Singularities in the optical response of cuprates

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(Received 15 January 2001; published 19 April 2001)

We argue that the detailed analysis of the optical response in cuprate superconductors allows one to verify the magnetic scenario of superconductivity in cuprates. For strong coupling charge carriers to antiferromagnetic spin fluctuations, the second derivative of optical conductivity should contain detectable singularities at $2\Delta+\Delta_{\text{spin}}, 4\Delta, \text{and } 2\Delta+2\Delta_{\text{spin}}$, where $\Delta$ is the amplitude of the superconducting gap, and $\Delta_{\text{spin}}$ is the resonance energy of spin fluctuations measured in neutron scattering. We argue that there is a good chance that these singularities have already been detected in the experiments on optimally doped Y-Ba-Cu-O.

DOI: 10.1103/PhysRevB.63.180510

The pairing state in cuprate superconductors is predominantly made out of Cooper pairs with $d_{x^2-y^2}$ symmetry.1 This salient universal property of all high-$T_c$ materials entails constraints on the microscopic mechanism of superconductivity. However, it does not uniquely determine it, leading to a quest for experiments which can identify “fingerprints” of a specific microscopic mechanism of $d$-wave superconductivity, a strategy similar to the one used in conventional superconductors.2

Several recent experiments were interpreted as indirect evidence that $d_{x^2-y^2}$ pairing in cuprates is produced by an exchange of collective spin fluctuations peaked at or near antiferromagnetic momentum $Q=(\pi, \pi)$.3 In particular, the distance between the peak and the dip in the fermionic spectral function, $A_k(\omega)$, in angle-resolved photoemission spectroscopy (ARPES) experiments coincides with the frequency $\Delta_s$ of the resonance peak measured in neutron scattering.4,6 This is exactly what one should expect for fermions interacting with a resonating spin collective mode.6,6 (For phonon mediated superconductors, this is known as the Holstein effect.)7 Similarly, a peak-dip structure of the SINS tunneling conductance with peak-dip distance roughly consistent with $\Delta_s$ has been obtained in the measurements on break junctions by Zasadzinski et al. for various doping values.8 Carbotte et al.9 analyzed optical conductivity $\sigma(\omega)$ in magnetically mediated $d$-wave superconductors and argued that $\Delta_s$ can be extracted from the measurements of the second derivative of $\sigma(\omega)$.

In this paper we reexamine the behavior of the optical conductivity in superconductors with quasiparticles strongly coupled to their own collective spin modes. Our results partly agree and partly disagree with those by Carbotte et al.9 (see below). The key prediction of this paper is as follows: we argue that by measuring the conductivity, one cannot only verify the magnetic scenario, but, in principle, also independently determine both $\Delta_s$ and $\Delta$ in the same experiment.

Our argument goes as follows. For a superconductor, the real part of the conductivity, $\sigma_1(\omega)$, has a $\delta$-functional piece due to the presence of the superconducting condensate. A nonzero $\sigma_1(\omega)$ at a finite frequency is only possible if fermions have a finite lifetime. More precisely, one of the two fermions excited in the process causing the ac conductivity should have a finite scattering rate, while another should be able to propagate, i.e., its energy should be larger than $\Delta$. For clean, phonon-mediated superconductors, there are two sources for fermionic decay. One is a direct four-fermion interaction, which yields a threshold in the imaginary part of the self-energy, $\Sigma^i(\omega)$, at $\omega=\Delta$—the minimal energy necessary to pull all three fermions in the final state out of the condensate of Cooper pairs. Another is the interaction between an electron and an optical phonon. It yields the onset of $\Sigma^i(\omega)$ at $\omega=\Delta+\Omega_p$, where $\Omega_p$ is the frequency of an optical phonon7 (for simplicity, we assumed that the phonon propagator has a single pole). For the values of the coupling constant used to interpret the tunneling data in strongly coupled conventional superconductors like Pb,10 $\Omega_p>2\Delta$, i.e., the onset of conductivity is at $3\Delta+\Delta=4\Delta$ (2$\Delta$ for dirty superconductors11), while the signatures of phonon-assisted damping only show up at a higher $2\Delta+\Omega_p$ and also at $2(\Delta+\Omega_p)$, both fermions in the conductivity bubble acquire a finite $\Sigma''$.

For spin-mediated superconductivity, the situation is different. In the one-band model for cuprates, which we adopt, the underlying interaction is solely a Hubbard-type four-fermion interaction. Spin excitations appear as collective modes of fermions, and their velocity $v_s$ is comparable to $v_F$. For $v_s \sim v_F$, the low frequency spin dynamics is dominated by a decay process into a particle-hole pair and is purely relaxational in the normal state, with nearly featureless $\chi''(Q, \omega)$.6 (For phonon superconductors the relaxation is also present but is strongly reduced due to a smallness of the sound velocity compared to $v_F$.)

Below $T_c$, fermions acquire a gap, and a decay in a particle-hole pair becomes impossible for energies below $\Delta_s$. The direct four-fermion interaction then yields a threshold in $\Sigma''$ at $3\Delta$ which gives rise to a singularity in the conductivity at $\omega=4\Delta$.12 If $\chi''(Q, \omega)$ remained strictly zero below $\Delta$, this would be the only effect. However, several authors have demonstrated that the residual attraction in a $d$-wave superconductor binds a particle and a hole into a spin exciton at an energy $\Delta_s<2\Delta$. This effect gives rise to a peak in $\chi''(Q, \omega)$ at $\omega=\Delta_s$ and makes it look like the spectral function for optical phonons. Accordingly, the conductivity acquires another threshold at $2\Delta+\Delta_s$. Formally, this is analogous to the phonon case, but in distinction to phonons, $\Delta_s<2\Delta$. Then $2\Delta+\Delta_s<4\Delta$, i.e., in clean systems, the

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the singularities in \( s \)-wave superconductivity, the optical conductivity is given by

\[
\sigma_{s}(\omega) = \text{Re} \left\{ \frac{1}{\omega + i \delta} \right\} \int d\theta \Pi_s(\theta, \omega),
\]

where \( \Pi_s(\theta, \omega) \) is the fully renormalized current-current correlator. In Matsubara frequencies, it is given by

\[
\Pi_s(\omega_n) = \frac{1}{\beta} \sum_m \int \frac{d^3k}{(2\pi)^3} \left[ G_k(i\omega_n + i\omega_m)G_k(i\omega_m) + F_k(i\omega_n + i\omega_m)F_k(i\omega_m) \right],
\]

and the normal and anomalous Green’s functions are

\[
G_k(\omega_m) = \frac{\Sigma_k(\omega_m) + \varepsilon_k}{\Sigma_k^2(\omega_m) - \Phi_k^2(\omega_m) - \varepsilon_k^2},
\]

\[
F_k(\omega_m) = \frac{\Phi_k(\omega_m)}{\Sigma_k^2(\omega_m) - \Phi_k^2(\omega_m) - \varepsilon_k^2},
\]

\[
\Pi_s(i\omega_n) \propto \int d\omega_m d\theta \frac{\Sigma_n + \Phi_n \Phi_{\pm} + D_n D_{\pm}}{D_n D_{\pm} + D_{\mp}},
\]

[we adsorbed a bare \( i\omega_n \) term into \( \Sigma_n(i\omega_m) \).]

As an input for the computation of \( \Pi_s \), we need the forms of the fermionic self-energy \( \Sigma_k(i\omega_m) \) and the anomalous vertex \( \Phi_k(i\omega_m) \). We obtained these forms in Ref. 16 by deriving and solving a set of Eliashberg equations within the spin-fermion model. This model adequately describes the interaction between low-energy fermions and their collective spin degrees of freedom, at energies smaller than \( E_F \).

The full dynamical spin susceptibility peaked at (or near) \( Q \) mediates \( d_{x^2-y^2} \) superconductivity. As discussed, this susceptibility is by itself affected by low-energy fermions via a decay process into a particle and a hole, and has to be computed together with the fermionic self-energy and the pairing vertex.

The justification of the Eliashberg approach for the spin-mediated superconductivity was discussed earlier by Carbotte and our group, and we just quote the result: at strong dimensionless spin-fermion coupling \( \lambda \), vertex corrections and \( v_F^{-1} d\Sigma/dk \), where \( k \) is the component of the momentum transverse to the Fermi surface, are small compared to \( d\Sigma/d\omega \) by log \( \lambda \). In what follows we will neglect these corrections, i.e., approximate \( \Sigma_k(i\omega_n) \) and \( \Phi_k(i\omega_m) \) by \( \Sigma_k(i\omega_n, \theta) = \Sigma(i\omega_n, \theta) \) and \( \Phi(i\omega_n, \theta) \). This approximation also allows one to neglect vertex correction to the conductivity bubble as the latter are obviously related to \( d\Sigma/dk \).

As our goal is to study the singularities in \( \sigma_s(\omega) \), we first perform calculations assuming that \( \Sigma \) and \( \Phi \) are independent on \( \theta \) (i.e., that the superconducting gap is flat near the hot spots), and then analyze the results for a true \( d \)-wave gap. For a flat gap, the momentum integration in Eq. (2) is straightforward. Substituting \( k \) integration by integration over \( \varepsilon_k \), and performing it, we obtain at \( T = 0 \) and \( \omega \neq 0 \),

\[
\Pi_s(i\omega_n) \propto \int d\omega_m d\theta \frac{\Sigma_n + \Phi_n \Phi_{\pm} + D_n D_{\pm}}{D_n D_{\pm} + D_{\mp}}.
\]

Here, \( \Sigma_n = \Sigma(i\omega_n, \theta) \), \( \Phi_n = \Phi(i\omega_n, \theta) \), and \( D_n = (\Phi_n^2 - \Sigma_n^2)^{1/2} \), where \( \omega \pm = \omega' \pm \omega/2 \). The conductivity is obtained by converting this expression to the real axis. The singular piece in \( \sigma_s(\omega) \) near \( 2\Delta + \Delta_s \) can be obtained without a precise knowledge of \( \Sigma(\omega) \) and \( \Phi(\omega) \): the only information we need is that in a \( d \)-wave superconductor, \( \chi^v(\Phi, \omega) \) has a \( \delta \)-functional singularity at \( \omega = \Delta_s \). This is what we found solving a set of three Eliashberg equations. Using this as an input and applying a spectral representation for \( \Sigma_n^v \) and \( \Phi_n^v \), we obtain that \( \Sigma_n^v(\omega) \) and \( \Phi_n^v(\omega) \) are zero up to \( \omega = \Delta + \Delta_s \), and undergo finite jumps at this frequency. By Kramers-Kronig relation, \( \Sigma^v \) and \( \Phi^v \) diverge as \( |\log(\omega - \omega_0)| \) where \( \omega_0 = \Delta + \Delta_s \). The prefactor is the same for \( \Sigma^v \) and \( \Phi^v \). Substituting these forms of \( \Sigma(\omega) \) and \( \Phi(\omega) \) into Eq. (2), we obtain after simple algebra that the conductivity emerges above \( 2\Delta + \Delta_s \) as \( e^{1/2} \log^2 \varepsilon \), where \( \varepsilon = \omega - (2\Delta + \Delta_s) \). This singularity obviously causes a divergence in the derivatives of the conductivity at \( \varepsilon = 0 \).
In Fig. 1(a) we show the result for the conductivity obtained by numerically solving Eq. (2) using $\Sigma(\omega)$ and $\Phi(\omega)$ from Ref. 16. We clearly see the expected threshold at $2\Delta + \Delta_s$. The inset shows the behavior of the relaxation rate $1/\tau(\omega) = (\omega^2/4\pi) \Re \{1/\sigma(\omega)\}$ where $\omega_m$ is the plasma frequency. Observe that $1/\tau(\omega)$ is linear in $\omega$ over a rather wide frequency range. This agrees with the earlier study of the normal state conductivity.\(^{18}\)

We next demonstrate that the position of the singularity is not affected by the angular dependence of the gap. Indeed, let the maximum value of the gap correspond to $\theta = 0$ and symmetry related points. At deviations from $\theta = 0$, both $\Delta$ and $\Delta_s$ decrease. The decrease of $\Delta$ is obvious, the decrease of $\Delta_s$ is due to the fact that resonance is a feedback from superconductivity, and its frequency scales as $(\Delta(\theta))^{1/2}$. Since both $\Delta$ and $\Delta_s$ are maximal at a hot spot, we can expand $\omega_0(\theta) = \Delta(\theta) + \Delta_s(\theta)$ as $\omega_0(\theta) = \omega_0 - \alpha \theta^2$, where $\alpha > 0$. The singular pieces in $\Sigma(\omega)$ and $\Phi(\omega)$ then behave as $[\log(\omega_0 - \omega - \alpha \theta^2)]$. Substituting these forms into Eq. (2) and integrating over $\theta$, we find that the conductivity itself and its first derivative are continuous at $\omega = 2\Delta + \Delta_s$, but the second derivative of the conductivity diverges as $d^2\sigma/d\omega^2 \propto 1/[e \log^2 e]$ where, we remind, $e = \omega - (2\Delta + \Delta_s)$. We see that the singularity is weakened by the angular dependence of the gap, but it is still located at exactly $2\Delta + \Delta_s$.

The same reasoning is also applied to a region near $4\Delta$. We found that the singularity at $4\Delta$ is also weakened by the angular dependence of the gap, but is not shifted and still should show up in the second derivative of the conductivity.

We now discuss the second derivative of the conductivity in more detail. In Fig. 2 we present our numerical results for $W(\omega) = d^2/d\omega^2 \omega \Re \{1/\sigma(\omega)\}$ [we followed Ref. 9 and used the same $W(\omega)$ as for phonon superconductors]. We clearly see that there is a sharp maximum in $W(\omega)$ near $2\Delta + \Delta_s$ followed by a deep minimum. We also see that $W(\omega)$ has extra extrema at $4\Delta$ and at $2\omega_0 = 2\Delta + 2\Delta_s$.

The experimental result for $W(\omega)$ in Y-Ba-Cu-O is shown in the inset. We see that the theoretical and experimental plots of $W(\omega)$ look rather similar, and the relative intensities of the peaks are at least qualitatively consistent with the theory. By the reasons which we display below, we identify $2\Delta + \Delta_s$ with the deep minimum in $W(\omega)$. This yields $2\Delta + \Delta_s \approx 100$ meV. Identifying the extra extrema in the experimental $W(\omega)$ with $4\Delta$ and $2\Delta + 2\Delta_s$, respectively, we obtain $4\Delta \approx 130$ meV, and $2\Delta + 2\Delta_s \approx 150$ meV. We see that three sets of data are self-consistent and yield $\Delta \approx 30$ meV and $\Delta \approx 40$–45 meV. The value of $\Delta$ is in good agreement with tunneling measurements,\(^{20}\) and $\Delta_s$ agrees well with the resonance frequency extracted from neutron measurements.\(^{21}\) We caution, however, that determination of a second derivative of a measured quantity is a very subtle procedure. The good agreement between our theory and the experiment is promising but has to be verified in further experimental studies. Nevertheless, our calculation...
clearly demonstrates the presence and observability of the “higher harmonics” of the optical response at $4\Delta$ and $2\Delta + 2\Delta_f$.

So far we have considered only the singular part of $\sigma_1(\omega)$. In Fig. 1(b) we compare our results for $\sigma_1(\omega)$ (ignoring the contributions from the nodes) directly with the experimental data by Puchkov et al.\textsuperscript{19} for optimally doped YBa$_2$Cu$_3$O$_{6+\delta}$. We used $\hbar\omega_c = 1.6 \times 10^4$ cm$^{-1}$, similar to that in Ref. 19, $\lambda = 1$ and the overall energy scale $\hbar\omega$ $\sim$ 150 meV which yields $\Delta \sim 30$ meV and $\Delta_f \sim 45$ meV as the solution of the Eliashberg set. As in earlier studies\textsuperscript{14,18} we had to add a small constant $6 \times 10^{-4}$ Ω cm to $(\sigma_1(\omega))^{-1}$ to match the magnitude of the conductivity. We see that the frequency dependence of the conductivity at high frequencies agrees well with the data. The measured conductivity drops at about 100 meV in rough agreement with $2\Delta + \Delta_f \approx 100$ meV in our theory. We view the good agreement between theory and experiment at $\hbar\omega > 2\Delta + \Delta_f$, as predominately an indication that the momentum dependence of the fermionic dynamics becomes irrelevant at high frequencies, and fermions from all over the Fermi surface behave as if they were at hot spots. The inset of Fig. 1(b) shows $\sigma_1^{-1}(\omega)$. We see that it is linear above 1000 cm$^{-1}$. This is consistent with the linear frequency behavior of the fermionic self-energy. Surprisingly, the linear behavior (both in theory and in the data) extends up to larger frequencies, where theoretical $\Sigma^-$ curves to $\sqrt{\omega}$ behavior. At frequencies of about 1 eV, our theory is clearly inapplicable and the agreement with the data is most likely accidental.

Finally, we comment on the position of the $2\Delta + \Delta_f$ peak and compare our results with those by Carbotte et al.\textsuperscript{9} Theoretically, at $T = 0$ and in clean limit, the maximum and minimum in $W(\omega)$ are at the same frequency. We found, however, that at finite $T$, they quickly move apart (see Fig. 2).

Carbotte et al.\textsuperscript{9} focused on the maximum in $W(\omega)$ and argued that it is located at $\Delta + \Delta_f$ instead of $2\Delta + \Delta_f$. We also found that the maximum in $W(\omega)$ shifts to a lower frequency with increasing temperature, already at $T$ where the temperature dependence of the gap may be neglected. On the other hand, the minimum in $W(\omega)$ moves very little with increasing $T$ and virtually remains at the same frequency as at $T = 0$. This is our reasoning to use the minimum in $W(\omega)$ as a much more reliable feature for the comparison with experiments. This reasoning is in agreement with recent conductivity data on optimally doped Bi2212 (Ref. 22) — $W(\omega)$ extracted from these data shows strong downturn variation of the maximum in $W(\omega)$ with increasing temperature, but the minimum in $W(\omega)$ is located at around 110 meV for all temperatures.

To conclude, in this paper we examined the singularities in the optical conductivity in $d$-wave superconductors assuming that the pairing is mediated by overdamped spin fluctuations. We argued that $\sigma_1(\omega)$ should have singularities at $2\Delta + \Delta_f$, $4\Delta$ and $2\Delta + 2\Delta_f$, where $\Delta$ is the maximum value of the $d$-wave gap, and $\Delta_f < 2\Delta$ is the resonance spin frequency. The experimental detection of these singularities would be a strong argument in favor of the magnetic scenario. We argued that there is a good possibility that all three singularities have actually been detected in recent data on Y-Ba-Cu-O.

It is our pleasure to thank D. N. Basov, G. Blumberg, J. C. Campuzano, J. Carbotte, P. Coleman, O. Dolgov, P. Johnson, M. Norman, D. Pines, E. Schachinger, S. Shulga, and J. Zasadzinski for useful conversations. We are also thankful to D. N. Basov, C. Homes, M. Strongin, and J. Tu for sharing unpublished results with us. The research was supported by NSF DMR-9979749 (A.A. and A.Ch.) and by U.S. DoE W-7405-Eng-82 (J.S.).


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