Residual absorption at zero temperature in *d*-wave superconductors

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In a *d*-wave superconductor with elastic impurity scattering, not all the available optical spectral weight goes into the condensate at zero temperature, and this leads to residual absorption. We find that for a range of impurity parameters in the intermediate coupling regime between Born (weak) and unitary (strong) limit, significant oscillator strength remains which exhibits a cusplike behavior of the real part of the optical conductivity with upward curvature as a function of frequency, as well as a quasilinear temperature dependence of the superfluid density. The calculations offer an explanation of recent data on ortho-II $YBa_2Cu_3O_{6.5}$ which has been considered anomalous.

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I. INTRODUCTION

Recent measurements[1] of the microwave conductivity up to 21 GHz at low temperatures in single crystal oxygen ordered ortho-II $YBa_2Cu_3O_{6.5}$ (YBCO) have revealed that there remains significant absorption at $T=0$ in the superconducting state, while at the same time the inverse square of the penetration depth shows a linear in temperature behavior. In the regime where this happens, the real part of the optical conductivity $\sigma_1(\omega)$ shows an unusual characteristic upward curvature very different from a Drude-like form. Anomalous residual absorption has also been seen in the past in THz work on thin films of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) (Ref. 2) and in this case was interpreted as due to coupling to a collective mode, with the spectral weight of this mode tracking the temperature dependence of the superfluid density.

In a pure *d*-wave BCS superconductor all of the optical spectral weight will go into the condensate at $T=0$ providing a delta function to the real part of the conductivity at zero frequency. This follows from the Ferrell-Glover-Tinkham sum rule[3,4] which holds when the kinetic energy change between normal and superconducting state is negligible. When elastic impurity scattering is introduced into the system, this no longer holds. Some optical spectral weight will remain at finite frequency under the real part of the conductivity at $T=0$ and correspondingly, the superfluid density will be reduced below its pure limit value. At the same time, however, in the unitary (strong) limit of impurity scattering which is the most studied case so far, a switch from linear to quadratic behavior in temperature is expected for the penetration depth. In this work we consider the case when the impurity scattering strength falls in the intermediate regime between Born (weak) and unitary (strong) limit. We find that for a range of impurity parameters, i.e., concentration and strength of the potential measured in terms of the width of the electronic band, the residual, impurity induced absorption remains very significant, while at the same time the superfluid density obeys a quasilinear law over the entire low temperature range and, more importantly, $\sigma_1(\omega)$ shows anomalous behavior in agreement with the experimental observation in ortho-II YBCO.

II. FORMALISM

The general expression for the optical conductivity at temperature T and frequency ν is well known and has been given in many places.[5–9] It can be written as

$$\sigma(T,\nu)=-\frac{\Omega_p^2}{4\pi}\left\langle\left[-\int_0^\infty d\omega\tanh\left(\frac{\beta\omega}{2}\right)J_\theta(\omega,\nu)+\int_{-\nu}^\infty d\omega\tanh\left(\frac{\beta(\omega+\nu)}{2}\right)J_\theta(-\omega-\nu,\nu)\right]\right\rangle_\theta, \quad (1)$$

where Ω_p is the plasma frequency and the function $J_\theta(\omega,\nu)$ takes on the form

$$2J_\theta(\omega,\nu)=\frac{1}{E_1+E_2}[1-N(\theta,\omega)N(\theta,\omega+\nu)-P(\theta,\omega)P(\theta,\omega+\nu)]+\frac{1}{E_1^*-E_2}\times[1+N^*(\theta,\omega)N(\theta,\omega+\nu)+P^*(\theta,\omega)\times P(\theta,\omega+\nu)]. \quad (2)$$

In Eq. (1) $\beta=1/k_BT$, with k_B the Boltzmann factor and T the temperature. In Eq. (2)

$$E_1(\theta,\omega)=\sqrt{\tilde{\omega}^2(\omega+i0^+)-\tilde{\Delta}^2(\theta,\omega)},$$

$$E_2(\theta,\omega,\nu)=E_1(\theta,\omega+\nu),$$

and

$$N(\theta,\omega)=\frac{\tilde{\omega}(\omega+i0^+)}{E_1(\theta,\omega)},\quad P(\theta,\omega)=\frac{\tilde{\Delta}(\theta,\omega)}{E_1(\theta,\omega)}.$$

Here θ is the angle giving the direction of momentum on the Fermi surface in the two-dimensional CuO_2 Brillouin zone. In BCS the gap does not depend on frequency ω and has the form $\tilde{\Delta}(\theta,\omega)=\Delta(T)\cos(2\theta)$ with $\Delta(T)$ a temperature dependent amplitude. The angular bracket $\langle\cdots\rangle_\theta$ indicates an average over angle θ.

The renormalized frequencies $\tilde{\omega}(\omega)$ do not depend on angle but are changed because of the elastic impurity scattering which is the only scattering processes accounted for. The equation for $\tilde{\omega}(\omega+i0^+)$ in a *t*-matrix approximation is[6–10]

$$\tilde{\omega}(\omega+i0^+)=\omega+i\pi\Gamma^+\frac{\langle N(\theta,\omega)\rangle_\theta}{c^2+\langle N(\theta,\omega)\rangle_\theta^2}. \tag{3}$$

Γ^+ is proportional to the impurity concentration and $c=1/[2\pi N(0)V_{\rm imp}]$ with $N(0)$ the normal band density of states at the Fermi surface and $V_{\rm imp}$ the impurity potential. An important parameter is γ defined as $\mathrm{Im}\,\tilde{\omega}(\omega+i0^+)$ at $\omega=0$ which is shown in the bottom frame of Fig. 4. For small values of $V_{\rm imp}$, Born's approximation applies and $c\to\infty$ with $t^+=\Gamma^+/c^2$ and the impurity term in Eq. (3) becomes proportional to $\langle N(\theta,\omega)\rangle_\theta$, its real part is the superconducting state density of states $[N_s(\omega)]$, while for large values of $V_{\rm imp}$, $(c\to 0)$ it is inversely proportional to $\langle N(\theta,\omega)\rangle_\theta$ (unitary limit). Both Born and unitary limit are extreme and a finite c is more realistic. As $N(0)$ is roughly inversely proportional to the electronic band width (W), we have $V_{\rm imp}\simeq W/(2\pi c)$. For $c=0.2$ the corresponding $V_{\rm imp}$ is 1.3 times the band width.

III. RESULTS AND DISCUSSION

The quasiparticle density of states $N_s(\omega)$ for a *d*-wave superconductor in the case of a finite value of $c=0.2$ is shown in Fig. 1 (top frame). The gap amplitude was set at $24\sqrt{2}$ meV and the impurity parameter Γ^+ was varied from $\Gamma^+=0.01$ meV (solid), $\Gamma^+=0.05$ meV (dashed), $\Gamma^+=0.1$ meV (dotted), and $\Gamma^+=0.15$ meV (dash-dotted). Clearly, impurities affect most strongly the low energy region near $\omega=0$ up to, say, 10 meV. The pure limit, a straight line through the origin is approached as Γ^+ is reduced, but even for the smallest value of $\Gamma^+=0.01$ meV, changes in $N_s(\omega)$ persist up to $\omega\simeq 4$ meV. It is the behavior of $N_s(\omega)$ in the low-energy range which determines low-temperature properties such as the specific heat. The behavior found for a finite c could not be inferred from a knowledge of the unitary or Born limit. In the Born limit the deviation from linearity would only occur at an exponentially small value of ω. Results for the unitary limit are shown in the middle frame and are seen to be very different from the top frame. The energy dependence of the quasiparticle lifetime of Eq. (3) $\mathrm{Im}\,\tilde{\omega}(\omega+i0^+)$ is shown in the bottom frame of Fig. 1. For $c=0$, the scattering rate has its maximum at $\omega=0$ and then drops monotonically as ω increases. For the larger values of c shown here this is no longer the case. A maximum in scattering rate occurs around $\omega\lesssim 8$ meV which is much larger than its value at $\omega=0$ (denoted γ).

The real part of the optical conductivity for a *d*-wave BCS superconductor is shown in Fig. 2 in units of $\Omega_p^2/8\pi$. Five values of temperature are considered, namely $T=0$ K (short dotted line) $T=5$ K (solid), $T=10$ K (dashed), $T=15$ K (dotted), and $T=20$ K (dash-dotted). The *d*-wave gap amplitude was set at $24\sqrt{2}$ meV. The top frame applies to an intermediate scattering case with $\Gamma^+=0.01$ meV and $c=0.3$. The bottom frame is for comparison and shows unitary limit results $(c=0)$. The real part of the optical conductivity $\sigma_1(T,\omega)$ vs ω up to 1 meV is radically different in the two cases. For $c=0.3$ the finite T curves are concave up and drop rapidly with increasing ω and show a very narrow halfwidth in qualitative agreement with the experiments by Turner *et al.*[1] and Hosseini *et al.*[11] The concave upward nature of these curves is due to the energy dependence of the quasiparticle scattering rate obtained from Eq. (3). These curves all correspond to the temperature dominated regime $T\gg\gamma$ (see Fig. 4, bottom frame). Their half width is not related to the value of γ but rather to temperature which samples the important energy dependence in $\mathrm{Im}\,\tilde{\omega}(\omega+i0^+)$. The $T=0$ curve is impurity dominated and, consequently, shows a qualitatively different behavior. It cannot be obtained from an extrapolation to $T=0$ of the finite T curves shown. These conductivity curves are in qualitative agreement with the experimental findings.[1] In the unitary limit the curves show instead a concave downward behavior at small ω and a broad half-width. This can be traced to the fact that the zero frequency scattering rate γ, is a rapidly increasing function of decreasing c as is seen in the bottom frame of Fig. 4. For the unitary limit γ is greater than its normal state

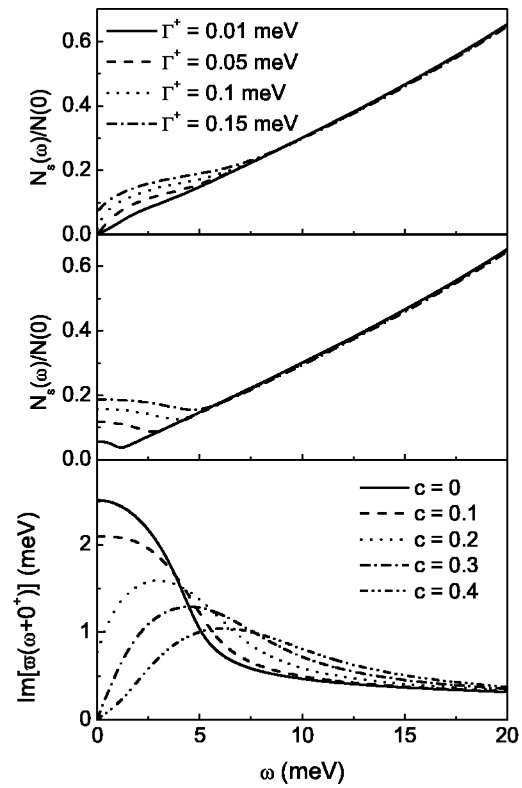

FIG. 1. The quasiparticle density of states $N_s(\omega)/N(0)$ vs ω, $\Delta_0=24\sqrt{2}$ meV. The top frame is for $c=0.2$, and the middle frame is for the unitary limit $c=0$. The bottom frame gives $\mathrm{Im}[\tilde{\omega}(\omega+0^+)]$ vs ω for $\Gamma^+=0.15$ meV and various values of c.

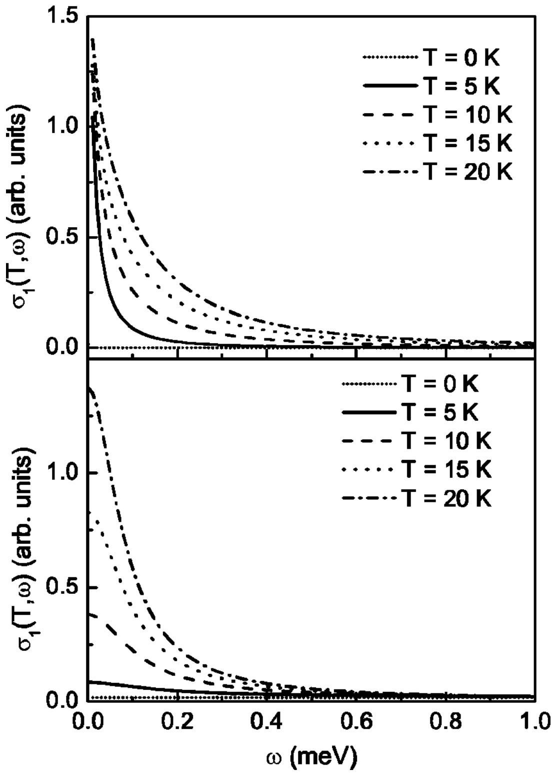

FIG. 2. The real part of the optical conductivity $\sigma_1(T,\omega)$ vs ω for five temperatures. The gap amplitude $\Delta_0 = 24\sqrt{2}$ meV and the impurity parameter $\Gamma^+ = 0.01$ meV. The top frame is for $c = 0.3$ and the bottom for $c = 0$. The computer units on the conductivity are such that a factor of $\Omega_p^2/8\pi$ needs to be applied.

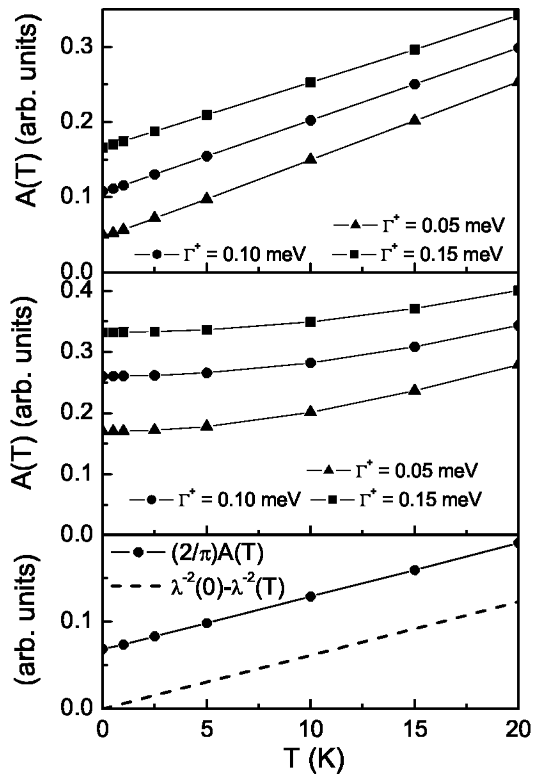

FIG. 3. Top frame: the remaining spectral weight $A(T) = \int_{0^+}^{\infty} d\omega\, \sigma_1(T,\omega)$ as a function of temperature T in the range 0 to 20 K for gap $\Delta_0 = 24\sqrt{2}$ meV. The impurity potential is characterized by $c = 0.3$ (to be compared with $c = 0$ for the unitary limit in the middle frame). The bottom frame compares $(2/\pi)A(T)$ with $\lambda^{-2}(0) - \lambda^{-2}(T)$ for the case $\Gamma^+ = 0.1$ meV and $c = 0.3$.

value $\pi\Gamma^+$ and is given by the well known relation $\gamma \simeq 0.63\sqrt{\pi\Delta_0\Gamma^+}$ while in the Born limit γ is exponentially dependent on Γ^+ [$\gamma(c\to\infty) = 4\Delta_0 \exp(-\Delta_0/2\Gamma_N)$ with $\Gamma_N = \Gamma^+/c^2$].

The quantity of interest is the total spectral weight remaining under the real part of the optical conductivity at temperature T, $A(T) = \int_{0^+}^{\infty} d\omega\, \sigma_1(T,\omega)$. Numerical results are presented in Fig. 3 which consists of three frames. The top frame is for $c = 0.3$ while the middle frame, included for comparison, is for the unitary limit. In both frames $\Delta_0 = 24\sqrt{2}$ meV and the temperature range considered is up to 20 K ($t = T/T_c \simeq 0.11$). The solid squares are for $\Gamma^+ = 0.15$ meV, solid circles $\Gamma^+ = 0.1$ meV, and solid triangles $\Gamma^+ = 0.05$ meV. The curves show a quasi linear temperature dependence over the entire temperature range considered. This is in sharp contrast to the results in the middle frame. The temperature dependence is now quadratic which is the behavior expected in the unitary limit. In the bottom frame we compare $A(T)$ vs T with the corresponding results for the penetration depth $\lambda^{-2}(0) - \lambda^{-2}(T)$ vs T. We see that the two curves are parallel and that the dotted curve goes through zero at the origin. This follows directly from the Ferrell-Glover-Tinkham sum rule which is satisfied to within our numerical accuracy. In our computer units the sum rule is

$$\lim_{\omega\to 0} \omega\sigma_2(T,\omega) + \frac{2}{\pi}\int_{0^+}^{\infty} d\omega\, \sigma_1(T,\omega) = 2, \qquad (4)$$

where σ_2 is the imaginary part of the conductivity. While we have not attempted a best fit to experiment, the results of the bottom frame of Fig. 3 are in qualitative agreement with the findings of Turner *et al.*[1]

Zero temperature values for $A(0)$ are shown in the top frame of Fig. 4. The lines are a guide to the eye through numerical results based on full conductivity calculations. The points are solid down triangles for $\Gamma^+ = 0.3$ meV, solid squares for $\Gamma^+ = 0.15$ meV, solid circles for $\Gamma^+ = 0.1$ meV, solid up-triangles for $\Gamma^+ = 0.05$ meV, and solid diamonds for $\Gamma^+ = 0.01$ meV. In all cases $A(0)$, which is entirely due to impurities, drops with increasing c. It is largest in the unitary limit but remains significant even when c has increased to 0.4 provided Γ^+ is not too small. In the bottom frame we show $\gamma(c)$ vs c, and stress that it becomes small more rapidly than does $A(0)$ as c increases; consequently, significant absorption can remain even with small γ. As can be seen in the top frame of Fig. 2, the value of $A(0)$, which gives the optical weight under $\sigma_1(\omega)$, samples importantly the quasiparticle scattering rate away from $\omega = 0$ and, thus, $A(0)$ is not directly related to $\gamma(c)$. There is much more absorption than would be indicated by the value of $\gamma(c)$ at the larger values of c considered here. This is emphasized by the solid gray line in the top frame of Fig. 4 which corresponds to the results of the approximate formula $A(0) \simeq (\gamma/\Delta_0)\ln(4\Delta_0/\gamma)$ obtained by approximating the

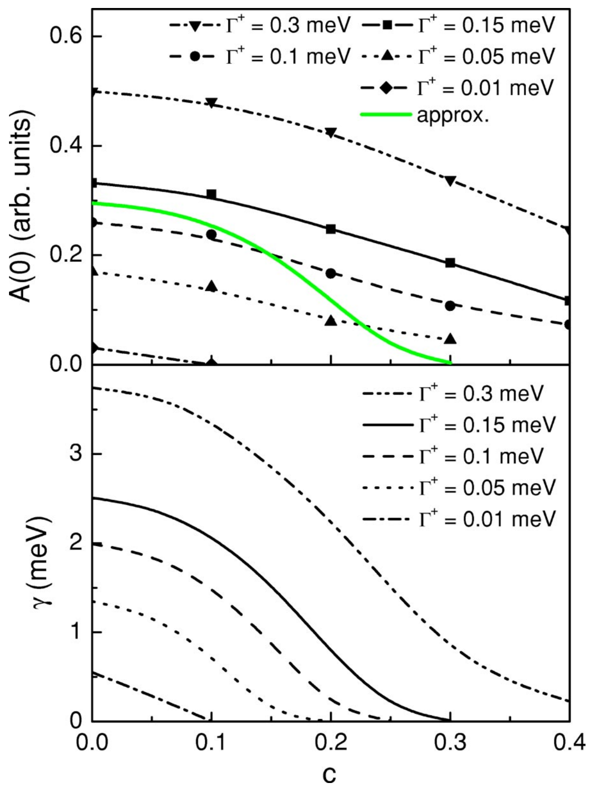

FIG. 4. Top frame: remaining spectral weight $A(0) = \int_{0^+}^{\infty} d\omega\, \sigma_1(0,\omega)$ as a function of the impurity potential strength c. The bottom frame gives the zero frequency value of the effective scattering in the superconducting state $\gamma(c)$ as a function of c. The solid gray line represents the results of the approximate formula for $\Gamma^+ = 0.15$ meV.

ω-dependent quasiparticle scattering rate in the exact expression by its $\omega=0$ value, i.e.: by $\gamma(c)$. Here $\Gamma^+ = 0.15$ meV. Comparison with the full results (solid squares) reveals that the agreement is reasonable for $c \leqslant 0.1$, i.e., the region for which the quasiparticle scattering rate has its maximum at $\omega=0$, but fails when its maximum falls instead at finite ω (see Fig. 1, bottom frame).

In their analysis of optical conductivity of thin films of Bi2212 Corson *et al.*[2] found a remaining spectral weight at $T=0$ of about 30% of the corresponding value of the superfluid density. In our language this corresponds to a value of $A(0) \gtrsim 0.5$. Corson *et al.*[2] also found that the remaining optical weight was distributed over a width of order 12 K independent of temperature. Reference to the theoretical curves in Fig. 4 shows that this value of $A(0)$ (top frame) is rather high for the observed value of the width $\sim\gamma$ (bottom frame); the data suggests $c \gtrsim 0.4$ and Γ^+ of the same order as was required[13] to fit the single crystal infrared optical data of Tu *et al.*[12] in Bi2212, $\Gamma^+ = 0.61$ meV. While Corson *et al.* interpret their data in terms of extra absorption due to a collective mode, part if not all is due instead to the impurity induced absorption discussed in this paper.

We mention the previous work on films of $YBa_2Cu_3O_{7-\delta}$ by Hensen *et al.*[14] in which the sizable surface resistance observed at low temperatures and attendant quasilinear temperature dependent superfluid density is seen to be consistent with d-wave and impurity scattering with a phase shift intermediate between Born and unitary limit. This work, however, is limited to the consideration of a single microwave frequency, namely, 87 GHz, and thus remains silent on the unusual frequency dependence of $\sigma_1(\omega)$ vs ω found also to be the characteristic of this regime in our theoretical work and in the experimental data of Turner *et al.*[1]

IV. CONCLUSION

For impurity scattering with a phase shift intermediate between 0 and $\pi/2$ we have found a regime in which considerable residual absorption can remain at zero temperature while at the same time the superfluid density is quasilinear in temperature. In addition, and more importantly, in this regime, the real part of the optical conductivity $\sigma_1(\omega)$ exhibits a distinctly non-Drude dependence on frequency in the microwave region. At low, but finite, temperatures $\sigma_1(\omega)$ vs ω has a cusplike dependence on ω out of $\omega=0$, followed by a rapid drop (concave upward curvature) as ω increases. The width at half maximum of $\sigma_1(\omega)$, which can be very small, varies strongly with temperature. This behavior is traced to the strong energy dependence of quasiparticle lifetime which is sampled in the temperature dominated regime discussed in this work. All aspects of this work are in good qualitative agreement with recent data in ortho-II $YBa_2Cu_3O_{6.5}$.

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