Magnetic resonance at $41\,\mathrm{meV}$ and charge dynamics in $\mathrm{YBa_2Cu_3O_{6.95}}$

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Abstract. – We report an Eliashberg analysis of the electron dynamics in $\mathrm{YBa_2Cu_3O_{6.95}}$. The magnetic resonance at 41 meV couples to charge carriers and defines the characteristic shape in energy of the scattering rate $\tau^{-1}(T,\omega)$, which allows us to construct the charge-spin spectral density $I^2\chi(\omega,T)$ at temperature T. The T-dependence of the weight under the resonance peak in $I^2\chi(\omega)$ agrees with experiment as does that of the London penetration depth and of the microwave conductivity. Also, the $T = 0$ condensation energy, the fractional oscillator strength in the condensate, and the ratio of gap-to-critical temperature agree well with the data.

A hallmark of the spin dynamics of several classes of high-T_c superconductors is a magnetic resonance observed around $40\,\mathrm{meV}$ by means of spin-polarized inelastic neutron scattering. The position in energy of the peak scales with the critical temperature both in $\mathrm{YBa_2Cu_3O_{6.95}}$ (Y123) and $\mathrm{Bi_2Sr_2CaCu_2O_8}$ (Bi2212) superconductors [1]. The analysis of the optical conductivity shows that the charge carriers are strongly coupled to the magnetic excitations with a coupling strength sufficient to account for superconducting transition temperatures $\simeq 90\,\mathrm{K}$ [2]. Thus, neutron scattering data combined with optical conductivity results, signal the prominence of the resonance mode for superconductivity in the cuprates. The analysis of additional optical data by Schachinger and Carbotte [3] showed that similar magnetic resonances are expected to be found in many other high-T_c materials with $T_c \simeq 90\,\mathrm{K}$ and that this phenomenon is not restricted to bilayer materials. At the moment some of these cannot be investigated with neutrons due to minuscule crystal size.

Because the spectral weight under the resonance is maximized at $T \ll T_c$ and vanishes at $T \simeq T_c$ [4] (at least in optimally doped Bi2212 and Y123), coupling of the conducting carriers to the magnetic mode ought to influence the temperature dependence of a variety of

properties including the London penetration depth and microwave absorption. In this work we determine the charge-spin spectral density $I^2\chi(\omega)$ at various T from the inversion of the optical constants. The T-dependence of the spectral weight under the resonance we obtain matches well the neutron data [4] on the temperature evolution of the magnetic resonance. We employ Eliashberg formalism to calculate the T-dependence of the penetration depth, of the microwave conductivity and the fractional optical oscillator strength that condenses in the superfluid density at $T = 0$. These results along with calculations of the zero-temperature condensation energy and the ratio of gap-to-critical temperature agree with experiment. This establishes the pivotal role played by the magnetic resonance mode in the charge dynamics as well as in the thermodynamic properties of the cuprates.

In a previous publication [2] we showed that an appropriately defined second derivative [5] of the optical scattering rate $\tau^{-1}(\omega)$ as a function of frequency gives an absolute measure of the spin excitation spectrum weighted by their coupling to the charge carriers. While the second-derivative technique is not exact and, for instance, does not account for the anisotropy of the relaxation rate on different segments of the Fermi surface [6], it, nevertheless, allows one to construct a good first estimate of the frequency dependence of the underlying charge carrier-spin excitation spectral density. Here we apply this analysis to study the temperature dependence of the spectral weight under the spin resonance in optimally doped Y123.

Eliashberg theory, on the other hand, is a highly successful extension of the BCS model for the case of an electron-phonon mechanism [7]. While the theory was formulated for the electron-phonon case, it can be used as a first approximation for other boson exchange mechanisms, the main limitation being that vertex corrections may become more important and therefore the theory less accurate. With the symmetry of the gap (d-wave) explicitly introduced into the formalism, the only material parameter that enters is the electron-spin excitation spectral density $I^2\chi(\omega)$.

In fig. 1 (top frame) we present the raw experimental results for the optical scattering rate spectra $\tau^{-1}(\omega)$ obtained for twinned samples of optimally doped YBCO single crystals [8]. Here $\tau^{-1}(\omega) = \Omega_p^2 \Re\{\sigma^{-1}(\omega)\}/4\pi$, where $\sigma(\omega)$ is the infrared conductivity and Ω_p is the plasma frequency. The low-T spectra reveal a threshold structure starting around $\omega \simeq 60$ meV which is a common signature of the electromagnetic response of the CuO_2 planes in a variety of high-T_c superconductors [9]. With increasing T this feature weakens and at $T > T_c$ the scattering rate assumes a nearly linear ω-dependence which is the counterpart of the linear resistivity, and is characteristic of the marginal Fermi liquid [10]. The second-derivative technique [2,3] shows more clearly the threshold structure and helps to unravel its microscopic origin. This technique applies to a d-wave superconductor which is described by a charge carrier-spin excitation spectral density $I^2\chi(\omega)$ within a generalized Eliashberg formalism [11,12]. A peak in the spectral density at energy ω_{sr} of the spin resonance, gives a peak at $\omega \simeq \Delta + \omega_{sr}$ (where Δ is the energy gap) in the second derivative of $\omega\tau^{-1}(\omega)$. A first approximation to the spectral density which applies, however, only to the region of the resonance peak (beyond it $W(\omega)$ has a negative region, not part of the spectral density which is positive definite) is given by the function $W(\omega)/2$, with ω appropriately shifted by Δ, and [5]

$$W(\omega) = \frac{1}{2\pi} \frac{\mathrm{d}^2}{\mathrm{d}\omega^2} \left[\frac{\omega}{\tau(\omega)} \right]. \tag{1}$$

The spectra for $W(\omega)$ (bottom frame of fig. 1) indeed reveal a peak at $\simeq 70$ meV at 10 K. Also, with increasing T, this peak softens by about 20 meV but this shift coincides with the temperature dependence of the gap, so that the energy of the spin resonance is temperature independent and the spectral weight confined under the peak is gradually reduced to zero as
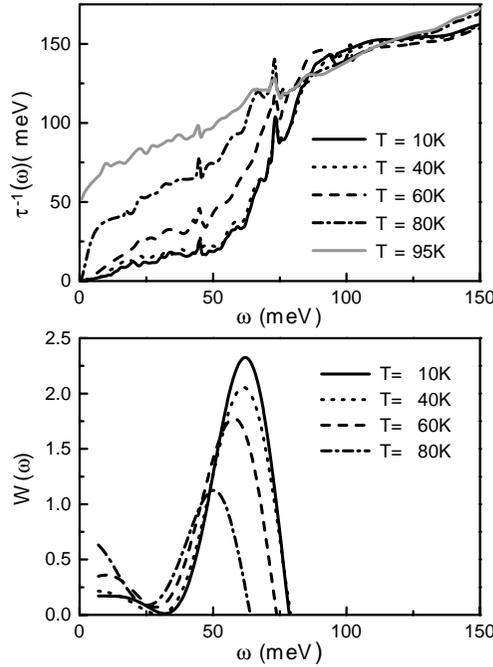
Fig. 1 – Top frame: optical scattering rate $\tau^{-1}(T, \omega)$ in meV for optimally doped twinned Y123 single crystals. Bottom frame: function $W(\omega)$ *vs.* ω in the region of the spin resonance.

T approaches T_{c}, and shows a temperature dependence similar to the strength of the spin resonance (top frame of fig. 2). These observations suggest that the spin resonance is responsible for the rise in the optical scattering rate. Recent ARPES data [13] show quasiparticle peaks along the BZ-diagonal (most relevant to in-plane transport) with width that displays a similar behaviour to the optical rates.

The data shown in the bottom frame of fig. 1 can be used to construct a charge carrier-spin excitation spectral density according to the following prescription. It is found that the scattering rate shown at $T = 95\,\mathrm{K}$ can be fit with the form [14]

$$I^2\chi(\omega) = G \frac{\omega/\omega_{\mathrm{SF}}}{1 + (\omega/\omega_{\mathrm{SF}})^2}\,, \tag{2}$$

where the single-spin fluctuation energy $\omega_{\mathrm{SF}} = 20\,\mathrm{meV}$ produces a good fit to the ω-dependence of the $T = 95\,\mathrm{K}$ data for $\tau^{-1}(\omega)$ with G adjusted to get the correct magnitude when a cut-off of $400\,\mathrm{meV}$ is applied. In the superconducting state the spectrum of $I^2\chi(\omega)$ given by eq. (2) is modified only at small ω [2,3], with the spin resonance at $41\,\mathrm{meV}$ added according to the data given in the lower frame of fig. 1. The area under the main resonance peak in $I^2\chi(\omega)$ is defined as $A(T)$ and the normalized area $A(T)/A(10\,\mathrm{K})$ is plotted in the top frame of fig. 2 as the solid line. This compares well with the solid circles for the normalized area under the neutron resonant peak obtained by Dai *et al.* [4] denoted by $\langle m_{\mathrm{res}}^2(T)\rangle/\langle m_{\mathrm{res}}^2 T = 10\,\mathrm{K}\rangle$. The agreement is good and shows that the variation in neutron peak intensity with T is reflected accurately in the transport data.

Once a model spectral density $I^2\chi(\omega)$ is specified, superconducting properties follow from the solution of the d-wave Eliashberg equations [11,12]. Here we report on two such properties.
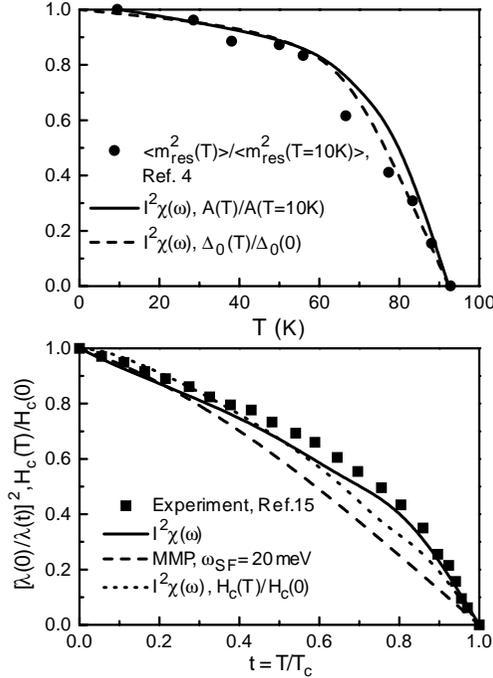
Fig. 2 – Top frame: spectral weight under the spin resonance as a function of temperature (solid line) obtained from the optical data of fig. 1 (top frame) (5 temperatures only). The solid circles are the data of Dai *et al.* [4] obtained by neutron scattering. The dashed curve gives our calculated $\Delta_0(T)/\Delta_0(0)$. Bottom frame: the normalized London penetration depth squared $(\lambda(0)/\lambda(T))^2$ *vs.* reduced temperature $t = T/T_\mathrm{c}$ (solid line) compared with the experimental results of Bonn *et al.* [15]. The dashed line does not include the spin resonance and is for comparison. The dotted curve gives thermodynamic critical field $H_\mathrm{c}(T)/H_\mathrm{c}(0)$ *vs.* t.

In the bottom frame of fig. 2 we show our results for the normalized London penetration depth $[\lambda(0)/\lambda(t)]^2$ as a function of reduced temperature t and compare with experimental results obtained by Bonn *et al.* [15] (solid squares). The dashed line was obtained with a spectral density taken as temperature independent and fixed to its $T = T_\mathrm{c}$ value; calculation details are given in ref. [11]. The agreement with the data is poor but can be significantly improved if we use the model for $I^2\chi(\omega)$ which includes the spin resonance. The solid line reproduces the essential features of the experimental data. It is the growth in strength with decreasing T of the 41 meV peak and the loss of spectral weight at small ω in the superconducting state that accounts for the bulging upward of the solid curve in the region above $t \simeq 0.3$.

Another quantity of interest is the temperature dependence of the microwave conductivity below T_c. A large peak [15] is observed in $\sigma_1(\omega)$ for $\omega = 0.144$ meV around 30 K. This peak has been attributed to the collapse of the inelastic scattering as T is lowered in the superconducting state. If the important scattering has its origin in correlations effects, as it does in a spin fluctuation mechanism, it is expected to be strongly affected by the onset of superconductivity, thus $I^2\chi(\omega)$ should be gapped. This mechanism is already included in our work with the spin resonance determining the low ω part of the spectral density. Our theoretical results for $\sigma_1(\omega = 0.144$ meV$)$ as a function of temperature are shown as solid circles in fig. 3 and are found to be close to previous theoretical results [11]. The arrow shows the point at which the
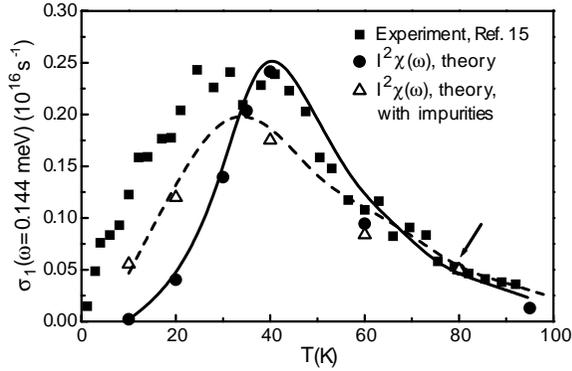
Fig. 3 – Temperature dependence of the conductivity $\sigma_1(\omega)$ at microwave frequency $\omega = 0.144\,\text{meV}$. The solid circles are results based on our model spectral density with the solid curve a guide to the eye. The open triangles include impurities with the dahsed line to guide the eye. The solid squares represent experimental data by Bonn *et al.* [15].

theoretical calculations have been made to agree exactly with the measurements of Bonn *et al.* [15] (solid squares). As for the T-dependence of $\sigma_1(\omega = 0.144\,\text{meV})$, the agreement with experiment is good at the higher temperatures, but the theoretical peak is too narrow. This discrepancy can be removed by including a small amount of impurity scattering which yields the open triangles. We note that the temperature dependence of the microwave conductivity reflects most importantly the reduction to near zero of $I^2\chi(\omega)$ at small ω which accompanies the formation of the resonance peak rather than the peak directly. Previous work [11] which included a low-frequency cut-off but no resonance peak was equally able to describe the data and fell close to the solid and dashed lines of fig. 2.

The plasma frequency Ω_p which does not enter our theoretical work can be found by scaling theoretical infrared conductivity data to experiment [16]. A value of 2.36 eV is found (see table I) which compares well with experiment.

A further comparison of our model with the infrared data is provided by the analysis of the fraction of the total normal-state spectral weight which condenses into the superfluid: n_s/n. Indeed, strong electron-boson coupling reduces the spectral weight of the quasiparticle component of the electronic spectral function $A(\boldsymbol{k}, \omega)$ compared to its non-interacting value by a factor of Z leading at the same time to the appearance of an incoherent component. It is the latter component which is responsible for the Holstein band in the optical conductivity whereas the coherent quasiparticle part gives rise to the Drude term at $T > T_\text{c}$ and to superfluid density

TABLE I – *Some superconducting properties of the twinned* Y123 *sample:* $\Delta F(0)$ *is the condensation energy at* $T = 0$ *in* meV/Cu-atom, n_s/n *is the superfluid to total carrier density ratio,* Ω_p *is the plasma frequency in* eV.

	Theory	Experiment	Ref.
$\Delta F(0)$	0.287	0.25	[17, 18]
n_s/n	0.33	0.25	[19]
Ω_p	2.36	2.648	[20]
$2\Delta_0/k_\text{B}T_\text{c}$	5.1	5.0	[21]

at $T = 0$ in the spectra of $\sigma_1(\omega)$ [22]. The values of n_s/n and hence $(Z - 1)$ yield an estimate of the strength of renormalization effects in the interacting system. Tanner *et al.* [19] obtained $n_s/n \simeq 0.25$ in crystals of Y123 and Bi2212. This compares well with the value $\simeq 0.33$ which corresponds to $Z \simeq 3$ (at low temperatures) generated in our analysis. The resonance peak alone accounts for 75% of the renormalization effect.

We have also calculated the condensation energy [7] as a function of temperature. Its value at $T = 0$ follows from the normal-state electronic density of states which we take from band structure theory equal to 2.0 states/eV/Cu-atom (double spin) around the middle of the calculated range of values [23]. This gives a condensation energy $\Delta F(0) = 0.287 \, \text{meV}/\text{Cu} - \text{atom}$ which agrees well with the value quoted by Norman *et al.* [17] from the work by Loram *et al.* [18]. (See table I.) This is equivalent to a thermodynamic critical field $\mu_0 H_c(0) = 1.41 \, \text{T}$ with $H_c(T)$ defined through $\Delta F(T) = H_c^2(T)/8\pi$. The normalized value $H_c(T)/H_c(0)$ is shown as the dotted line in the bottom frame of fig. 2 and is seen to follow reasonably, but not exactly, the T-dependence of the normalized penetration depth. Another quantity that comes out directly from our calculations is the temperature dependence of the gap. It follows closely the temperature dependence of the resonance intensity $A(T)/A(T = 10 \, \text{K})$ as shown (dashed curve) in the top frame of fig. 2. One further quantity is the ratio of the gap amplitude to the critical temperature which in BCS theory is $2\Delta_0/k_B T_c = 4.2$. In Eliashberg theory the gap depends on frequency. In this case an unambiguous definition of what is meant by Δ_0 is to use the position in energy of the peak in the quasiparticle density of states which is how the gap Δ_0 is usually defined experimentally for a d-wave superconductor. We get a theoretical value of $2\Delta_0/k_B T_c \simeq 5.1$ in good agreement with experiment, as shown in table I.

The analysis presented above argues for the prominence of the spin resonance in the charge dynamics and thermodynamics of Y123 (and Bi2212) [24]. Results from other experimental techniques which also probe the charge related properties of the high-T_c superconductors have also been described in terms of coupling to a collective mode. ARPES results in Bi2212 [25,26] as well as certain features of tunneling spectra [27] are examples.

The analysis of optical data gives the charge carrier-spin excitation spectral density $I^2\chi(\omega)$ which determines the superconducting properties of the system within a generalized d-wave Eliashberg formalism. $I^2\chi(\omega)$ depends significantly on T because of feedback effects expected in theories of electronic mechanisms [28]. We obtained agreement with experiment for the T-dependence of the London penetration depth, of the peak in the microwave conductivity, and of the spectral weight under the 41 meV spin resonance. The size of the zero-temperature condensation energy is also understood as is the observed value of the fractional oscillator strength in the condensate and the ratio of gap-to-critical temperature.

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