Interlayer optical conductivity of a superconducting bilayer

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We employ the Bardeen-Cooper-Schrieffer theory to calculate the frequency-dependent interlayer conductivity of a superconducting bilayer, the two layers of which are coupled by weak single-particle tunneling. The effect of the superconducting transition on the normal-state absorption band is to blue-shift and broaden it, while causing the peak absorption to be reduced and the line shape to become asymmetric.

In this paper we present a calculation of the interlayer optical conductivity of a superconducting bilayer in a cuprate superconductor such as $YBa_2Cu_3O_{7-\delta}$.[1] We assume that each layer of the bilayer is described by a Bardeen-Cooper-Schrieffer[2] (BCS) reduced Hamiltonian, and that the states of the layers are coupled by weak single-particle tunneling between the layers. This model implies, of course, that coupling to other bilayers is negligible. Anderson[3] has proposed that, due to strong electron correlation effects, coherent single-particle interlayer tunneling is blocked even though the bare interlayer hopping integral $t_\perp$ is finite [$t_\perp \sim 0.05$ eV (Ref. 4)]. In principle, this assertion of single-particle "confinement" can be tested experimentally by measurement of the frequency-dependent conductivity $\sigma_\perp(\omega)$ in the c-axis direction. The present calculation of $\sigma_\perp(\omega)$ for the bilayer establishes a simple benchmark for what should be the *conventional* behavior of this quantity as the temperature T is lowered through the mean-field superconducting transition temperature T_c of the bilayer. A recent experimental analysis of $\sigma_\perp(\omega)$ for $YBa_2Cu_3O_{7-\delta}$ has been undertaken by Homes *et al.*[5]

In the simple model we study $\mathrm{Re}\sigma_\perp(\omega)$ above T_c consists of a single absorption band due to electronic transitions between the "bonding" and "antibonding" states of the bilayer. The energies of these excitations are typically $\hbar\omega = 2t_\perp$. Below T_c, we find that the oscillator strength of the latter excitations is increasingly transferred to pair excitations with typical energies $\hbar\omega = 2\sqrt{t_\perp^2+\Delta^2}$, where Δ denotes the magnitude of the superconducting order parameter. At $T=0$, all of the oscillator strength has been transferred to the pair excitations. The main effect of the superconducting transition is therefore to blueshift the normal-state absorption band to higher frequencies. This effect, which also leads to a broadened and asymmetric line shape (and, hence, reduced peak absorption) in the superconducting state, would be observable if the dispersion in the value of $t_\perp$ due to the actual three-dimensional electronic structure of the cuprate is not too large by comparison to Δ.

We assume the bilayer to consist of two parallel monolayers each of area A ($A \to \infty$), labeled "a" and "b," and separated by a distance d in the c direction. We take the Hamiltonian H describing the bilayer to be

$$\begin{aligned} H = & \sum_{k,\sigma} (\epsilon_k - \mu)(a_{k\sigma}^\dagger a_{k\sigma} + b_{k\sigma}^\dagger b_{k\sigma}) \\ & - \sum_{k,\sigma} t_k (a_{k\sigma}^\dagger b_{k\sigma} + \mathrm{H.c.}) \\ & - (1/N) \sum_{k,k'} V_{k,k'} (a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger a_{-k'\downarrow} a_{k'\uparrow} \\ & + b_{k\uparrow}^\dagger b_{-k\downarrow}^\dagger b_{-k'\downarrow} b_{k'\uparrow}) . \end{aligned} \quad (1)$$

The first and third terms of H describe, respectively, the intralayer band energy and BCS pairing interactions of the isolated monolayers, while the second term specifies the coupling of the layers via a single-particle hopping matrix element t_k. $V_{k,k'}$ denotes the pairing matrix element, ϵ_k the energy of the Bloch state with two-dimensional wave vector k, and spin polarization σ ("$\uparrow$" or "$\downarrow$"). N ($N \to \infty$) denotes the number of unit cells in a monolayer while μ denotes the chemical potential of the bilayer. The fermion operators $a_{k\sigma}^\dagger$, $a_{k\sigma}$, $b_{k\sigma}^\dagger$, $b_{k\sigma}$ create and destroy electrons in the Bloch state of the layers a and b, respectively. The interlayer current implied by H is

$$J = (ed/i\hbar) \sum_{k,\sigma} t_k (a_{k\sigma}^\dagger b_{k\sigma} - b_{k\sigma}^\dagger a_{k\sigma}) , \quad (2)$$

where e denotes the electronic charge. $\mathrm{Re}\sigma_\perp(\omega)$ is conveniently obtained from the Kubo formula

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$$\mathrm{Re}\sigma_\perp(\omega)=\frac{1}{Ad}\frac{1-\exp(-\hbar\omega/k_BT)}{2\hbar\omega}\times\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle J(t)J(0)\rangle\,, \quad (3)$$

where k_B denotes Boltzmann's constant, $J(t)$ is the current operator at time t, and $\langle A\rangle$ denotes the ensemble average of the operator A. We shall assume that the interlayer tunneling constitutes only a weak coupling of the layers, i.e., $|t_k/\mu|\ll 1$. Then the main temperature dependence of μ is of second order in t_k and, consequently, we will neglect it. Moreover, $|t_k|$ will later be assumed small by comparison with the energy range within which the attraction of electrons occurs in Eq. (1) which is ω_D in conventional electron-phonon models.

The first two terms of H are immediately diagonalized by transformation to the bonding and antibonding states $\alpha_{k\sigma}=(1/\sqrt{2})(a_{k\sigma}+b_{k\sigma})$ and $\beta_{k\sigma}=(1/\sqrt{2})(a_{k\sigma}-b_{k\sigma})$. In terms of these states the Hamiltonian of the coupled bilayer becomes

$$H=\sum_{k,\sigma}\{(\xi_k-t_k)\alpha^\dagger_{k\sigma}\alpha_{k\sigma}+(\xi_k+t_k)\beta^\dagger_{k\sigma}\beta_{k\sigma}\}-(1/2N)\sum_{k,k'}V_{k,k'}(\alpha^\dagger_{k\uparrow}\alpha^\dagger_{-k\downarrow}+\beta^\dagger_{k\uparrow}\beta^\dagger_{-k\downarrow})\times(\alpha_{-k'\downarrow}\alpha_{k'\uparrow}+\beta_{-k'\downarrow}\beta_{k'\uparrow})+H'\,. \quad (4)$$

In Eq. (4) we have introduced notation $\xi_k=\epsilon_k-\mu$. H' contains terms of the form $\alpha^\dagger_{k\uparrow}\beta^\dagger_{-k\downarrow}$ and can be shown to be irrelevant for the minimum-free-energy state in the mean-field approximation. The rest of the Hamiltonian in Eq. (4) then describes the classic problem of two-band superconductivity,[6] the mean-field solution of which is as follows.

Corresponding to the bonding and antibonding bands of Eq. (4) there are two quasiparticle (QP) excitation bands. These have excitation energies

$$E_\alpha(k)=\sqrt{(\xi_k-t_k)^2+|\Delta_k|^2}\,,$$
$$E_\beta(k)=\sqrt{(\xi_k+t_k)^2+|\Delta_k|^2}\,,$$

where Δ_k is the superconducting order parameter of the *bilayer*. The latter is defined by

$$\Delta_k=(1/2N)\sum_{k'}V_{k,k'}\langle\alpha_{-k'\downarrow}\alpha_{k'\uparrow}+\beta_{-k'\downarrow}\beta_{k'\uparrow}\rangle$$

from which follows the gap equation

$$\Delta_k=(1/2N)\sum_{k'}V_{k,k'}\Delta_{k'}\left[\frac{\tanh[E_\alpha(k')/k_BT]}{2E_\alpha(k')}+\frac{\tanh[E_\beta(k')/k_BT]}{2E_\beta(k')}\right]. \quad (5)$$

We note that if $t_k\to 0$, Eq. (5) reduces to the BCS gap equation for the isolated monolayer.

In order to simplify our subsequent discussion of $\mathrm{Re}\sigma_\perp(\omega)$ we will take $V_{k,k'}=V$ and $t_k=t_0$, where V and t_0 are positive constants. However, we will later allow for the dispersion in t_k by averaging our result for $\sigma_\perp(\omega,t_0)$ over a Gaussian distribution of values of t_0. In this way we avoid tying our results to a specific model for the k dependence of t_k. The Gaussian distribution also may be regarded as including the additional dispersion in the electronic band structure which results from the weak electronic coupling (t_i) between bilayers. This is so because the effect of the latter is to cause the interband gap E_{ib} to depend weakly on the Bloch-state wave vector k_z in the c direction. (Explicitly, $E_{ib}=2[t_0^2+t_i^2+2t_0t_i\cos(k_zb)]^{1/2}$ where $t_i\ll t_0$ and b is the separation between bilayers.) With these simplifications it follows from Eqs. (2) and (3) that, in the normal state,

$$\mathrm{Re}\sigma_\perp(\omega,t_0)=[2\pi N_F(v_0e)^2/d]\delta(2t_0-\hbar\omega)\,, \quad (6)$$

where we have introduced $v_0=t_0d/\hbar$, and the Fermi surface density of states per unit area N_F of the isolated layer. In the superconducting state ($T<T_c$), however, Eqs. (2) and (3) lead to the result

$$\mathrm{Re}\sigma_\perp(\omega,t_0)=(2\pi v_0^2e^2/Ad\hbar\omega)\left[\sum_{\xi_k>0}A_k^2\delta[E_\beta(k)-E_\alpha(k)-\hbar\omega][f_\alpha(k)-f_\beta(k)]+\sum_{\xi_k<0}A_k^2\delta[E_\alpha(k)-E_\beta(k)-\hbar\omega][f_\beta(k)-f_\alpha(k)]+\sum_k B_k^2\delta[E_\alpha(k)+E_\beta(k)-\hbar\omega][1-f_\alpha(k)-f_\beta(k)]\right]. \quad (7)$$

Here, $f_i(k)=\{1+\exp[E_i(k)/k_BT]\}^{-1}$, where $i=\alpha,\beta$. A_k and B_k are the coherence factors:

$$A_k=u_\alpha(k)u_\beta(k)+v_\alpha(k)v_\beta(k)\,, \quad (8)$$

$$B_k=u_\beta(k)v_\alpha(k)-u_\alpha(k)v_\beta(k)\,, \quad (9)$$

in which $u_i^2=[1+\xi_i(k)/E_i(k)]/2$ and $v_i^2(k)=[1-\xi_i(k)/E_i(k)]/2$. In the latter we have introduced the quantities $\xi_i(k)=\xi_k-t_0$ for $i=\alpha$, and $\xi_i(k)=\xi_k+t_0$ for $i=\beta$.

The first two terms of Eq. (7) describe interband excitations of thermally excited QP's. The excitation energy is

$$\hbar\omega=|\sqrt{(\xi_k+t_0)^2+\Delta^2}-\sqrt{(\xi_k-t_0)^2+\Delta^2}|$$

so that $\hbar\omega$ lies in the range $0<\hbar\omega<2t_0$. On the other

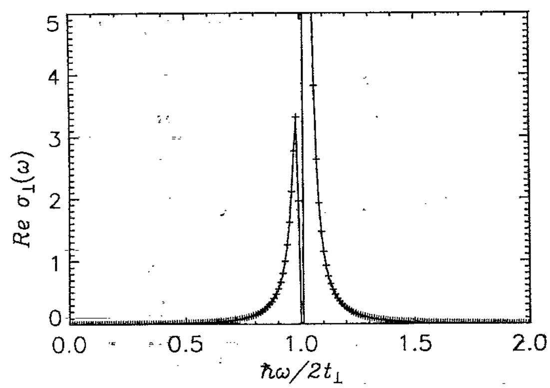

FIG. 1. Interlayer optical absorption (in arb. units) as a function of the reduced frequency for the nondispersive-t_k, Δ_k case. Here $\Delta/t_\perp=0.2$ and $T/t_\perp=0.2$.

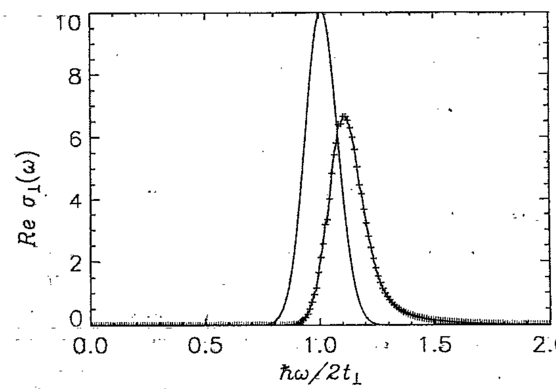

FIG. 2. Interlayer optical absorption as a function of the reduced frequency for the broadened t_0 case. Broadening parameter $w/t_\perp=0.1$. Compared are the absorption at $T=0$, $\Delta_0/t_\perp=0.4$ (the line marked with crosses) and the normal-state absorption.

hand, the third term of Eq. (7) describes pair excitations of energy

$$\hbar\omega=\sqrt{(\xi_k-t_0)^2+\Delta^2}+\sqrt{(\xi_k+t_0)^2+\Delta^2}\ .$$

The energies of these excitations begin at the threshold value $\hbar\omega_0=2\sqrt{t_0^2+\Delta^2}$, at which it may be shown from Eq. (7) $\mathrm{Re}\sigma_\perp(\omega,t_0)$ has a square-root singularity. At higher frequencies $\mathrm{Re}\sigma_\perp(\omega)$ falls off as ω^{-5}. We note that there is an energy gap equal to $2(\sqrt{t_0^2+\Delta^2}-t_0)$ between the spectra of the interband and pair excitations. As T is reduced, oscillator strength is increasingly transferred from the interband excitations to the pair excitations. A characteristic behavior of this two-band absorption at intermediate T for the ideal, nondispersive t_k and $\Delta_k=\Delta$ case is illustrated in Fig. 1.

In order to allow for the dispersion in the values of t_k we introduce a Gaussian distribution of t_0 values and calculate $\sigma_\perp(\omega)$ as

$$\sigma_\perp(\omega)\propto\int dt_0\sigma_\perp(\omega,t_0)\frac{1}{w}\exp\left[-\frac{(t_0-t_\perp)^2}{w^2}\right],$$

where w and $t_\perp$ are constants. This smears out the fine structure of $\sigma_\perp(\omega,t_0)$ below T_c and gives, of course, a finite width to the normal-state absorption band defined in Eq. (6). Figure 2 shows $\mathrm{Re}\sigma_\perp(\omega)$ calculated for $T\geq T_c$ and for $T=0$ for the parameter choices $\Delta_0=0.4t_\perp$ and $w=0.1t_\perp$, where Δ_0 is the value of Δ at $T=0$. The latter choice of w produces a total width for the normal-state absorption that is approximately equal to $t_\perp$ and hence of the order $2\Delta_0$. It is seen from Fig. 2 that for these parameter values the blueshift obtained in the superconducting state is still well resolved. We note that the transfer of the oscillator strength of the interband excitations of the normal state to the pair excitations of the superconducting state leads to the broadening of the line shape and, hence, decreased peak absorption in the superconducting state. In general, it leads also to a "right-shoulder-like" asymmetry of the absorption line. Of course, when the dispersion of t_k is very large by comparison to Δ_0 even these broad features become unresolvable.

In conclusion, it is interesting to note that the interlayer conductivity $\sigma_\perp(\omega)$, in principle, yields direct information on the superconducting gap. This is a consequence of the new combination of BCS coherence factors, defined in Eqs. (8) and (9), which are unique to the bilayer system. Experimentally,[5] the presence of a *distinct* interband absorption in $\sigma_\perp(\omega)$ in the normal state of $YBa_2Cu_3O_{7-\delta}$ is not observed, however, although a broad and approximately constant absorption representing a significant portion of the oscillator strength of $\mathrm{Re}\sigma_\perp(\omega)$ is. It is possible that this absorption is the sum of a rather wide interband absorption and a temperature-dependent Drude contribution. This is consistent with the measurements of $\sigma_\perp(\omega)$ at $T=10$ K ($T\ll T_c$),[5] which reveal the presence of a pseudogap in the absorption which, allowing for experimental error, may be placed in the range 200–300 cm^{-1}. This could mark the onset of the interband absorption or, as suggested by Homes *et al.*,[5] correspond to the pseudogap of a spin-gap phase[7,8] of a highly correlated two-dimensional (2D) metal. If the former interpretation is adopted it would appear that for $YBa_2Cu_3O_{7-\delta}$ the effective dispersion in t_0 is too large for the effect we have calculated to be observable.

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