Optical conductivity of d-wave superconductors

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PACS. 74.20.-z – Theories and models of superconducting states.
PACS. 74.25.Fy – Transport properties.
PACS. 74.25.Gz – Optical properties.

Abstract. – We study theoretically the optical conductivity of d-wave superconductors like in high temperature cuprates in the presence of impurities. We limit ourselves at $T = 0\, \text{K}$ and focus on the frequency dependence of both $\sigma_1(\omega)$ and $\omega\sigma_2(\omega)$ for $\omega \lesssim 2\Delta$. When the impurity scattering is in the unitary limit, we find a peak in $\sigma_1(\omega)$ with $\omega/\Delta \simeq 0.1 \sim 0.5$, which may account for the peak seen by Basov et al. in Zn-substituted YBCO.

Introduction. – Now $d_{x^2-y^2}$-wave superconductivity is well established in both hole-doped and electron-doped high temperature cuprate superconductors. Further superconductivity in organic conductors in $\kappa-(ET)_2$ salts appears to be of d-wave. In spite of these developments, the optical conductivity in d-wave superconductors appears to be not well understood. For example Hirschfeld et al. considered the microwave conductivity in d-wave superconductors in the presence of impurity in the unitary limit. However they were more interested in the temperature dependence rather than the frequency dependence. Similarly Sun and Maki and Graf et al. studied only some aspect of the optical conductivity. On the other hand, a recent infrared conductivity in Zn-substituted YBCO exhibits a peak around $\omega/\Delta \simeq 0.1 \sim 0.2$, which cannot be accounted for the above theories. The object of this paper is to study the in plane optical conductivity focusing on the frequency dependence at $T = 0\, \text{K}$. As a model we take d-wave superconductors (with gap function $\Delta(k) = \Delta \cos(2\phi)$, $\phi$ is the in plane angle measured from the $k_x$ direction) in the presence of impurities in the unitary and Born limit. We assume that the former describes the Zn impurity while the latter the Ni impurity. In the following we summarize what we needed for the model, then we calculate $\sigma_1(\omega)$ and $\omega\sigma_2(\omega)$ for impurities in the unitary and the Born limit for several impurity concentrations. Indeed, for the impurity in the unitary limit $\sigma_1(\omega)$ develops a peak around $\omega/\Delta \simeq 0.1 \sim 0.2$, somewhat similar to the one observed in Zn-substituted YBCO. On the other hand, $\sigma_1(\omega)$ in the Born limit develops a broad bump around $\omega/\Delta \sim 1.5$. © EDP Sciences
The effect of impurity scattering is incorporated by renormalizing the frequency in the quasi-particle Green’s function [13, 14]:

$$\frac{\omega}{\Delta} = u + \alpha \frac{\pi}{2} \frac{1 - u^2}{uK(\sqrt{1 - u^2})},$$  \hspace{1cm} (1)

$$\frac{\omega}{\Delta} = u - \alpha \frac{2}{\pi} \frac{u}{\sqrt{1 - u^2}} K \left( \frac{1}{\sqrt{1 - u^2}} \right)$$  \hspace{1cm} (2)

for the unitary and the Born limit, respectively, where $u = \tilde{\omega}/\Delta$, $\alpha = \Gamma/\Delta$, $K(z)$ is the complete elliptic integral of the first kind and $\Gamma$ is the scattering rate. Making use of the gap equation the superconducting transition temperature ($T_c$) in the presence of impurity is given:

$$-\ln \left( \frac{T_c}{T_{c0}} \right) = \Psi \left( \frac{1}{2} + \frac{\Gamma}{2\pi T_c} \right) - \Psi \left( \frac{1}{2} \right),$$  \hspace{1cm} (3)

where $T_{c0}$ is the one in the absence of impurity and $\Psi(z)$ is the di-gamma function. This is the same as the Abrikosov-Gor’kov formula for s-wave superconductors in the presence of magnetic impurities [15]. Also it is independent of whether the impurity is in the unitary limit or in the Born limit. Further we note the AG formula is universal in the sense that it applies to all unconventional superconductors (p-wave, d-wave, f-wave etc.) and independent on whether the scattering is in the unitary or the Born limit. Now at $T = 0K$ the gap equation yields [12–14]

$$-\ln \left( \frac{\Delta(0, \Gamma)}{\Delta_{00}} \right) = 2\left( f^2 \text{arcsinh} \left( \frac{C_0}{f} \right) \right) -$$

$$-2\frac{\Gamma}{\Delta} \int_{C_0}^{\infty} dx \frac{1}{x^2} \left( 1 - \frac{E}{K} \right) \left( 1 + x^2 \right) \frac{E}{K} - x^2,$$  \hspace{1cm} (4)

and

$$-\ln \left( \frac{\Delta(0, \Gamma)}{\Delta_{00}} \right) = 2\left( f^2 \text{arcsinh} \left( \frac{C_0}{f} \right) \right) +$$

$$+2 \left( \frac{2}{\pi} \right)^2 \frac{\Gamma}{\Delta} \int_{C_0}^{\infty} dx (K - E) \left( E - \frac{x^2}{1 + x^2} K \right)$$  \hspace{1cm} (5)

for the unitary limit and the Born limit, respectively and $C_0$ is given by

$$C_0^2 = \frac{\pi \Gamma}{2\Delta} \sqrt{1 + C_0^2} \left[ K \left( \frac{1}{\sqrt{1 + C_0^2}} \right) \right]^{-1}$$  \hspace{1cm} (6)

and

$$\sqrt{1 + C_0^2} = \frac{2\Gamma}{\pi \Delta} K \left( \frac{1}{\sqrt{1 + C_0^2}} \right)$$  \hspace{1cm} (7)

for the unitary limit and the Born limit, respectively, and $f = \cos(2\phi)$, $\Delta_{00} = \Delta(0, 0)$, $\langle \ldots \rangle$ means average of $\phi$ and $K = K(1/\sqrt{1 + x^2})$ and $E = E(1/\sqrt{1 + x^2})$. Finally the residual density of states (i.e. the density of states on the Fermi surface) is given by

$$\frac{N(0, \Gamma)}{N_0} = \frac{2}{\pi} \frac{C_0}{\sqrt{1 + C_0^2}} K \left( \frac{1}{\sqrt{1 + C_0^2}} \right) = \begin{cases} \frac{\Gamma}{\Delta C_0} & \text{unitary limit} \\ \Delta C_0/\Gamma & \text{Born limit} \end{cases}$$  \hspace{1cm} (8)

We show in fig. 1 and fig. 2 $T_c/T_{c0}$, $\Delta(0, \Gamma)/\Delta_{00}$ and $N(0, \Gamma)/N_0$ versus $\Gamma/\Gamma_c$ for the unitary and Born limit respectively, and $\Gamma_c = 0.8819T_{c0}$. 


Fig. 1 – $\Delta(0, \Gamma)/\Delta_{00}$ (dashed line), $T_c/T_c^0$ (solid line) and $N(0, \Gamma)/N_0$ (dashed-dotted line) are shown as a function of $\Gamma/\Gamma_c$ in the unitary limit.

Fig. 2 – $\Delta(0, \Gamma)/\Delta_{00}$ (dashed line), $T_c/T_c^0$ (solid line) and $N(0, \Gamma)/N_0$ (dashed-dotted line) are shown as a function of $\Gamma/\Gamma_c$ in the Born limit.

Quasi-particle density of states and optical conductivity. – The quasi-particle density of states in the presence of impurities is given by

$$N(0, \Gamma) = N_0 \text{Re} \left( \frac{u}{\sqrt{u^2 - f^2}} \right).$$

We show the quasi-particle density of states for $\Gamma/\Delta = 0.01, 0.05, 0.1, 0.2$ and 1 for the unitary and Born limit in fig. 3 and 4 respectively. These figures are consistent with the earlier results in [10, 12–14]. In particular in the Born limit there is little density of states at $E = 0$ until $\Gamma/\Gamma_c \geq 0.5$. This result is consistent with tunneling conduction data from Ni substituted Bi$_2$2212 [16].

Now the optical conductivity is expressed as $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$:

$$\omega \sigma_2(\omega) = -\frac{e^2 n}{m \pi \Delta} \text{Im} \left( I(\omega) + 2 \int_{-\infty}^{\infty} \frac{1}{e^{\beta x} + 1} F(u(x), u(x - \omega)) dx \right),$$

where

$$I(\omega) = \int_{-\infty}^{\infty} \frac{1}{2} \left( \tanh \left( \frac{\beta x}{2} \right) - \tanh \left( \frac{\beta (x + \omega)}{2} \right) \right) \times (F(u(x + \omega), \pi(x)) - F(u(x + \omega), u(x))) dx$$
Fig. 3 – The density of states is shown for different $\Gamma/\Delta(\Gamma)$ in the unitary limit: 0.01 (thin solid line), 0.02 (dashed line), 0.1 (dashed-dotted line), 0.2 (thin dotted line) and 1 (thick solid line).

Fig. 4 – The density of states is shown for different $\Gamma/\Delta(\Gamma)$ in the Born limit: 0.01 (thin solid line), 0.02 (dashed line), 0.1 (dashed-dotted line), 0.2 (thin dotted line) and 1 (thick solid line).

and

$$F(u, u') = \frac{1}{u' - u} \left( \frac{u'}{\sqrt{1 - u'^2}} K\left(\frac{1}{\sqrt{1 - u'^2}}\right) - \frac{u}{\sqrt{1 - u^2}} K\left(\frac{1}{\sqrt{1 - u^2}}\right) \right).$$

It is worth noting, that the imaginary part of the integral of the second $F$ function in $I(\omega)$ is zero. In evaluating $F(u, u')$, we included self energy corrections from impurities, but the vertex corrections vanished in the long wavelength limit because of s-wave scattering [17, 18]. At zero frequency, $\sigma_1(\omega)$ reduces to:

$$\sigma_1(0) = \frac{e^2 n}{m\pi\Delta(0, \Gamma)} \frac{E\left(\frac{1}{\sqrt{1+C_0^2}}\right)}{\sqrt{1+C_0^2}},$$

which is valid in both limits. $E(z)$ is the complete elliptic integral of the second kind. At $\Gamma_c$, $\sigma_1(0)$ reaches $\pi/0.8244$ times its pure value. See fig. [3]. Note the vertical axis in fig. [3] can be rewritten as $\sigma_1(0)/\sigma_n = \lim_{T \to 0} \kappa/\kappa_n$, where $\kappa$ is the thermal conductivity and $\sigma_n$ and $\kappa_n$ are the conductivity and the thermal conductivity in the normal state. In the vortex state of d-wave superconductors the Wiedeman-Franz law still holds [9, 12, 19]. Then fig. [3] shows the deviation from Lee’s universality relation [20]. Indeed this deviation from the universality is verified later in Zn-substituted YBCO by measuring the low temperature thermal conductivity [21].

In fig. [3] and [4], we show $\sigma_1(\omega)$ at $T = 0K$ for the previously investigated scattering rates in the unitary and Born limit. In the unitary limit $\sigma_1(\omega)$ develops a small peak around $\omega/\Delta \simeq 0.1 \sim 0.2$ for $\Gamma/\Delta < 0.1$, this may be related to the small peak seen in Zn substituted Y(124) [11]. On the other hand in the Born limit $\sigma_1(\omega)$ initially drops monotonously with
Fig. 5 – The DC conductivity is shown as a function of $\Gamma/\Gamma_c$ in the unitary (dashed line) and the Born (solid line) limit.

Fig. 6 – Real part of the optical conductivity is plotted for different $\Gamma/\Delta(\Gamma)$ in the unitary limit: 0.01 (thin solid line), 0.02 (dashed line), 0.1 (dashed-dotted line) and 0.2 (thin dotted line).

Fig. 7 – Real part of the optical conductivity is plotted for different $\Gamma/\Delta(\Gamma)$ in the Born limit: 0.01 (thin solid line), 0.02 (dashed line), 0.1 (dashed-dotted line) and 0.2 (thin dotted line).
increasing $\omega$, then develops a broad bump around $\omega/\Delta \sim 1.5$. In either case there is no clear feature around $\omega/\Delta \sim 2$. This implies perhaps the single particle rather than the pair breaking scattering dominates $\sigma_1(\omega)$.

In fig. 8 and 9 we show $\omega \sigma_2(\omega)$ at $T = 0K$ for the unitary and the Born limit. We note that

$$\lim_{\omega \to 0} \omega \sigma_2(\omega) = \frac{e^2 n}{m} \rho_s(0, \Gamma),$$

where $\rho_s(0, \Gamma)$ is the superfluid density. Further $\lim_{\omega \to \infty} \omega \sigma_2(\omega) = e^2 n / m$ independent of $\Gamma$ and of whether in the unitary limit or the Born limit. This means that $\omega \sigma_2(\omega)$ should have a dip at $\omega = 0$ as seen in these figures as well as in Fig. 1. In the Born limit, there is a small peak at $\omega/\Delta = 1$ for small scatterers, which is unobservable in our figure due to its scale. Also in the unitary limit this dip like structure appears to develop steps. In a future study we shall discuss the temperature dependence of these quantities.

**Conclusion.** – We find a simple closed form expression of the complex conductivity for d-wave superconductors which applies for both the unitary and the Born limit. In the unitary limit $\sigma_1(\omega)$ exhibits a small peak around $\omega/\Delta \simeq 0.1 \sim 0.2$ which may describe a similar feature observed experimentally. Finally we discover that a dip in $\omega \sigma_2(\omega)$ at $\omega = 0$ is the universal feature of the unconventional superconductors, which has been overlooked until now.

Finally the present model will apply as well to the superconductivity in $Sr_2RuO_4$, if the superconductivity is one of 2D-f-wave states ($\Delta(k) \sim e^{\pm i\phi} \cos(2\phi)$, $e^{\pm i\phi} \sin(2\phi)$ without the vertex renormalization and $e^{\pm i\phi} \cos(k_z c)$) considered by Hasegawa et al. [22–25]. However, both anisotropy in the upper critical field in a planar magnetic field [26,27] and the magnetic thermal conductivity in a planar magnetic field [28,29] indicate extremely small angular depen-
dence (∼3%). Clearly these data show that $\Delta(k) \sim e^{\pm i\phi} \cos(2\phi)$ and $e^{\pm i\phi} \sin(2\phi)$ are incompatible with this observation. Therefore at this moment we are left with $\Delta(k) \sim e^{\pm i\phi} \cos(k_x c)$ as the only candidate. However this suggests a rather strong interlayer spin coupling, which is very puzzling.

We thank Dimitri Basov for useful discussion on the optical data of Zn-substituted YBCO and providing us with some of his unpublished data. We are benefited also from useful discussions with and help of Hyekyung Won. One of the authors (B. D.) gratefully acknowledges the hospitality at the University of Southern California, Los Angeles, where part of this work was done. This work was supported by the Hungarian National Research Fund under grant numbers OTKA T032162 and T029877, and by the Ministry of Education under grant number FKFP 0029/1999.

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