# Interference of superconducting and dielectric correlations in the IR spectra of high-temperature superconductors

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Features caused in the IR spectra of a system with dielectric and superconducting correlations by the quasiparticle state density might be mistaken as implying a nonstandard temperature dependence of the gap and an upper biased value of $2\Delta/T_c$.

Most of the experimental work on the optical properties of high-temperature superconductors has consisted of an attempt to determine the magnitude and temperature dependence of the energy gap $2\Delta$ from the IR reflection spectra. The value of the parameter $2\Delta/T_c$ has been found to be[1] $\approx 8$ for $YBa_2Cu_3O_{7-x}$ single crystals and $\approx 5$

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(Ref. 2) or 9.5 (Ref. 3) for 1–2–3 films. The values of $2\Delta/T_c$ for polycrystalline samples are lower by a factor of two or three; this result can be explained in terms of an effective averaging of an anisotropic gap in optical experiments carried out on ceramics.[2] The results found on the temperature dependence of the gap, $\Delta(T)$, have been contradictory, ranging from a BCS behavior[4] to a weak dependence[5] and even an independence of the gap from the temperature up to $T \sim T_c$ (Refs. 2 and 6).

The IR spectra of high-temperature superconductors were interpreted in Refs 1–3, 5, and 6 on the basis of Mattis and Bardeen's study,[7] itself based on the BCS model. For high-temperature superconductors, however, dielectric correlations are apparently important, leading to a charge density wave or a spin density wave in the nonsuperconducting phase. In Ref. 8, for example, the relatively high superconducting transition temperature $T_c = 12$ K in $BaPb_xBi_{1-x}O_3$ was linked with a charge density wave which was observed. These correlations are described either in the Hubbard model or in band models with a "nesting." Evidence in favor of the latter models comes from the experimental observation of a nesting in 1–2–3 samples.[9] Rusinov *et al.*[10] used a two-band model (to which a nesting model can be reduced) to analyze (1) a transition of a semimetal (the "regular" phase) into the phase of a degenerate semiconductor, accompanied by the appearance of a gap in the spectrum of the regular phase, as a manifestation of dielectric correlations and (2) a transition of the semiconductor into a high-temperature superconducting state as a result of intraband and interband Cooper pairing.

Our analysis of the IR spectra of the high-temperature superconductors is based on Ref. 10 for the case of singlet electron-hole (dielectric) and Cooper pairings. The phases of the superconducting order parameters of the different bands are equal (the *s* wave in a nesting model).[10] One might expect that in the case of a triplet dielectric pairing (a spin density wave), in which the superconducting order parameters of the different bands have different signs (the *d* wave in a nesting model), the results presented below would remain the same.

Figure 1 shows polarization diagrams describing the response of a system to an external electromagnetic field. Expressions for the Green's functions of the system were given in Ref. 10. The anomalous functions $F_{ij}$, where $i, j = 1,2$ are the band indices of the regular phase, arise from intraband ($i = j$) and interband ($i \neq j$) superconducting correlations. The functions $G_{ij}$ $(i \neq j)$ arise from dielectric correlations.

Figure 2 shows the spectrum of elementary excitations of the system. The branches shown by the dashed lines in Fig. 2 exist only in the superconducting phase. At points of extrema the state densities have root (one-dimensional) singularities,


FIG. 1. Polarization diagrams.

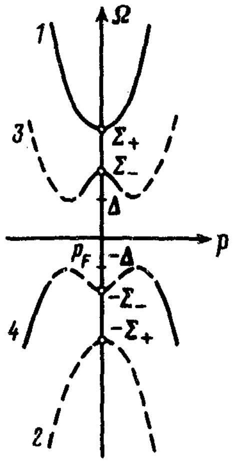


FIG. 2. Spectrum of elementary excitations. Ω—Energy of quasiparticles; $p$—momentum; $p_F$—Fermi momentum of the "regular" phase.

which appear with dielectric ($2\Sigma$) and superconducting ($2\Delta$) gaps. We call the corresponding singularities "dielectric" (at the points $\pm\Sigma_{\pm}$ in Fig. 2) and "superconducting" (at the points $\pm\Delta$) singularities. Frequencies corresponding to transitions between extrema of the branches may turn out to be critical in terms of a manifestation of the singularities of the state density in the IR absorption spectrum (we are dealing with the "dirty" limit; i.e., indirect transitions are also possible). In the case $T = 0$, for which we are carrying out this calculation, only the transitions from branches 2 and 4 to branches 1 and 3 contribute to the absorption.

The absorption of the system is determined not simply by a composite state density, as in the case of a direct optical transition, but by an integral over the energy of the product of the state densities of the corresponding branches and a matrix element or coherence factor, which requires a dependence on the integration variable because of the dielectric and superconducting correlations.

Here are expressions for the contributions $\mathrm{Im}\Pi_{kl}(\omega)$ from the transitions from the $k = 4$ branch to the $l = 3$ branch (Fig. 2) to the imaginary part of the polarization operator $\Pi(\omega)$ near the critical frequencies of the external field, $\omega$ (we are omitting nonsingular terms):

$$\mathrm{Im}\,\Pi_{43}(\omega) = -\frac{\pi(3\pi+2)}{8}\left(\frac{\omega}{2}-\Delta\right), \quad \frac{\omega}{2}-\Delta \ll \Delta \tag{1}$$

$$\mathrm{Im}\,\Pi_{43}(\omega) = \pi\int_{\Delta}^{\Sigma_-} \rho_+(\Omega)\rho_-(\omega-\Omega)\left(1-\frac{\Sigma^2}{(\mu-E(\Omega))(\mu+E(\omega-\Omega))}\right)$$

$$\times\left(1+\frac{E(\omega-\Omega)E(\Omega)-\Delta^2}{\Omega(\omega-\Omega)}\right)d\Omega, \qquad \omega=\Delta+\Sigma_- . \tag{2}$$

Here $\Sigma_{\pm} = \sqrt{(\mu\pm\Sigma)^2+\Delta^2}$; $E(\Omega) = \sqrt{\Omega^2-\Delta^2}$; $\mu$ is the shift of the Fermi level due to the doping; and the functions $\rho_{\pm}(\Omega)$, given by $\rho_{\pm}(\Omega)$

$= \Omega(E(\Omega) \mp \mu)/\sqrt{E(\Omega)((E(\Omega) \mp \mu)^2 - \Sigma^2)}$; represent the state densities which we have been discussing. Among the contributioins to $\mathrm{Im}\Pi_{kl}(\omega)$ not written out in (1) and (2), a term in $\mathrm{Im}(\Pi_{41}(\omega) + \Pi_{23}(\omega))$ at $\omega = \Sigma_- + \Sigma_+$ has a singularity. An expression for it can be found from (2) by replacing $\rho_-(\omega - \Omega)$ by $\rho_+(\omega - \Omega)$ and by replacing $E(\omega - \Omega)$ by $-E(\omega - \Omega)$ in the coherence factor.

In the derivation of (1) and (2) it was assumed that the relation $\Sigma > \Delta$ holds. In the limit $\Delta/\Sigma \to 0$ the singular part of $\mathrm{Im}(\Pi_{41}(\omega) + \Pi_{23}(\omega))$ vanishes, while contribution (2) loses its singularity but remains finite, describing an intraband absorption by free carriers of the nonsuperconducting phase. The term which describes the interband absorption in the latter phase in the limit $\Delta/\Sigma \to 0$ goes into the nonsingular part of $\mathrm{Im}(\Pi_{41}(\omega) + \Pi_{23}(\omega))$ and has not been written out here.

The quantity in (1), which corresponds to absorption near the threshold frequency $\omega = 2\Delta$, is small because of the suppression of a singularity of the state density by the coherence factor. In (2), the superconducting and dielectric singularities "interfere," intensifying each other at the upper integration limit, $\Omega = \Sigma_-$. The coherence factor remains finite, and the integrand diverges as $(\Sigma_- - \Omega)^{-1}$, leading to a discontinuity of the integral at the frequency $\omega = \Delta + \Sigma$. A corresponding discontinuity at $\omega = \Sigma_- + \Sigma_+$ occurs in the singular term in $\mathrm{Im}(\Pi_{41}(\omega) + \Pi_{23}(\omega))$, but here two dielectric singularities are interfering; one of them (at the point $-\Sigma$) exists only in the superconducting phase. In actuality, these discontinuities are manifested as maxima in the absorption spectrum, since the scattering blurs the singularity in the state density.

The reflection coefficient of this system, $R$, can be expressed in terms of the surface impedance $Z$ in the form $R = 1 - 4\,\mathrm{Re}\,Z$. The frequency dependence of the real part of the impedance of the superconductor is given in the dirty limit by[11]

$$\mathrm{Re}Z(\omega) \sim -(\omega/|\Pi(\omega)|)^{1/3} \sin(\arctan\,(\mathrm{Im}\Pi(\omega)/\mathrm{Re}\,\Pi(\omega))/3).$$

It can be seen from these expressions that the maxima at the critical frequencies in the absorption spectrum are also manifested as maxima in the reflection spectrum, at frequencies close to the corresponding critical frequencies. The effect is to shift the region $R_s/R_n > 1$ ($R_{s,n}$ are the reflection coefficients of the superconducting and normal phases, respectively) to a frequency region high in comparison with $2\Delta$. The size of the superconducting gap was estimated in Refs. 1–3, 5, and 6 on the basis of a certain characteristic point (e.g., a maximum[1–3]) of the dependence of $R_s/R_n$ in the frequency region with $R_s/R_n > 1$. When that method is used to analyze the spectra, the parameter $2\Delta/T_c$ may be substantially overestimated.

The dependence $\Delta(T)$ was found in Refs 2, 5, and 6 from the frequency shift of a characteristic point in the $R_s/R_n$ spectrum as the temperature was changed. In the limit $T \to T_c$ ($\Delta/\Sigma \to 0$) the singularities associated with the state density disappear from the spectrum, as we have already mentioned. As the temperature is raised from $T = 0$ to $T \sim T_c$, however, these maxima shift less along the frequency scale than the theshold $\omega = 2\Delta$ does, because of the terms $\mu \pm \Sigma$ in $\Sigma_\pm$, which are large in comparison with $\Delta$ and which vary only slightly in this temperature interval. This effect might be erroneously interpreted as a temperature dependence of the gap which is weak in comparison with the BCS temperature dependence.[2,5,6]

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