v_2 + v_1u_2)^2[f_1 + f_2 - 1] \right\rangle, \end{aligned} \tag{8}$$

where $f_{1,2} = 1/(e^{\frac{E_{1,2}}{T}} + 1)$ is the Fermi function, $A(T)$ relates to the superconducting feature and is required for the optical sum rule. P_C stands for Cauchy principal value.

The optical absorption rate of thin metallic films $\sigma_{1s}(\omega, T)$ is given by the real part of the conductivity in Eq. (8) at arbitrary $|\omega| > 0$ and temperature, for any given random potential configuration. The configuration average over a given probability function $P(v)$ can be done numerically to any desired accuracy. Here we present the results for *Lorentzian* distribution $P(v) = (\Gamma/\pi)/(v^2+\Gamma^2)$, which is typical. The disorder parameter Γ is assumed to be momentum independent. It measures the rms strength of the random potential $\sqrt{\langle v^2\Phi\rangle} \sim \Gamma$.

The energy scale of BCS theory in weak coupling is set by the Debye temperature ω_D: $T_c(\Gamma = 0)/\omega_D = 1.13e^{-\frac{1}{\lambda}}$ is fixed by the coupling constant λ, for which we shall assume a typical value $\frac{1}{3}$ here.

Given these parameters, $\sigma_{1s}(\omega, 2T/T_c = 0.1)$ is shown in Fig. 1 for three Γ's, representing clean, intermediate, and dirty limits, respectively, in the unit of ne^2/m. The inset, $T_c(\Gamma)/T_c(0)$ at zero temperature, relates T_c to Γ. Normal state conductivity $\sigma_{1n}(\omega)$'s [6] are included for comparison. (The *temperature* dependence of σ_{1n} is negligible in a narrow range $0 < T < T_c$.) Note that each $\Delta(\Gamma, T)$ has to be determined self-consistently as a function of disorder and temperature in our generalized gap equation [6].

At zero temperature and $\omega < 2\Delta(\Gamma, 0)$, $\sigma_{1s}(\omega) = 0$. However, at finite T, small but nonvanishing absorption appears for $\omega < 2\Delta(\Gamma, T)$ even though $\lim_{\omega\to 0}\sigma_{1s}(\omega, T) = 0$ for $T < T_c$. Note that the delta function contribution $A\delta(\omega)$ is excluded from this analysis, as it relates only to the Meissner effect and not to dissipative phenomena. This is shown in Fig. 2 for two different temperatures $2T/T_c(\Gamma) = 0.5, 0.9$ at $\Gamma/\omega_D = 0.2$. Only when T approaches T_c does the small absorption at low frequency become noticeable.

It is interesting to compare the dirty limit ($\Gamma \to \infty$) in the present model to the Mattis-Bardeen result. Figure 3 shows the ratio of the superconducting to normal absorption rate σ_{1s}/σ_{1n} as a function of frequency for several Γ, from the clean to the dirty limit. The curves saturate at $\Gamma/\omega_D = 0.8$, where they approach the Mattis-Bardeen result [1] (included in dashed line) as a lower bound.

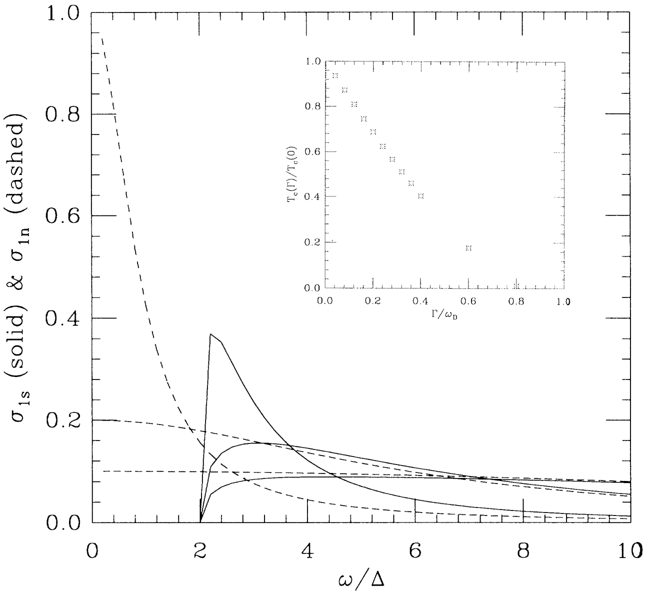

FIG. 1. Solid curves: $\sigma_{1s}(\omega, 2T/T_c = 0.1)$ as a function of $\omega/\Delta(\Gamma, T)$ for $\Gamma/\omega_D = 0.04, 0.20, 0.40$ (from top to bottom just above $\omega = 2\Delta$). Dashed curves: $\sigma_{1n}(\omega)$ for comparison. Note that curves σ_{1s} and σ_{1n} of given disorder have the same asymptotic behavior at large frequency. Inset: $T_c(\Gamma)/T_c(0)$ as a function of disorder at $T = 0$.

The remaining difference (our result indicates a larger absorption than does the Mattis-Bardeen theory) above $\omega = 2\Delta$ can be explained by the fact that backward scattering causes current to decay faster than the isotropic scattering mechanism as in Ref. [1], and moreover acts as a "pair breaker" in the superconducting phase. We also see that in the clean limit $\Gamma/\omega_D \ll 0.2$, the absorption at $\omega \approx 2\Delta$ becomes unremarkable, consistent with a variety of experimental data on high-T_c superconductors. No features are seen at $\omega = 4\Delta$, and neither is the Holstein structure.

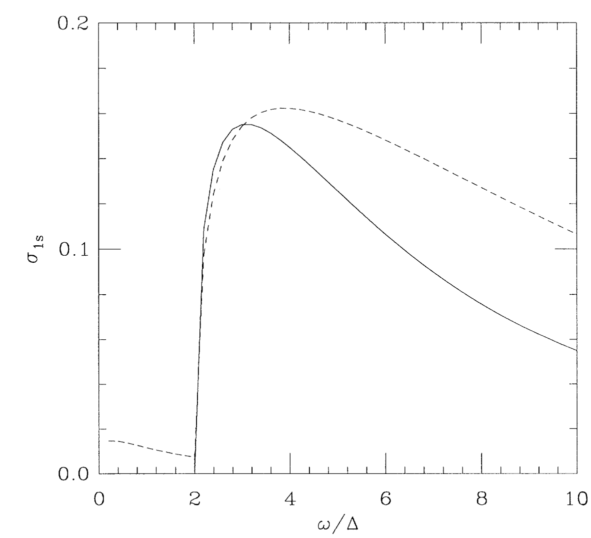

FIG. 2. $\sigma_{1s}(\omega, T)$ as a function of $\omega/\Delta(\Gamma, T)$ for $2T/T_c = 0.5$ (solid), 0.9 (dashed) at fixed $\Gamma/\omega_D = 0.20$.

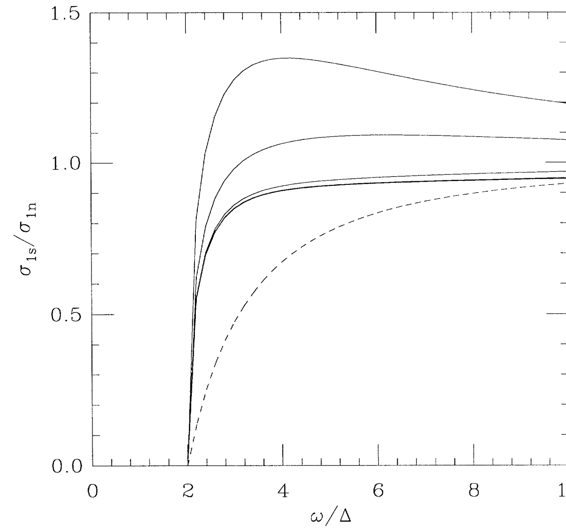

FIG. 3. σ_{1s}/σ_{1n} as a function of $\omega/\Delta(\Gamma, 2T/T_c = 0.1)$ from the clean (top curve) to the dirty limit: $\Gamma/\omega_D = 0.12, 0.2, 0.4, 0.6, 0.8$. The dashed line is the Mattis-Bardeen result.

In summary, we have exactly evaluated the Kubo formula in the superconducting state for the optical conductivity as a function of frequency, temperature, and disorder within the backward-scattering model. All interesting features can be reproduced with the use of this simple scattering mechanism. Our results approach something like the Mattis-Bardeen result in the dirty limit. Generalization to strong-coupling theory is straightforward.

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