Coupling strength of charge carriers to spin fluctuations in high-temperature superconductors

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In conventional superconductors, the most direct evidence of the mechanism responsible for superconductivity comes from tunnelling experiments in which a clear image of the electron-phonon interaction is revealed. The observed structure in the current voltage characteristics at the phonon energies can be used to measure, through inversion of the Eliashberg equations, the electron phonon spectral density $\alpha^2 F(\omega)$. The coherence length in conventional materials is long and the tunnelling process probes several atomic layers into the bulk of the superconductor. On the contrary, in the high $T_c$ oxides, particularly for c-axis tunneling, the coherence length can be quite short and in an optical experiment or in neutron scattering experiments the bulk of the sample is probed. Therefore, these spectroscopies become the methods of choice for the investigation of mechanisms of high-$T_c$ superconductivity. Accurate reflectance measurements in the infrared range and precise polarized neutron scattering data are available for a variety of oxides.

In this paper we show that conducting carriers studied by means of infrared spectroscopy reveal strong coupling to a resonance structure in the spectrum of spin fluctuations examined with neutron scattering. The coupling strength inferred from experiment is sufficient to account for high values of $T_c$ which signals the prominent role of spin excitations in the superconductivity of oxides.

There have been many suggestions as to the mechanism involved in the superconductivity of the oxides. While, so far, no consensus has yet emerged, the state itself is widely accepted to have $d$-wave symmetry with the gap on the Fermi surface vanishing along the main diagonals of the two-dimensional Brillouin zone. In YBCO there also exists extensive spin polarized inelastic neutron scattering data. These experiments reveal that spin excitations persist on a large energy scale over several 100 meV, but are mainly confined around the $(\pi, \pi)$-point in momentum space. Also, in the superconducting state, a new peak emerges out of, or is additional to, the spin excitation background which is often referred to as the 41 meV resonance (Fig. 1). This peak has received much attention but its origin remains uncertain.

In one view, it is due to a readjustment in the spin excitation spectrum due to the onset of superconductivity. Such a readjustment of spectral weight with a reduction below twice the superconducting gap value $\Delta_s$ is expected on general ground and is generic to electronic mechanisms. A second view is that it is a resonance in the $SO(5)$ unification of magnetism and superconductivity.

If the spin excitations are strongly coupled to the charge carriers they should be seen in optical experiments. The normal state optical conductivity $\sigma(\omega)$ as a function of frequency (\omega) depends on the electron self energy $\Sigma(\omega)$ which describes the effect of interactions on electron motion. In an electron-phonon system the electron-phonon interaction spectral density, $\alpha^2 F(\omega)$, is approximately but not exactly equal to $W(\omega)$, a second derivative of the inverse of the normal state optical conductivity

$$\alpha^2 F(\omega) \approx W(\omega) = \frac{1}{2\pi} \frac{d^2}{d\omega^2} \left[ \omega \Re \left( \frac{1}{\sigma(\omega)} \right) \right].$$

In the phonon energy range, the correspondence is remarkably close and determines $\alpha^2 F(\omega)$ with good accuracy. At higher energies, additional, largely negative wiggles come into $W(\omega)$ which can simply be ignored as they are not part of $\alpha^2 F(\omega)$. Note that (1) is dimensionless and so determines the absolute scale of the electron-phonon interaction spectral density as well as its shape in frequency. This fact is important as it allowed Marsiglio et al. to determine the $\alpha^2 F(\omega)$ of K$_x$C$_60$ from its optical conductivity by inversion (2) and to conclude from a solution of the Eliashberg equations that it is large enough to explain the observed value of critical temperature.

$(T_c$ is related to the mass enhancement factor $\lambda$, twice the first inverse moment of $\alpha^2 F(\omega)$). The formalism for the normal state conductivity can also be applied to spin excitations. If we ignore anisotropy as a first approximation, we can proceed by introducing an electron-spin excitation spectral density denoted by $T^2 \chi(\omega)$ with its scale set by the coupling strength to the charge carriers, $T^2$, and $\chi(\omega)$ the imaginary part of the spin susceptibility measured in spin
polarized inelastic neutron scattering experiments averaged over all momentum in the Brillouin zone. At low temperatures \( \chi(\omega) \) contains the 41 meV resonance observed in the superconducting state. To illustrate our main point we will use here \( \chi(\omega) \) directly from experimental results on a YBa\(_2\)Cu\(_3\)O\(_{6.92}\) sample with \( T_c = 91 \) K, near optimum doping and for which results exist at the temperatures \( T = 100 \) K and \( T = 5 \) K.]\(^{13}\) both properly calibrated in units of \( \mu_B^2/\text{eV} \) (\( \mu_B \) is the Bohm magneton) as shown in Fig. 1. We multiply \( \chi(\omega) \) at \( T = 100 \) K by a constant coupling \( I^2 \) fixed to get \( T_c = 100 \) K.\(^{13}\) The mass enhancement factor \( \lambda \) (twice the first inverse moment of \( I^2\chi(\omega) \) obtained is 2.6 and is, to within 10 percent, the same as obtained from the \( W(\omega) \) derived from the normal state experimental data of Basov et al.\(^{14}\) in YBa\(_2\)Cu\(_3\)O\(_{6.95}\) and from our calculated \( W(\omega) \) at \( T_c \). In a preliminary attempt to invert Collins et al.\(^{14}\) found a \( \lambda \) of three which is greater than our value. Their twinned crystals exhibited a higher optical scattering rate than our untwinned crystal and consequently they obtained about 50% more weight in the main peak of \( I^2\chi(\omega) \) around 30 meV.

In order to access lower temperatures, we need to understand how the \( I^2\chi(\omega) \) structure enters the superconducting state optical conductivity. To this end, we have done a series of calculations of the superconducting state \( \sigma(\omega) \) for a d-wave superconductor including inelastic scattering. Details have been presented in the work of Schachinger et al.\(^{15}\). We used their prescription to calculate the theoretical \( \sigma(\omega) \) using the neutron data taken for YBa\(_2\)Cu\(_3\)O\(_{6.92}\) (at 5 K) as \( \chi(\omega) \) multiplied by the same value of the coupling strength \( I^2 \) previously determined to obtain a \( T_c \) of 100 K from the normal state neutron data. We then inverted this theoretical \( \sigma(\omega) \) data using Eq. 4. The result of this inversion is compared in the top frame of Fig. 2 (solid line) with our input spectral density \( I^2\chi(\omega) \) (solid triangles) shifted in energy by the gap \( \Delta_0 = 27 \) meV of our theoretical calculations.\(^{13}\)

The absolute scale of \( I^2\chi(\omega) \) in the resonance region is well given by the peak value in the solid curve. This peak is followed by negative wiggles which are not in the original input spectrum because \( W(\omega + \Delta_0) \) is not exactly \( I^2\chi(\omega) \). Nevertheless, such a procedure allows us to see quite directly by spectroscopic means some of the features of \( I^2\chi(\omega) \) and, more importantly gives us information on its absolute value at maximum. The long tails in \( I^2\chi(\omega) \) at higher energy extending well beyond the resonance are not resolved in \( W(\omega) \) but cause \( \tau^{-1}(\omega) \), defined as \( \text{Re} \{ \sigma^{-1}(\omega) \} \), to rise in a quasi linear fashion at high frequencies\(^{13}\) in both normal and superconducting state, as is observed. This quasilinear rise was the motivation for the marginal Fermi liquid mode\(^{13}\) which gives \( \tau^{-1}(\omega) \propto \omega \) and a constant spectral density for \( \omega > T \) extending to high energies. If we approximate the normal state experimental \( \tau^{-1}(\omega) \) data\(^{13}\) at \( T_c \) by a straight line for \( 0 \leq \omega \leq 200 \) meV, we get 0.3 as the weight of the spectral density for all frequencies \( \omega > T \) and a \( \lambda \) of 2.8 quite consistent with our previous estimates. It is important to realize that, in as much as the 41 meV resonance is near \( 2\Delta_0 \), the density of quasiparticle states (not shown here), has structure at \( 3\Delta_0 \) in our calculations, a well established feature of tunnelling data particularly in Bi2212.\(^{13}\)

In the bottom frame of Fig. 2, we show experimental
results obtained from the data by Basov et al. on application of the prescription [1] to a-axis conductivity data on an untwinned single crystal. The 41 meV resonance is clearly resolved as a peak at approximately 69 meV in the solid curve (the gap is 27 meV). The height of this peak is about 3 and gives an absolute measure of the coupling between charge carriers and spin excitations. On comparison with the top frame of Fig. 2 we see that the coupling to the 41 meV resonance is larger in the experiment than the value assumed in the calculations that generated the theoretical results of that frame. This is not surprising since we have used the spin polarized inelastic neutron scattering data set measured on a near optimum 91 K sample of YBa$_2$Cu$_3$O$_{6.92}$ while the neutron results for slightly overdoped YBCO are very different although the $T_c$ value is hardly affected. This large dependence of $\chi(\omega)$ on the sample can be used to argue against their role in establishing $T_c$. However, the function that controls the conductivity is a complicated weighting of the spin susceptibility involving details of the Fermi surface and points in the Brillouin zone away from ($\pi$, $\pi$) as well as the coupling to the charge carriers. Thus, the correspondence between $I^2\chi(\omega)$ and $\chi(\omega)$ is complicated. What optical experiments reveal is that $I^2\chi(\omega)$ is not as strongly dependent on doping as is $\chi(\omega)$.

In Fig. 2, bottom frame, we present experimental results for $W(\omega)$ in underdoped, untwinned YBa$_2$Cu$_3$O$_{6.6}$ (dashed line) and compare with the optimally doped case (solid line). It is interesting to note that the peak in the underdoped case is slightly reduced in height reflecting a reduction in $T_c$. It is also shifted to lower energies. Some experiments [10, 11] indicate a reduction in gap value with underdoping in YBCO while many experiments show an important increase in Bi2212 [12]. Even if the gap is assumed to stay the same at 27 meV, the spin polarized neutron resonant frequency is known to decrease with doping [13]. Accounting for this gives almost exactly the downward shift observed in our experimental data of Fig. 2 (bottom frame).

Very recently, inelastic neutron scattering data in Bi2212 [14] have been published. They show a resonance peak at 43 meV in the superconducting state and establish a similarity with the earlier results in YBCO. We have inverted the optical data of Puchkov et al. [15] in this case and find that coupling at low temperatures to the observed superconducting state spin resonance peak is a general phenomena in both YBCO and Bi2212.

Spin excitations are seen in an appropriately chosen second derivative of the superconducting state optical conductivity and the strength of their coupling to the charge carriers determined from such data. The coupling to the excitations including the 41 meV resonance is large enough in YBCO that it can account for superconductivity at that temperature. At $T_c$ the spectrum obtained from experiments gives a value of the mass enhancement parameter $\lambda$ which is close to the value used in our model calculations to obtain a critical temperature of 100 K.

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