Bosons in high-temperature superconductors: an experimental survey

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Abstract
We review a number of experimental techniques that are beginning to reveal fine details of the bosonic spectrum $\alpha^2 F(\Omega)$ that dominates the interaction between the quasiparticles in high-temperature superconductors. Angle-resolved photoemission spectroscopy (ARPES) shows kinks in electronic dispersion curves at characteristic energies that agree with similar structures in the optical conductivity and tunnelling spectra. Each technique has its advantages. ARPES is momentum resolved and offers independent measurements of the real and imaginary part of the contribution of the bosons to the self-energy of the quasiparticles. The optical conductivity can be used on a larger variety of materials and with the use of maximum entropy techniques reveals rich details of the spectra including their evolution with temperature and doping. Scanning tunnelling spectroscopy offers spatial resolution on the unit cell level. We find that together the various spectroscopies, including recent Raman results, are pointing to a unified picture of a broad spectrum of bosonic excitations at high temperatures which evolves, as the temperature is lowered, into a peak in the 30–60 meV region and a featureless high-frequency background in most of the materials studied. This behaviour is consistent with the spectrum of spin fluctuations as measured by magnetic neutron scattering. However, there is evidence for a phonon contribution to the bosonic spectrum as well.

(Some figures in this article are in colour only in the electronic version)

This article was invited by L H Greene.

1. Introduction
At the 25th anniversary of the discovery of high-temperature superconductivity (Bednorz and Müller 1986) we still lack a complete understanding of this astonishing phenomenon. However, we can take a look back at the history of low-temperature superconductivity to get some perspective on this apparent lack of progress. The original formulation of the Bardeen–Cooper–Schrieffer (BCS) theory (Bardeen et al 1957a, 1957b) treated the interaction between a pair of electrons with up and down spins of equal and opposite momentum at the Fermi energy by a constant average matrix element. While it was clear from the isotope effect on the transition temperature $T_c$ that phonons were involved, it took high-resolution tunnelling experiments by McMillan and Rowell (1965) to accurately resolve the underlying bosonic structure of the electron–phonon spectral density denoted by $\alpha^2 F(\Omega)$ and relate it to the phonon spectrum as determined by inelastic neutron scattering (Brookhouse et al 1962). A further important step was to calculate this function from band theory and phonon dynamics (Leung et al 1976, Tomlinson and Carbotte 1976) and more recently in MgB$_2$ by Choi et al (2002a, 2002b), Golubov et al (2002) and Brinkman et al (2002)). Nevertheless,
even with all this detailed understanding of low-temperature superconductivity, we are still treated to surprising new superconductors, not predicted by theory, such as the recent discovery of MgB$_2$ with a $T_c$ of the order of 40 K (Nagamatsu et al 2001).

The situation in high-$T_c$ cuprates is not at all clear. In a recent Science article, Anderson (2007) raised the issue of the very existence of pairing ‘bosonic glue’ in this case, be it phonons (Johnston et al 2010a), perhaps modified by strong correlation physics (Kulić 2000), or some other boson exchange mechanism such as spin fluctuation (Chubukov et al 2008) within a nearly antiferromagnetic Fermi liquid model (Millis et al 1990, Monthoux and Pines 1994, Branch and Carbotte 1999).

Returning to the question of whether or not the Cooper pair binding may involve only high energy dynamics on the scale of the Hubbard $U$ (>>eV) or the antiferromagnetic exchange coupling $J$ (~0.12eV) or rather on the smaller scale of the spin fluctuations, the work of Maier et al (2008) is instructive. The critical question is one of dynamics and the energy scale associated with the pairing interaction. These authors find that for both Hubbard and t-J models the dominant contribution to the pairing reflects this smallest energy scale and so one can speak of a spin-fluctuation glue. It is useful to quantify their pairing with the help of the imaginary part $\phi_2(k,\omega)$ of the electron–phonon spectral function $\alpha^2 F(\omega)$.

This quantity measures the contribution to the pairing coming from excitation energies in the range 0–$\omega$ and by construction, $I(k,\omega)$ saturates to value one at $\omega \rightarrow \infty$.

Figure 1 shows the results of Maier et al (2008) for the case of the BCS superconductor Pb which can be described by an isotropic electron–phonon spectral density $\alpha^2 F(\omega)$ shown as the dashed spectrum in the left frame and a Coulomb repulsion $\mu^*$ of 0.1 which accounts for the electron–electron interactions. This involves the introduction of a pseudopotential rather than a bare Coulomb repulsion as described by Morel and Anderson (1962). Solutions of the Eliashberg equations for the complex gap gives the solid curve for $\phi_2(\omega)/\phi_1(0)$. The results for $I(\Omega)$ are presented in the right-hand side frame (b). We see the structure at the sum of the gap $\Delta_0$ plus the main transverse phonon frequency $\omega_L$ in $\alpha^2 F(\Omega)$ as well as at $\Delta_0+\omega_L$ which gives the main longitudinal frequency. Most of the glue occurs in this energy range. In fact, as $\Omega$ increases $I(\Omega)$ first becomes larger that even higher $\Omega$. This behaviour is traced to the non-retarded repulsive Coulomb term $\mu^*$.

Turning to the cuprates in figure 2, we reproduce from Maier et al (2008) their results for the Hubbard model. In this case the complex gap depends on momentum as well as energy $\omega$ and in the top frame (a) $k = k_A = (0,\pi)$ with a doping of $n = 0.8$, where $n = 1$ corresponds to half-filling. Three values of $U$ are used as labelled. It is clear that all cases show pairing glue with $I(k_A,\Omega)$ reaching ~95% of its saturated value for $\Omega/t \sim 7$, where $t$ is the first nearest neighbour hopping parameter of the model. In the lower frame the d-wave projection of the spin susceptibility is plotted for $U = 10$ and we note that its energy scale corresponds closely to the energy scale for the contribution of the pairing glue to the pairing strength which suggests that spin fluctuations form the glue. There have been other similar calculations, among these the work...
coupling is much smaller than its quasiparticle counterpart which provides a direct explanation of the observation that the resistivity is linear in $T$ in the normal state above $T_c$ (Zeyher and Kulič 1996). Recent local density approximation (LDA) calculations in YBa$_2$Cu$_3$O$_y$ (YBCO) (Heid et al 2008, 2009) and in La$_{2−x}$Sr$_x$CuO$_4$ (LSCO) (Giustino et al 2008) have found, however, very small values of coupling in the d-channel and conclude that the electron–phonon interaction is too small to provide the glue for Cooper pair formation. Also quasiparticle mass enhancement factor renormalizations are small as is its transport counterpart. Renormalization due to electron correlations beyond LDA are not expected to considerably enhance these values (Zeyher and Kulič 1996) although some have argued that this need not necessarily be the case (Reznik et al 2008). A review emphasizing the role of phonons in angle-resolved photoemission spectroscopy (ARPES) has been given by Johnston et al (2010b). A discussion of a possible combined role of spin fluctuations plus a phonon part is found in Johnston et al (2010a). Another approach to the origin of kinks in ARPES spectra is that of Byczuk et al (2007) who discuss the role of Hubbard subbands in strongly correlated electronic systems. Bauer and Sangiovanni (2010) consider dispersion kinks in a Hubbard model supplemented with electron–phonon coupling in a Holstein model using dynamical mean-field theory. They also consider the effect of including antiferromagnetic correlations on the electron–phonon interaction and find that it enhances the phonon effect in the electronic dispersions. As described by Datta et al (2007), kinks also exist in the ‘effective’ dispersion curves defined by the peaks in the hole spectral density at fixed $\omega$ in the momentum distribution curve of ARPES within Tomonaga–Luttinger liquid models which exhibit spin–charge separation. In view of all these possible effects, it is important to turn to experiment to understand better what signatures of boson structure are present and how they might be interpreted. This is the main aim of this review.

To get fine details of the electron–boson interaction, tunnelling has been the spectroscopy of choice in the past. However, the same spectral density can be obtained by other experimental techniques. For example, for the elemental BCS superconductor lead, optics has given (Joyce and Richards 1970, Farnworth and Timusk 1974, 1976) results for $\alpha^2 F(\Omega)$ in excellent agreement with calculations of $\alpha^2 F(\Omega)$ (Tomlinson and Carbotte 1976) and with tunnelling (McMillan and Rowell 1965). In addition to optics, a spectroscopic technique that has been particularly important in the study of cuprate high-temperature superconductors is ARPES. More general reviews of this powerful technique already exist (Damascelli et al 2003, Campuzano et al (2004), Eschrig 2006, Chubukov et al 2008, Garcia and Lanzara 2010, Kordyuk et al 2010). While optics and ARPES will be our main focus, scanning tunnelling spectroscopy (STS) (for a review, see Fischer et al 2007) and break junction tunnelling will also be considered as well as the very recent Raman scattering data (Muschler et al 2010).

2. Angle-resolved photoemission spectroscopy

Modern ARPES is based on the classical photoelectric effect. A high-energy photon impinges on the surface of a single

![Figure 2. (a) The cumulative pairing interaction spectral weight $I(\mathbf{k}_A, \Omega)$ versus $\Omega/t$ for the Hubbard model. Reprinted with permission from Maier et al (2008). Copyright 2008 by the American Physical Society. (b) The d-wave projected spin susceptibility $\chi_d(\Omega)$ versus $\Omega/t$ for the same model. We note that the major contribution to the gap function comes from low-frequency excitations with an additional attractive interaction at the 5% level from high-frequency excitations.](image-url)
Figure 3. ARPES spectroscopy. Reprinted with permission from Damascelli et al (2003). Copyright 2003 by the American Physical Society. (a) A photon is absorbed by the sample and emits a photoelectron in the direction specified by the angles \( \theta \) and \( \phi \). Its momentum parallel to the surface equals the momentum of the hole in the filled band (grey area in (b)). An analyser has a slit that accepts electrons with different \( k \) vectors and spreads them in energy with an electric field perpendicular to the slit. The electrons are collected in a fluorescent screen that will display a two-dimensional plot of the energy versus momentum along the slit. (b) shows a non-interacting electron system (with a single energy band dispersing across \( E_F \)). (c) An interacting Fermi liquid system. Note the broad sideband due to bosonic interactions in addition to the sharp peak.

crystal cleaved in situ in ultrahigh vacuum. The energy of the photo-ejected electron and the direction of its velocity are determined. Conservation of momentum demands that the momentum component parallel to the crystal surface of the emerging electron must be equal and opposite to the momentum of the hole created in the sample. In this way the energy and momentum relationship of the occupied states below the Fermi surface of a two-dimensional system can be mapped out. This is illustrated in figure 3 from Damascelli et al (2003). At present a resolution in energy of better than 1 meV and 0.1° in angle is possible (Garcia and Lanzara 2010). The photo current intensity \( I(k, \omega) \) is given by the product of three factors:

\[
I(k, \omega) = |M(k, \omega)|^2 f(\omega) A(k, \omega).
\]

The first is a dipole matrix element \( M(k, \omega) \) that depends on the initial and final electronic states, incident photon energy and polarization. While some attention needs to be paid to this factor, the other two factors are of most general interest and combine to make the technique a powerful tool that yields a detailed picture of the energy and momentum dependence of the electronic structure of the occupied states below the Fermi surface. The first of these factors is the Fermi–Dirac (FD) distribution function \( f(\omega) \) which states that at zero temperature only states below the Fermi energy \( E_F \) are accessible and at finite \( T \) the thermal tail of the FD distribution provides some limited information on unoccupied states. The second factor, which is the most important one, is the spectral density of the charge carriers \( A(k, \omega) \). It is related to the imaginary part of the electron Green’s function \( G(k, \omega) \). In terms of the electronic self-energy \( \Sigma(k, \omega) \) the spectral density is written as

\[
A(k, \omega) = \frac{1}{\pi} \frac{\Sigma''(k, \omega)}{[\epsilon_k - \Sigma'(k, \omega)]^2 + \Sigma''(k, \omega)^2},
\]

where \( \Sigma' \) and \( \Sigma'' \) are, respectively, the real and imaginary parts of \( \Sigma(k, \omega) \). For free electrons, \( A(k, \omega) \) reduces to a Dirac delta function on the band structure dispersion curves, \( \epsilon_k \) versus \( k \) as shown in figure 3(b). When interactions are included, the quasiparticle energies are renormalized and they acquire a finite lifetime and an incoherent side band develops

\[
E_k - \epsilon_k - \Sigma'(k, E_k) = 0
\]

and these can be measured in ARPES experiments. In figure 4 we show the results (Kaminski et al 2001) for the ARPES experiment.

Figure 4. (a) The ARPES intensity \( I(k, \omega) \) for optimally doped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) for \( k \) along the diagonal line in the \( k_x, k_y \) plane of the Brillouin zone shown in the inset. Reprinted with permission from Kaminski et al (2001). Copyright 2001 by the American Physical Society. The curved line is the Fermi surface. MB is the main band and SL a superlattice image. (b) and (c) show, respectively, a constant \( \omega \) cut (MDC) and constant \( k \) cut (EDC) from (a).
Figure 5. The variation of ARPES intensity along selected cuts in the $k_y$ direction for optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (shown in the zone inset of figure 4). Left panel: the normal state ($T = 140$ K). Middle panel: the superconducting state ($T = 40$ K). Right panels: EDCs at locations marked by the vertical lines in the middle panels. Reprinted with permission from Kaminski et al (2001). Copyright 2001 by the American Physical Society. These data show the increase in coupling to a bosonic mode at $\approx 70$ meV as one moves from the nodal direction (lower panels) towards the antinodal direction (upper panels) both in the normal and superconducting states.

intensity $I(k, \omega)$ as a function of $k$ and $\omega$ for incident photon energy $h\nu = 22$ eV and temperature $T = 40$ K. Frame (a) gives a 3D plot while frames (b) and (c) give, respectively, a constant energy curve called the momentum distribution curve (MDC) and a constant $k$ cut called the energy distribution curve (EDC). MB denotes the main band and SL is a superlattice image. For (b) the frequency $\omega = 0$ and hence the peak in the curve is at $k = k_F$ (the Fermi momentum in this direction). Data on $k_F$ in different directions in the Brillouin zone will determine the Fermi surface. The line in the MDC spectrum is symmetric and close to Lorentzian in shape with only a small background. By contrast (c) is far from Lorentzian and has a large tail extending to a high binding energy (negative values). These tails, also called the ‘dip–hump’ structure, reflect inelastic processes where, in addition to the creation of a hole in the valence band, a bosonic excitation has been created. An analysis of these tails can yield information on the bosonic spectrum that interacts with the holes. Figure 3(c) gives a schematic illustration of these processes. The widths of the MDCs can be analysed to yield frequency-dependent scattering rates $1/\tau(\omega)$ which are proportional to the imaginary part of $\Sigma(k, \omega)$. Modelling of the self-energy with a synthetic bosonic spectrum to get a fit to the dispersion curves can be used to yield the real part of $\Sigma(k, \omega)$.

While the MDCs are more straightforwardly interpretable using equation (4) with the inverse quasiparticle lifetime $1/\tau$ related to $\Sigma''(k, \omega)$, historically the EDCs were first used in the interpretation of ARPES dispersion curves. In figure 5 the results for the dispersion curves are reproduced from Kaminski et al (2001). From top to bottom, we go from the antinodal to...
the nodal direction along lines shown in the inset of figure 4(a) where one quarter of the Brillouin zone is shown along with the Fermi contour (solid black curve). The left panels show the normal state dispersion curves. Note the changes in slope at low energies which are called kinks in dispersion, a signature of interaction with bosonic modes. In the middle panels for the superconducting state these features become stronger and we see two dispersion branches which overlap in momentum with the lower energy branch showing almost no dispersion (change of energy) with $k$ while the higher energy branch varies more, although it too remains quite flat. These dispersions correspond to the energy of the sharp peaks seen in the EDC (right panel) while the second branch corresponds to the ‘hump’ separated from the larger sharp peak at lower energy by the ‘dip’ (Engelsberg and Schrieffer 1963). We note the evolution of the dispersion curves in the superconducting state (SC): there is a gradual closing of the gap between the two branches until a single branch emerges but with a distinct ‘kink’ remaining in the nodal direction. Two observations are made by Kaminski et al (2001). First, the energy of the gap structure which evolves into the kink is reasonably fixed along the Fermi surface. Interpreting the kink as a signature of an interaction with a bosonic excitation suggests that this excitation has a fixed and well-defined energy. Second, the normal state dispersions are comparatively smooth which is taken as evidence that the mechanism involved is coupling to a collective mode which vanishes at temperature $T = T_c$, as does the well-known spin resonance seen in inelastic neutron scattering at 41 meV in optimally doped YBa$_2$Cu$_3$O$_{6+\delta}$. It is also clear from this figure and this is noted by Kaminski et al (2001) that the coupling to the collective mode increases as one progresses from the nodal to the antinodal direction. We need to keep this in mind in the discussions of the origin of the boson involved. However, as we have already noted, a more careful examination of the normal state dispersions, as we will see below in more detail, shows that strong bosonic interactions are present in the normal state.

The peak–dip–hump structure in the antinodal direction (at $(\pi, 0)$ in the Brillouin zone) has a long history (Dessau et al 1991, 1992, Shen and Dessau 1995 and Ding et al 1996). It was interpreted by many to be distinctively related to the coupling to the spin-one resonance seen in inelastic magnetic neutron scattering experiments. An early formulation was given by Norman et al (1997) and a detailed comparison between the charge carrier self-energy due to a sharp boson mode of momentum $(\pi, \pi)$ and the results in figure 5 was made (Eschrig and Norman 2000) with excellent qualitative agreement noted. An independent but closely related formulation of the relation between ARPES data and the neutron resonance peak was given by Abanov and Chubukov (1999) with almost the same conclusions. This work was questioned by Kee et al (2002) on the grounds that the spin resonance had too small a spectral weight and coupling to charge carriers to have a strong effect on the electronic self-energy. A response by Abanov et al (2002) provides results of calculations that show that even though the resonance has a small spectral weight, this weight is confined to a small region in momentum space and energy and consequently this resonance can provide clear signatures in electronic properties. More details can be found in Eschrig and Norman (2003). An important fact underlying these calculations is the disappearance of the resonance at $T_c$ in many systems although for underdoped materials a remanence remains up to a higher temperature $T^*$, the pseudogap energy scale. The evolution of the self-energy as one moves from the $(\pi, 0)$ to the $(\pi, \pi)$ direction is also an important feature of the data. Later we will return to this issue and discuss how eventually it was recognized that bilayer splitting can have a strong effect on ARPES results in the antinodal direction and this needs to be accounted for before the dispersion curves can be analysed for self-energy effects. Modifications of the picture just described are needed but some elements of the explanation given remain valid. Finally, we note the experimental study of Campuzano et al (1999) who extended the work to doping as well as momentum and temperature dependences and found that the hump scales with the peak and persists above $T_c$ in the pseudogap state. Also the inferred mode energy has the same doping dependence as does the magnetic resonance peak position seen in inelastic neutron scattering (Fong et al 1999, He et al 2001). They conclude that the peak–dip–hump structure arises from the electronic interaction with a collective mode with wave vector $(\pi, \pi)$. As we will see below, the sharp resonance that appears at $T_c$ is only a part of the bosonic spectrum. In addition, there is a broad background of excitations that is present in the normal state and will be the ultimate trigger of superconductivity at $T_c$. However, before we review further the recent ARPES studies of the bosonic spectra, we must address the problem of bilayer splitting which needs to be considered as it could mask intrinsic self-energy effects.

In systems with two copper-oxygen layers such as Bi$_2$Sr$_2$CaCu$_2$O$_{6+\delta}$, the family most studied with ARPES, the degeneracy of the two bands is split into a bonding band and an antibonding band. An unfortunate coincidence is that this splitting energy is of the same order as the energy of the bosonic excitations discussed previously. Illustrated in figure 6 are the ARPES results by Feng et al (2001) on the Fermi surface of overdoped Bi-2212 ($T_c = 65$ K). We see clearly the bonding (BB) and the antibonding (AB) bands as well as their superstructure replicas. Note that in this sample no splitting is observed in the nodal direction.

However, in figure 7 we show nodal direction renormalized electronic dispersion curves as a function of angle (instead of momentum) for YBa$_2$Cu$_3$O$_{6+\delta}$ from the work of Borisenko et al (2006) for an underdoped sample UD35 with $T_c \approx 35$ K at a temperature of 30 K. Three photon energies $h\nu = 50, 53$ and 55 eV are employed. In the left frame (photon energy 50 eV) we clearly see two different dispersion curves, bonding and antibonding. With increasing photon energy a single bonding band dominates in the right-hand frame. This shows that photon energy has a significant effect on the photoemission matrix elements that determine the admixture of the antibonding versus the bonding bands. It should be clear that different admixtures of bonding and antibonding bands could be mistaken for self-energy effects when in reality the structure is due to bilayer splitting. For additional discussion of bonding and antibonding bands see
Figure 6. The effect of bilayer splitting on ARPES data on overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Reprinted with permission from Feng et al (2001). Copyright 2001 by the American Physical Society. (a) False colour plot of the spectral weight mapping near $E_F$ ($\sim$20 meV, 10 meV) of OD65 taken at 22.7 eV (lower right half, $T = 75$ K) and 20 eV (upper left half, $T = 80$ K) (note they are from different experiments). The Fermi surface is plotted for antibonding states (AB, triangles) and bonding states (BB, circles). A second set of states arises from superstructure with antibonding states (AB$'$, squares) and bonding states (BB$'$, diamonds). (b) ARPES spectra along the cut indicated by the arrow in (a).

Figure 7. The effect of incident photon energy on ARPES photoemission intensity in YBCO. Note the decrease in the antibonding band intensity at 53 and 55 eV incident photon energy. The inset schematically shows the LDA-predicted Fermi surface and a cut in the $k$ space along which the data have been taken. Reprinted with permission from Borisenko et al (2006). Copyright 2006 by the American Physical Society.

among others Chuang et al (2001), Yamasaki et al (2007), Kordyuk et al (2002), Borisenko et al (2003), Kim et al (2003) and for a review Kordyuk et al (2010).

Gromko et al (2003) provide a detailed analysis of the bilayer effect in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ yielding information on self-energy effects without contamination by bilayer issues. They find that the kink in the bonding band in overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ is stronger in the $(\pi, 0)$ direction and appears at a lower energy $\approx$40 meV for overdoped samples, and is only seen in the superconducting state as expected if the mode structure is due to the magnetic resonance mode. In figure 8 we display their results for the temperature evolution for the bonding band energy in their overdoped sample with $T_c = 71$ K of the $(\pi, 0)$ kink and the inset gives the self-energy derived from these data using equation (5) ($\text{Re} \Sigma(\omega)$). The amplitude of the maximum in $\text{Re} \Sigma(\omega)$ as a function of temperature is plotted in figure 8(b) as red circles. Also shown for comparison is the leading edge superconducting gap $\Delta_{LE}$, blue squares. We see that both sets of data track each other and the peak in the self-energy difference between the superconducting state and the normal state, modelled by a straight line (see frame (a)), vanishes at $T_c$ with the vanishing of the gap $\Delta_{LE}$. The evolution of the superconducting state structures with momentum for the same overdoped $T_c = 71$ K sample is shown in figure 9 for four points in the Brillouin zone with the left panel near $(\pi, 0)$ and the right panel near $(\pi, \pi)$ as labelled in the figure. It is clear that the dispersion curve structure remains around 40 meV but becomes much weaker.
Figure 8. The \((\pi, 0)\) kink strength and its variation with temperature. Reprinted with permission from Gromko et al (2003). Copyright 2003 by the American Physical Society. (a) MDC dispersion from overdoped Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) along \((\pi, 0) - (\pi, \pi)\). The inset shows \(\text{Re} \Sigma\) after a linear term has been subtracted from the data showing a kink energy of \(\approx 40\) meV. (b) Temperature dependence of the amplitude of the maximum in \(\text{Re} \Sigma\) (red circles) from (a) and the superconducting gap \(\Delta_{\text{LE}}(T)\) (blue squares).

Figure 9. The change of the kink strength with \(k\) of a sample of overdoped Bi-2212. Reprinted with permission from Gromko et al (2003). Copyright 2003 by the American Physical Society. Here \(r\) is the radial distance from \((\pi, 0)\) which increases as we move from (a) to (d). The kink weakens as we move towards the node.

as one moves away from the antinodal direction and strong \((\pi, \pi)\) scattering such as is the case for the coupling to the spin-one resonance.

A different method of analysis aimed at eliminating artefacts arising from bilayer splitting effects has been developed which employs Kramers–Kronig (KK) consistent (Kordyuk et al 2002, 2004a, 2004b, 2005) procedures as a prominent element. The physical idea behind this procedure is simple: since the real and imaginary parts of the self-energy can be measured independently by EDC and MDC, they should be related by KK transformations. The method allows the simultaneous extraction of self-energy and the bare dispersion. This technique has been applied by Kordyuk et al (2006) to the study of the 70 meV kink in Bi-2212 in the nodal direction. The authors separate the self-energy obtained from experiment into two components (‘primary’ and ‘secondary’) as shown in figure 10 by thick red and blue dashed lines for \(\Sigma_1\) and \(\Sigma_2\), respectively. The coupling in \(\Sigma_2\) is to a single boson mode while the structure in \(\Sigma_1\) represents Coulomb repulsion. An important conclusion made by these authors is that the primary \(\Sigma_1\) is structureless and largely independent of temperature and doping, while the secondary \(\Sigma_2\) depends strongly on doping and temperature in agreement with coupling to spin fluctuations.

Returning to equation (5) we see that subtracting a bare dispersion curve \(\epsilon_k\) from the renormalized energy \(E_k\) of ARPES gives the real part of the quasiparticle self-energy \(\Sigma'(k, \omega)\) versus \(\omega\) for a fixed value of \(k\). Johnson et al (2001) have done this for the nodal direction and several doping levels in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\). Their results are shown in figure 11; from top to bottom three doping levels, underdoped with \(T_c = 69\) K, optimally doped with \(T_c = 91\) K and overdoped with \(T_c = 55\) K denoted as UD69, OP91 and OD55, respectively. In each case they show two temperatures, one in the normal state (open red diamonds), and the other in the superconducting state (solid blue circles) as well as the difference \(\omega = \omega_{\text{sc}}\) shown as solid green triangles. It is clear that the self-energy is dominated by a broad background at all temperatures but there is a peak in the superconducting state which does not exist in the normal state for the UD and OP samples. For the overdoped sample the peak is absent. The authors also plot the position in energy of the peaks in the self-energy \(\Sigma'(k, \omega)\) at \(\omega = \omega_{\text{sc}}\) and in the difference \(\omega = \omega_{\text{sc}}\) as a function of \(T_c^\text{max} - T_c\) and find that these go approximately as
Figure 10. Splitting of the nodal self-energy into two components $\Sigma_1$ and $\Sigma_2$ based on the data for the optimally doped sample. Reprinted with permission from Kordyuk et al. (2006). Copyright 2006 by the American Physical Society. Top panel: the real part. Bottom panel: the imaginary part. The authors associate the $\Sigma_1$ component with a temperature-independent Coulomb repulsion and the $\Sigma_2$ component with a bosonic excitation.

$\omega \approx 6k_B T_c$. This law is close to the spin-one resonance mode seen in neutron scattering which gives $E_n \approx 5.4k_B T_c$ (Fong et al. 1999, He et al. 2001). This correspondence lends support to the idea that the peak seen in figure 11 is associated with coupling to the spin resonance mode. This interpretation is further supported by the fact that the real part of the self-energy from ARPES, $\text{Re } \Sigma_1(\omega = \omega_0^E)$ for the UD69 sample tracks closely the intensity of the neutron mode in a similar sample of YBa$_2$Cu$_3$O$_{6+x}$ with $T_c = 74$ K (Dai et al. 1999) as a function of temperature. The most rapid change in intensity occurs for temperatures below the superconducting critical temperature $T_c$ and some intensity remains up to a higher temperature $T^*$ (the pseudogap temperature). Finally, we note that the doping dependence of the mass renormalization $\lambda$ is found to decrease with increasing doping. The coupling constant $\lambda'$ follows from the self-energy $\Sigma(k, \omega)$.

A different interpretation of the ARPES nodal kink, as it has become known since its initial discovery (Valla et al. 1999a, 1999b, Kaminski et al. 2000, Bogdanov et al. 2000), has been put forward by Lanzara et al. (2001). These results are summarized in figure 12 for a variety of materials (see also the review by Garcia and Lanzara (2010)). Lanzara et al. (2001) note that the energy of the kink, indicated by the heavy horizontal arrow, is close to 70 meV in all the different materials. Also, as shown in frame (f) the coupling constant $\lambda'$ is found to decrease with increasing doping. In the absence of any knowledge of the bare dispersion curve, $\lambda'$ is estimated from the ratio of the group velocities above and below the kink energy $E_F$. We have neglected any small momentum dependence in $\Sigma(k, \omega)$.

Figure 11. The real part of the self-energy of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ as measured by Johnson et al. (2001) for the superconducting (blue dots) and normal states (open red diamonds) for three doping levels starting with underdoped (top panel), optimally doped (middle panel) and overdoped (bottom panel). The solid lines through the normal state data represent fits to the data. The difference between the superconducting and the normal state self-energies for each level of doping is shown as green triangles. Gaussian fits to extract the peak energy $\omega_0^E$ (green line) show that there is a well-defined peak at 40–50 meV that is not present in the normal state and is absent in the overdoped sample at all temperatures. In all samples there is a second component to the self-energy in the form of a relatively temperature-independent background. Reprinted with permission from Johnson et al. (2001). Copyright 2001 by the American Physical Society.
Figure 12. The kink in ARPES dispersion in the nodal direction (except (b) inset, which is off this line) for a range of materials (a)–(c) from Lanzara et al (2001). The doping level is denoted by δ. The red arrow in (a) denotes the frequency of an optic phonon. (d) and (e) show the temperature dependence of the dispersions for optimally doped LSCO and Bi-2212. (f) shows doping dependence of λ′ the coupling constant to the bosonic excitations in different materials as a function of doping for LSCO (filled triangles) and NdLSCO (1/8 doping; filled diamonds), Bi-2201 (filled squares) and Bi-2212 (filled circles in the first Brillouin zone, and unfilled circles in the second zone). Note the presence of the kink in all the materials at roughly the same energy, denoted by the black arrow. Reprinted by permission from Macmillan Publishers Ltd: Nature Lanzara et al (2001), copyright 2001.

Figure 13. ARPES dispersion in YBa$_2$Cu$_3$O$_{6+x}$ as a function of doping from Borisenko et al (2006). Horizontal lines mark the energies of the kink, where dispersion starts to deviate from the straight line. Grey arrows show the position of the second high-energy kink. Note the shifting of the kink to higher frequency as the doping is increased.
The underlying bosonic function is temperature independent. In the normal state due to the closing of the superconducting gap. In the superconducting state at $T = 10^4 \text{ K}$ associated with the 70 meV mode while that in the superconducting state at $T = 10^3 \text{ K}$ is associated with the 36 meV mode. This interpretation, however, depends on the use of $\delta$-functions and does not consider possible changes brought about by extended spectra (Schachinger and Carbotte 2009). If sufficiently broad, such spectra do not necessarily show a significant shift due to the opening of a superconducting gap.

One can get additional information of the possible origin of the nodal direction kink structure in the renormalized quasiparticle dispersion curves from isotope substitution effects. Oxygen $^{16}\text{O}$ can be exchanged to $^{18}\text{O}$. Early experiments by Gweon et al (2004) showed relatively small changes in the dispersion curves in the nodal direction at low energy but unexpectedly large (much larger than the 6% energy shift expected for lattice vibrations involving oxygen) at higher energies. Even larger shifts were found away from the nodes in MDC as well as EDC distributions (Gweon et al 2006) with low energy photons and greatly improved spectral resolution compared with conventional ARPES (Koralek et al 2006). The expected isotope shift in boson frequency $\Delta \Omega / \Omega = (1 - \sqrt{16/18})$ is a few meV at most. Recent advances in ARPES resolution have made such measurements feasible. Results on optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ from Iwasawa et al (2008) are reproduced in figure 15. These new results do not confirm the large changes at high energies found by Gweon et al (2006). To extract the self-energy from ARPES dispersion curves a bare dispersion is needed. Three different forms were tried by Iwasawa et al and gave essentially the same results and are reproduced in figure 15 for the real part of the self-energy $\Re \Sigma(\omega)$ and corresponding results for $\Im \Sigma(\omega)$ are shown in frame (b). Both sets of results give almost the same shift of about 3.4 meV and 3.2 meV going from $^{16}\text{O}$ to $^{18}\text{O}$ as seen in (c) and (d), respectively. These shifts are in accord with an in-plane half-breathing phonon mode with $\Omega \approx 70 \text{ meV}$ as noted by Iwasawa et al (2008). On the other hand, for $\Omega \approx 70 \text{ meV}$ the necessary structure of $\alpha^2 F(\Omega)$ would have to be in the form of a distributed spectrum at this energy. Only in this case will the boson structure in $\Re \Sigma(\omega)$ and $\alpha^2 F(\Omega)$ be unshifted by the superconducting gap $\Delta$. We will return to our discussion of the isotope shift after we consider the inversion of ARPES data to recover a complete picture of the underlying electron–boson spectral density.

A difficulty in finding the boson spectral function lies in the fact that the experimentally determined quantity, the real part of the quasiparticle self-energy $\Re \Sigma(\epsilon, k, \omega)$, is related to the boson spectral density of Eliashberg theory $\alpha^2 F_1(\Omega)$ through a convolution integral. Such ‘inverse’ problems are inherently difficult and can result in ambiguous solutions.
Figure 15. (a) The effect of oxygen isotope substitution on the real part of the self-energy \( \text{Re}\{\Sigma(\omega)\} \) from ARPES data of Iwasawa et al. (2008). Five samples of \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) substituted with \(^{16}\text{O}\) (blue lines) and \(^{18}\text{O}\) (red lines) were measured along the nodal direction. The curves are offset for clarity. (b) Imaginary part of the self-energy \( \text{Im}\{\Sigma(\omega)\} \) determined from MDC full widths. ((c), (d)) Kink energy as a function of sample numbers both for \(^{16}\text{O}\) (blue line) and \(^{18}\text{O}\) (red line) from \( \text{Re}\{\Sigma(\omega)\} \) and \( \text{Im}\{\Sigma(\omega)\} \), respectively. Reprinted with permission from Iwasawa et al. (2008). Copyright 2008 by the American Physical Society.

A maximum entropy method (MEM) (Jaynes 1957) can be used to invert this equation and retrieve an estimate of the electron–boson spectral density. An early example of the application of this method to ARPES spectra was the work of Shi et al. (2004) who recovered an electron–phonon function on the surface of Be and Zhou et al. (2005) and Yoshida et al. (2007) who used the same method in their study of electron self-energy effects in \( \text{La}_{2−x}\text{Sr}_x\text{CuO}_4 \) as a function of doping \( x \). An analysis of nodal direction data in the normal state of underdoped samples yielded fine structures in the 23–29, 40–46, 58–63 and 75–85 meV energy ranges. A comparison of these results with inelastic neutron scattering data in the phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material. A related phonon spectrum leads these authors to support a phonon mechanism for superconductivity in this material.

The above observation should be contrasted with results on optimally doped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) in which Zhang et al. (2008a) have identified in the real part of the quasiparticle self-energy features at \( \approx 115 \) and \( \approx 150 \) meV in addition to the prominent feature at \( \approx 70 \) meV. Their results are reproduced in figure 16. The arrows (frame (a)) point to structures in the self-energy which gradually smear as the temperature is increased. This is seen better in frame (b) which shows the difference of the data at a temperature \( T = 128 \) K. High-energy features in ARPES have been discussed by many authors including Meevasana et al. (2007), Xie et al. (2007), Valla et al. (2007), Graf et al. (2007), Chang et al. (2008), Ikeda et al. (2009), Pan et al. (2006), Inosov et al. (2007) and Zhang et al. (2008b). As an example, the high-energy structure in the ARPES spectra of the cuprates has also been analysed in Valla et al. (2007) for several doping levels in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) and \( \text{La}_{2−x}\text{Ba}_x\text{CuO}_4 \). Frame 17 reproduces their results for one sample of \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) and \( \text{La}_{2−x}\text{Ba}_x\text{CuO}_4 \) at \( x = 1/8 \), the critical doping where, due to stripe formation, \( T_c \rightarrow 0 \) in this material. Frame (a) gives a model for the electron–boson spectral density which was chosen to reproduce the data for the real part of the self-energy shown in (b). In (c) the corresponding imaginary part is shown (heavy lines) and compared with the data (thin lines). A similar comparison for the \( \text{La}_{2−x}\text{Ba}_x\text{CuO}_4 \) sample is shown in (d)–(f). Here the solid red line is the spin-fluctuation spectrum determined from neutron magnet scattering by Tranquada et al. (2004) and the black dashes are the modified spectrum used to get
a better fit to the ARPES data (frame (e)). The authors conclude that this represents evidence for coupling to spin fluctuations. There have also been reports of additional low energy structures seen in ARPES spectra of optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ by Rameau et al (2009) who report coupling to a zero momentum optical out-of-plane $c$-axis even-phonon mode with energy 8 meV and a $\lambda \approx 0.5–0.4$. Recently several groups have reported new kink-like features in the ARPES dispersion curves at very low energies which depend on temperature and doping (Plumb et al 2010, Vishik et al 2010, Anzai et al 2010).

The nodal direction high-precision data of Zhang et al (2008a) in optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ was inverted using the maximum entropy (MaxEnt) technique by Schachinger and Carbotte (2008). They discuss finite band effects and obtain the results shown in panel (a) of figure 18 for four temperatures, namely 17 K (solid), 45 K (long dashed), 99 K (dotted) and 128 K (dashed–dotted). In their work the MaxEnt technique is used to get an estimate of the electron–boson spectral density using an approximate relationship between the self-energy and the bosonic spectral function. The resulting approximate electron–boson spectral density is then parametrized and used in the full Eliashberg equations included in d-wave symmetry and finally a least squares fit to the data is performed. The spectrum obtained evolves with temperature and the mass enhancement parameter $\lambda$ changes from 1.12 at 17 K to 0.73 at 128 K. The lowest $T$ case shows a peak around 65 meV which remains at 128 K but with reduced amplitude and its centre shifted to a higher frequency. A second component is a prominent background extending to $\approx 400$ meV. In the solid curve (at 17 K) we note a valley at $\approx 115$ meV and a second structure around 150 meV. A constant background for the spectral density is characteristic for the marginal Fermi liquid which displays quantum critical behaviour and was used early on to interpret ARPES spectra (Valla et al 1999a, 1999b, 2000). This model, however, is not consistent with a peak in the spectral density seen here around 65 meV. An explanation of this peak in terms of phonons has been advanced by Lanzara et al (2001). The role of phonons in generating the nodal peak will be discussed further in the next section, but it is worth noting here that a recent study attempts to explain, within a phonon model, the evolution of the spectral function with temperature, an effect not normally expected for phonons. Meevasana et al (2006) have made a comparative study by ARPES of an optimally doped and a strongly overdoped non-superconducting Bi$_2$Sr$_2$CuO$_6$ sample which is single-layered. They find a weakening of the self-energy renormalization as well as a shift to higher energies with overdoping, an effect they related directly to changes in the coupling to $c$-axis phonons which results from increased metallicity (increased screening).

The data of Zhang et al (2008a) were also analysed by Bok et al (2010). A maximum entropy inversion method was used and the results are reproduced in panel (b) of figure 18 for six directions, labelled from nodal at 0° to 25° in steps of 5°. The results are very similar to those of Schachinger and Carbotte (2008) for the nodal direction. Off the node there is little change at energies below 200 meV. The main changes with angle along the Fermi surface are in the location of the high-energy cutoff which starts around 400 meV at 0° and is reduced to roughly 250 meV at the largest angle considered, 25°. All this provides evidence that the mechanism involved in the charge carrier self-energy is not exclusively phonons and is in fact dominated by some higher energy electronic mechanism, possibly spin fluctuations. We return next to our discussion of the nodal direction isotope effect data of Iwasawa et al (2008).
Figure 17. ARPES self-energy fits to models in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Reprinted with permission from Valla et al (2007). Copyright 2007 by the American Physical Society. (a) A model bosonic spectrum used in fits to the data consisting of a peak and a high-frequency background. (b) Re $\Sigma$ measured in Bi-2212 (thin lines) and model Re $\Sigma$ obtained from the spectrum in (a) (bold line). (c) Corresponding Im $\Sigma$. (d)–(f) Same for La$_{2-x}$Ba$_x$CuO$_4$ at $x = 1/8$. Solid lines represent neutron scattering data from Tranquada et al and the self-energies derived from them. Dashed lines represent the excitation spectrum and derived self-energies that better model the high-energy region of measured self-energies (green circles) (near or nodal direction). Note the need for high-energy spectral weight beyond the spin excitations revealed by neutron scattering.

Schachinger et al (2009) (see also Schachinger and Carbotte 2010) have used the spectrum recovered from nodal direction ARPES data in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ which is displayed in panel (a) of figure 18 to calculate in the d-wave superconducting state the real part of the quasiparticle self-energy Re $\Sigma(\omega)$ expected when the isotope O$^{16}$ is substituted by O$^{18}$. In this calculation they assume that only the peak in $\alpha_k F_k(\omega)$ around $\omega \approx 60$ meV seen in panel (a) of figure 18 is due to coupling to an oxygen phonon. The background below this peak which also extends to 400 meV is assumed to be due to some other interaction. Applying an isotope shift of $\sqrt{16/18} = 0.94$ to this peak only, they are able to explain the shift seen in the data of Iwasawa et al (2008). They take this as evidence that in optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ phonons contribute $\sim 10\%$ to the area under the nodal direction electron–boson spectral density.

We return next to studies of boson structure away from the nodal direction towards the antinode. Studies across families of superconductors as well as away from the nodal direction can be helpful. One-, two- and three-layer Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n = 1, 2, 3$) are compared in the work of Sato et al (2003). Renormalized dispersion curves are shown in figure 19. Top to bottom are Bi-2201 ($n = 1$) UD (underdoped) $T_c = 18$ K, Bi-2212 ($n = 2$) OP (optimally doped) $T_c = 90$ K and Bi-2223 ($n = 3$) UD (underdoped) $T_c = 100$ K. The left columns are nodal data at various temperatures while the right columns give results for a cut closer to the antinodal direction as shown in the inset. In contrast to the single-layer case, for $n = 2$ and $n = 3$ there is a strong evolution of the dispersion curve kinks as one moves towards the antinode and lowers the temperature into the superconducting state. These features correlate with some of the features associated with the spin resonance. On the other hand for $n = 1$ almost no temperature dependence is observed. This would seem to imply that in this case there is no coupling to the resonance mode which gives rise to the strong temperature dependence in the other two cases. The authors further conclude that the kink in the nodal direction may have a different origin from that in the antinodal which is possibly the spin resonance. Lee et al (2009) have studied Tl compounds and find a similar behaviour. For this family, however, a spin-one resonance has been observed (He et al 2002) in its single layer version. This leads Lee et al (2009) to suggest that this disfavours strong coupling to the spin resonance in all cases and suggests that coupling to a c-axis phonon can provide a more natural explanation of the data. On the other hand, Wei et al (2008) have observed a peak–dip–hump structure in the
antinodal direction in an optimally doped Bi$_2$Sr$_{1.6}$La$_{0.4}$CuO$_6$ sample with $T_c = 34$ K. They find a peak–dip separation of only 19 meV in this system, much smaller than for multilayered samples. This scale is consistent with observed values of the spin excitations in single-layered cuprates. This leads the authors to favour a spin origin for their observations and reject the notion that it may be due to a phonon. Certainly all oxygen-related phonons have energies above 35 meV.

Terashima et al (2005) have studied the effect of substituting Ni or Zn for the in-plane Cu in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (see also Zabolotnyy et al (2006)). Their pristine sample has $T_c \sim 91$ K dropping to $80$–$85$ K for the 0.5–1.0% Zn–Ni substituted samples. With impurities, the off-diagonal kink is found to be noticeably weakened which is taken as an indication that the coupling to the boson involved is reduced. As a function of angle in the Brillouin zone the weakening is the largest in the antinodal direction and is almost zero in the nodal direction. As figure 20 shows the antinodal kink survives as a function of temperature well above $T_c$ for the Zn-substituted sample (non-magnetic impurity) but not in the pristine and Ni substituted (magnetic impurity) case. This observation parallels what is seen in inelastic polarized neutron scattering experiments in YBa$_2$Cu$_3$O$_{6.9-\delta}$ for the effect of Zn and Ni on the spin resonance shown in the right panel of figure 20. It is important to note that both Zn and Ni have a mass similar to that of Cu and would not be expected to change the lattice dynamics significantly.

Cuk et al (2004) among others have studied boson structure evolution as the antinodal direction is approached. Their optimum Bi$_2$Sr$_2$CaCu$_2$O$_{7.9}$ sample had a $T_c = 94$ K. They find a kink in the normal (above $T_c$) state at $\omega \sim 40$ meV for angles $22^\circ$ to $27^\circ$ off the antinodal direction. In the superconducting state at $T = 10$ K a peak–dip–hump structure is seen with boson signature at 70 meV, a value which agrees with 40 meV shifted by the superconducting gap value. They also note that for an underdoped sample with $T_c = 85$ K and a large superconducting gap the structure remains at $\sim 70$ meV, while for a deeply overdoped sample ($T_c = 65$ K or $\delta \geq 22\%$) the kink energy shifts to 40 meV consistent with a much smaller superconducting gap value. While some of these observations are consistent with a spin resonance interpretation of the boson involved, some are not. The 40 meV kink remains in the normal state and is sharp in the superconducting state of the overdoped $T_c = 65$ K sample. On the basis of this evidence and other facts, the authors suggest that the boson involved is the 40 meV B$_{1g}$ phonon involving out-of-plane motion of the in-plane oxygen (for more details see also Devreese et al (2004)). Sandvik et al (2004) have studied theoretically how the minimum dependence specific to coupling to a phonon or spin fluctuation manifests itself in ARPES. They find only qualitative changes between the two mechanisms and no easily recognized distinct signature which would unambiguously favour phonons or spin fluctuations.

Returning to the work of Borisenko et al (2006) we note that in their experiment on YBCO they compared their ARPES spectra with spin susceptibility measured with inelastic neutron scattering on exactly the same samples. Using a simple model these authors found that the various kinks, dips and humps in the ARPES spectra across the whole Brillouin zone were caused by spin fluctuations. It should be noted that several of the magnetic excitations, including a new high mode and continuum contributed to the spectra.

3. Optical properties

One of the simplest measurements that can be made on a metallic system is the dc resistivity. Right from the beginning it was obvious that the high-temperature superconductors were very different from ordinary metals (Gurvitch and Fiory 1987, Martin et al 1990). Their dc resistivity had a linear temperature dependence with a zero temperature intercept at zero resistivity. In simple metals where the electron–phonon interaction is the dominant scattering mechanism this intercept is approximately at $\theta_{DB} / 4$ and in a model system with an Einstein phonon at $\Omega_0$ one would expect the intercept to be at $\Omega_0 / 4$. These early observations motivated the search for scattering models with a continuous spectrum of bosonic excitations without an energy scale such as the
marginal Fermi liquid theory (Varma et al 1989) but studies of dc transport as a function of doping soon showed that the situation was much more complicated at doping levels away from optimal doping where this simple behaviour is seen: at low doping the pseudogap had a profound influence on dc transport while in the overdoped region a quadratic temperature dependence seemed to emerge, characteristic of electron–electron scattering. The optical conductivity offers deeper insight into the influence of bosonic excitations on the transport of charge in a metallic system. A comprehensive review of the optical properties of high-temperature superconductors can be found in Basov and Timusk (2005). In a metal the standard formula for the current $J$ in the presence of an electric field $E$ (Ziman 1972) is given by

$$J = \sigma \cdot E = \frac{e^2}{4\pi^3} \int dS_F \frac{\tau_k v_k v_k \cdot E}{v_k} \frac{1}{1 - i\tau_k \omega},$$

where $\sigma$ is the conductivity tensor, $E$ the applied field, $\tau_k$ the lifetime of state $k$ and $v_k$ its velocity. The integration is carried out over the Fermi surface. The conductivity is proportional to the component of the velocity in the direction of the applied field $E$ averaged over the Fermi surface and it is also proportional to the factor $\tau_k$ which can vary over the Fermi surface independently.

In a dirty metal where impurity scattering dominates $\tau$ is a constant and the classical Drude formula for the conductivity holds:

$$\sigma(\omega) = \frac{1}{4\pi} \frac{\omega_p^2}{1/\tau - i\omega}.$$  

The real part of $\sigma(\omega)$ is a Lorentzian at zero frequency with an oscillator strength $\omega_p^2/8$. For a spherical Fermi surface $\omega_p^2 = 4\pi n e^2/m_e$, where $n$ is the free-carrier density and $m_e$ is the electronic band mass. The imaginary part of $\sigma(\omega)$ is just the real part multiplied by $\omega\tau$. 

Figure 19. ARPES dispersion of one-, two- and three-layer superconductors. Reprinted with permission from Sato et al (2003). Copyright 2003 by the American Physical Society. Left panels are Brillouin zone cuts in the nodal direction, right panels are closer to the antinode (the arrow in each inset shows the cut). There is a systematic increase in the strength of the kink at 50 meV as one moves away from the node in all cases. Note that the kink is stronger as the number of layers increases.
If the electrons are scattered by bosonic fluctuations $\tau$ becomes frequency dependent, and the extended Drude model or memory function technique can be used (Mori 1965, Götze and Wölfle 1972, Allen and Mikkelsen 1977, Puchkov et al 1996). The extended Drude formula is written as

$$\sigma(\omega, T) = \frac{\pi}{4\tau} \frac{\omega^2}{\pi} \frac{1}{\tau^{\rho\rho}(\omega, T)} - \frac{\omega^2}{\pi} \frac{\omega^2}{\tau(\omega, T)},$$

where $1/\tau^{\rho\rho}(\omega, T)$ describes the frequency-dependent optical scattering rate and $\lambda^{\rho\rho}(\omega, T)$ is the optical mass enhancement factor. By analogy to the case of quasiparticles, an optical self-energy, $\Sigma^{\rho\rho}(\omega)$ can be defined with minus twice its imaginary part given by $1/\tau^{\rho\rho}(\omega)$ and the real part related to $\lambda^{\rho\rho}(\omega)$.

One can solve for $1/\tau^{\rho\rho}(\omega)$ and $1 + \lambda^{\rho\rho}(\omega)$ in terms of the experimentally determined optical conductivity to find

$$\frac{1}{\tau^{\rho\rho}(\omega)} = \frac{\omega^2}{4\pi} \text{Re} \left[ \frac{1}{\sigma(\omega)} \right].$$

The dc resistivity is the zero frequency limit $\rho_{dc}(T) = 1/\sigma_{dc}(T) = m_e/\tau(T)n_e^2$ since $\sigma(\omega)$ is real in the zero frequency limit. The mass enhancement factor $\lambda(\omega)$ is given as the imaginary part of $1/\sigma(\omega)$:

$$1 + \lambda(\omega) = -\frac{\omega^2}{4\pi} \frac{1}{\omega} \text{Im} \left[ \frac{1}{\sigma(\omega)} \right].$$

The total plasma frequency $\omega_p^2$ can be found from the sum rule $\int_0^\infty \sigma_1(\omega) d\omega = \omega_p^2/8$. Allen (1971) and Shulga et al (1991) give the following expressions for $1/\tau(\omega, T)$ and its $T = 0$ limit:

$$\frac{1}{\tau^{\rho\rho}(\omega, T = 0)} = \frac{2\pi}{\omega} \int_0^\omega d\Omega \alpha_p^2(\Omega) F(\Omega) \left( \frac{\omega - \Omega}{2T} \right)^2 + \frac{1}{\tau_{imp}}.$$

Here $\alpha_p^2(\Omega) F(\Omega)$ is a weighted phonon density of states appropriate to transport and $T$ is the temperature measured in frequency units. Transport and quasiparticle electron–boson spectral density differ through a factor that weights more strongly back scattering in transport as compared with quasiparticle scattering but we will not emphasize these differences here. The last term in equation (12) represents impurity scattering.

The simple approximations of Allen (1971) and Shulga et al (1991) can be justified through the use of the Kubo formula approach where the optical conductivity is related to the current–current correlation function which involves the overlap of two Green’s functions, one displaced in energy from the other by the photon energy $\Omega$. In the most general formulation vertex corrections also need to be considered. To include inelastic scattering by bosons, an energy-dependent self-energy needs to be included in the formalism written in real frequency axis formulation. An alternative is to stay on the imaginary Matsubara frequency axis and use analytical continuation using the Padé approximant (Nicol et al 1991). For numerical implementation on the real axis an efficient formula within Eliashberg theory including an s-wave superconducting gap was given by Marsiglio et al (1988). To go from the Green’s function to the frequency-dependent conductivity $\sigma(\omega, T)$ the necessary formula was given by Lee et al (1989). This was evaluated numerically by Akis et al (1991) who provided results for the real part of the conductivity including s-wave superconductivity, and Marsiglio et al (1996) who considered the imaginary part.
The calculations can also be generalized to the marginal Fermi liquid (Nicol and Carbotte 1991). The necessary generalization to d-wave superconductivity was given by Carbotte et al (1995) and by Jiang et al (1996). To consider a gap with d-wave symmetry, it was first necessary to include the possibility of different spectral densities $a^2 F(\Omega)$ entering the gap and the renormalization channels. In the simplest possible approximation the same shape $a^2 F(\Omega)$ is retained but its magnitude is allowed to be different in each channel with a parameter giving the ratio of d- to s-wave projections of the underlying spectral density (Carbotte and Jiang 1993, 1994). These equations have since been applied to the calculation of other related properties including phonon self-energies (Marsiglio et al 1992), penetration depth (Arberg et al 1993, Arberg and Carbotte 1994, Schachinger et al 1997), microwave conductivity (Schachinger and Carbotte 1998a), thermal conductivity (Schachinger and Carbotte 1998b) and Raman scattering (Jiang and Carbotte 1996). A comparison of quasiparticle self-energy effects and optical signature was given by Schachinger et al (2003) and by Carbotte et al (2005). Most formulations as described above involve the infinite band approximations with a constant density of states. There are corrections coming from finite band effects both in the normal state properties (Mitrović and Carbotte 1983a) and the superconducting ones (Mitrović and Carbotte 1983b) with the initial state position $(\phi, \theta)$ given by Schachinger (1998a,b) and Carbotte and Jiang (2005). Most formulations as described above involve the infinite band approximation with a constant density of states.

In the infinite band approximation with a constant density of electronic states the conductivity at temperature $T$ and frequency $\omega$ is given by

$$\sigma(T, \omega) = \frac{a^2 \bar{\omega}}{4\pi} \int_{-\infty}^{\infty} \frac{f(v) - f(v + \omega)}{\omega + \Sigma^*(\omega) - \Sigma(v + \omega)} dv,$$

where $a_0^2$ is the plasma frequency, $f$ the Fermi function and $\Sigma(\omega)$ the complex quasiparticle self-energy. At $T = 0$ this reduces to

$$\sigma(T = 0, \omega) = \frac{a_0^2}{4\pi} \int_{0}^{\omega} \frac{1}{\omega + \Sigma^*(\omega) - \Sigma(v)} dv,$$

where $\omega_p$ is the plasma frequency, $f$ the Fermi function and $\Sigma(\omega)$ the complex quasiparticle self-energy. At $T = 0$ this reduces to

$$\sigma(T = 0, \omega) = \frac{a_0^2 \bar{\omega}}{4\pi} \int_{0}^{\omega} \frac{1}{\omega + \frac{1}{\tau_{\text{imp}}} - \Sigma^*(\omega) - \Sigma(\omega - \nu)} dv,$$

where we have made the elastic impurity contribution to the imaginary part of the quasiparticle self-energy explicit with $1/\tau_{\text{imp}}^{\text{dp}} = 2/r_0^{\text{dp}}$, with $1/\tau_{\text{imp}}^{\text{el}}$ the quasiparticle elastic scattering rate. In deriving these equations it is assumed that the anisotropy in the electron–boson scattering rate can be neglected and the self-energy depends only on frequency and not on the direction or magnitude of the momentum. For many purposes this is perhaps a reasonable first approximation but it needs to be kept in mind that even in simple metals such as aluminum the electron–phonon interaction does exhibit anisotropy (see Leung et al 1976).

A multiple plane wave calculation of the electron–phonon interaction by Leung et al (1976) shows that the directional spectral density $a^2 F(\phi, \theta, \Omega)$ versus $\Omega$ varies considerably with the initial state position $(\phi, \theta)$ on the Fermi surface.

**Figure 21.** Bosonic spectral function $a^2 F(\Omega)$ from tunnelling data of Pb adapted by McMillan and Rowell (1965) (dotted curve) compared with a calculated $a^2 F(\Omega)$ (solid curve) based on a four plane wave electronic function (Tomlinson and Carbotte 1976). The phonons were modelled by a Born–von Karman model based on neutron scattering.

Note that

$$a^2 F(\Omega) = \frac{V}{8\pi^2 \hbar} \int_{S_k} \frac{dS_k}{\hbar v_k} \sum_{\lambda} |g_{k\lambda}|^2 \delta(\Omega - \Omega_{\lambda}(k' - k)),$$

where $dS_k$ is a Fermi surface element, $v_k$ the Fermi velocity, $V$ the volume, $\hbar$ Planck’s constant, $g_{k\lambda}$ the electron–phonon matrix element for scattering from initial state $k$ on the Fermi surface to all final states $k'$ again on the Fermi surface emitting a phonon of energy $\Omega_{\lambda}(k' - k)$ with $\lambda$, a branch index. The mass enhancement factor $\lambda_k$ associated with the directional $a^2 F(k, \Omega) F(k, \Omega)$ and given by $2 \int a^2 F(\Omega) F(k, \Omega) d\Omega / \Omega$ displays considerable anisotropy, of the order of 20%. The superconducting critical temperature of such a material is determined not by the directional $a^2 F(k, \Omega)$ but by its Fermi surface average

$$a^2 F(\Omega) = \frac{\int_{S_k} \frac{dS_k}{\hbar v_k} a^2 F(k, \Omega) F(k, \Omega)}{\int_{S_k} \frac{dS_k}{\hbar v_k}}$$

over all the initial states of the Fermi surface. Anisotropy can increase the value of the critical temperature but this is usually a very small effect. Impurities wash out anisotropy and conventional metals are often in the isotropic limit. For example, in figure 21 we show the results of multiple plane wave calculations of $a^2 F(\Omega)$ for Pb conducted by
Tomlinson and Carbotte (1976). The solid curve shows the result of the numerical calculation while the dotted curve given for comparison is the experimental results obtained from superconducting tunnelling experiments by McMillan and Rowell (1965). It is this average function which is most relevant to discussions of the mechanism of superconductivity. In this regard the experimentally measured optical conductivity, like the quasiparticle density of states of tunnelling, is an average property over all the electrons. Angle-resolved photoemission is momentum specific and yields a directionally specific spectral density which needs to be averaged over directions before it can be made the basis for a discussion of the magnitude of the critical temperature. This same average function determines the many properties of the superconducting state in real materials which differ from BCS predictions (Carbotte et al 1986, Marsiglio et al 1987, 1992, Mitrović et al 1980, Schachinger et al 1980). Carbotte et al (2005) have given a discussion of the relationship between optics and quasiparticle self-energy. While these are not the same they have some commonality.

In modern discussions of the optical conductivity it has become standard practice to represent the results of experiments as well as calculations based on the Kubo formula in the extended Drude form, equation (8). A very useful but approximate formula for $1/t^{\varphi}(\omega)$ was given by Allen (1971) and extended to finite temperatures by Shulga et al (1991) as equation (11) and equation (12), respectively. The Shulga formula, equation (12), was originally derived using ordinary perturbation theory without explicit reference to many-body theory and in particular to Eliashberg theory. Others (Marsiglio et al 1998, Marsiglio 1999) have given more analytical arguments that justify equation (12). Extensions to energy-dependent densities of states have been provided by Sharapov and Carbotte (2005) based on previous work of Mitrović and Fiorucci (1985).

In as much as the approximate equation (11) is applicable one immediately finds that

$$\alpha^2(\Omega)F(\Omega) \equiv W(\omega) \equiv \frac{1}{2\pi} \frac{d^2}{d\omega^2} \left[ \frac{\omega}{t^\varphi(\omega)} - 1 \right].$$

We can write the equation above in terms of the optical conductivity as follows using equation (9):

$$W(\omega) \equiv \frac{\omega^2}{8\pi^2} \frac{d^2}{d\omega^2} \left[ \omega \text{ Re} \left[ \frac{1}{\sigma(\omega)} \right] \right].$$

The validity and limitations of equation (17) can be tested against complete numerical calculations of the conductivity based on the Kubo formula and Eliashberg equations. The results are shown in figure 22 from Marsiglio et al (1998). The solid curve is the $\alpha^2F(\Omega)$ versus $\Omega$ obtained for Pb by McMillan and Rowell (1965) from tunnelling data. This function is then used as input for the normal state numerical calculation of the optical conductivity. The derivative indicated by equation (17) is carried out on the numeric data for the conductivity and $W(\Omega)$ (denoted $\alpha^2F(\Omega)$ in the figure) computed at $T = 1\, \text{K}$ (the dotted curve) agrees remarkably well with the input $\alpha^2F(\Omega)$ and shows that in this case at least, the optical conductivity can provide information on the underlying electron–boson spectral density in the system. Note the negative tails at higher energies which appear in $W(\Omega)$ but have to be ignored as they cannot be part of the spectral density, which by definition is positive definite. But in the phonon energy range, the second derivative $W(\Omega)$ and $\alpha^2F(\Omega)$ are very close to each other in shape and in absolute value. In this regard $W(\Omega)$ is a dimensionless function. Of course, while equation (17) was established only at $T = 0\, \text{K}$ and is approximate, it can be generalized to finite temperatures but for now we point out that a simple second derivative of the optical scattering rate starts to deviate more seriously from the spectral density we wish to know as we raise the temperature. At $T = 14\, \text{K}$ the curve for $W(\Omega)$ shows a single peak which is much broader than the two peak structure of the input function. Roughly speaking there is a thermal smearing which makes the simple correspondence between $W(\Omega)$ and $\alpha^2F(\Omega)$ less accurate and eventually, at higher temperatures, completely breaks down.

One can ask, can one obtain experimental data of sufficient accuracy to be able to extract from it a detailed and accurate image of $\alpha^2F(\Omega)$? The answer is yes as demonstrated by Farnworth and Timusk (1976). In figure 23 their optical results (solid curve) are compared with the dotted curve obtained from tunnelling. The agreement is very good and shows quite explicitly that the optical conductivity can yield the electron–phonon spectral density in the case of Pb. We note that the optical data seem to contain more details than do the tunnelling data and show in particular an image of phonon lifetime effects at twice the gap (structure labelled A).

In isotropic systems at low temperatures our results show that there exists a close relationship between the quasiparticle self-energy $\Sigma^{\varphi}(\omega)$ and the corresponding optical self-energy $\Sigma^{\sigma}(\omega)$ defined in terms of the generalized Drude formula equation (8). As we have verified that equation (17) holds with $1/t^{\varphi}$ given by equation (11) we see that $d/\omega[\omega/t^{\varphi}(\omega)] \equiv \pi \int_0^\infty \alpha^2F(\Omega) \, d\Omega$ which is...
features in the neutron density of states of lead. The peak A at the point C. The peaks B, D and F are in good agreement with the American Physical Society. The curves have been normalized at permission from Farnworth and Timusk (1976). Copyright 1976 by density of states (dashed line) in the same material. Reprinted with optical absorption (solid line) of Pb compared with tunnelling finite temperature generalization and Hwang the same approximation. Carbotte exactly equal to twice the quasiparticle scattering rate in Figure 23.

Figure 23. Electron–phonon spectral density $\alpha^2 F(\Omega)$ from the optical absorption (solid line) of Pb compared with tunnelling density of states (dashed line) in the same material. Reprinted with permission from Farnworth and Timusk (1976). Copyright 1976 by the American Physical Society. The curves have been normalized at the point C. The peaks B, D and F are in good agreement with features in the neutron density of states of lead. The peak A at $\omega = 2\Delta$ is associated with phonon lifetime effects.

eaxactly equal to twice the quasiparticle scattering rate in the same approximation. Carbotte et al (2005) provided a finite temperature generalization and Hwang et al (2007a) have considered the case when the density of electronic states is not constant as in finite bands. One can define an intermediate quantity $1/\tau^{\text{op}-\text{qp}}(\omega)$ directly through the measured conductivity scattering rate:

$$
\frac{1}{\tau^{\text{op}-\text{qp}}(\omega)} = \frac{d}{d\omega} \left[ \frac{\omega}{\tau^{\text{qp}}(\omega)} \right], \quad (19)
$$

and take this to provide a first estimate of the momentum-averaged quasiparticle scattering rate from which the real part of $\Sigma^{\text{op}}(\omega)$ follows by KK transformation. Complete numerical results based on the Eliashberg equation are presented in figure 24 for a three-delta function model of $\alpha^2 F(\Omega)$ with peaks at 0.04, 0.09 and 0.19 eV. The green dashed curve shows the results of a numeric calculation of the Kubo formula for the conductivity from which $\Sigma^{\text{op}}(\omega)$ is extracted. We see little boson structure in this curve. The solid red curve, however, is extracted from the green as $-d[\omega \Sigma^{\text{qp}}(\omega)]/d\omega$ and is to be compared with the blue dashed–dotted curve for the quasiparticle self-energy calculated for the same spectral density within the Eliashberg theory. The agreement with the solid red curve is good and shows that both methods are able to give the same results. Of course, this only holds if anisotropy can be neglected.

Thomas et al (1988) analysed their reflectivity data in YBa$_2$Cu$_3$O$_{6+x}$ with $T_c = 92$ K to recover a rough estimate of the underlying spectral density. Within the analysis they equate the optical scattering rate with its quasiparticle equivalence and recover a spectrum extending from 30 to 70 meV with a mass enhancement parameter of the order of 9. A similar calculation was performed by Collins et al (1989) who find a peak at about 33 meV and broad background that extends to rather high energies with a coupling constant $\lambda$ of about 2–3. Carbotte et al (1999) took a somewhat different approach taking guidance from measured spin-polarized neutron scattering of Bourges et al (1999). A spin resonance peak at 41 meV is observed around $(\pi, \pi)$ in momentum space. This peak occurs only below $T_c$. They used their Eliashberg analysis generalized to include approximately a superconducting transition to a d-wave gap to perform two calculations. In the first calculation they use a smooth spectrum without the low-temperature resonance peak to model an $\alpha^2 F(\Omega)$ function which they denote by $I^2 \chi(\Omega)$ to better reflect its inspiration from spin fluctuation theory and adjust its strength to get the measured $T_c$. The coupling between electrons and spin-fluctuations is then kept fixed but the shape of the spectrum is readjusted to include the measured spin resonance peak and the conductivity at 5 K in the superconducting state is calculated. In figure 25 (top frame) we show the model $I^2 \chi(\Omega)$ (solid triangles) used as well as the second derivative of the real part of the inverse of the conductivity which according to equation (18) serves as the definition of $W(\Omega)$ in the superconducting state. On theoretical grounds there is no reason why this derivative should agree with the input $I^2 \chi(\Omega)$. But it was found numerically that the resonance peak in $I^2 \chi(\Omega)$ agrees well with $W(\omega)$ provided its frequencies are displaced by the superconducting gap value. In the Eliashberg calculations the gap was 28 meV so that the resonance plus gap frequency was 69 meV. Processing the experimental data in the same way gives the solid curve in the upper frame of figure 25 which

Figure 24. Calculation by Hwang et al (2007a) that shows that an image of the quasiparticle self-energy $\Sigma^{\text{qp}}(\omega)$ can be extracted from optical self-energy via the derivative of $\omega \Sigma^{\text{qp}}(\omega)$ (solid red curve). It agrees well in magnitude and detailed structure with the exact theoretical curve for $\Sigma^{\text{qp}}$ (dashed–dotted blue). The optical self-energy itself (dashed green) is almost structureless and does not agree with the $\Sigma^{\text{qp}}$ curve. Copyright 2007 by the American Physical Society.
Figure 25. Inversion of the superconducting state optical conductivity for YBCO from Carbotte et al (1999). (a) Comparison of a model calculation of the bosonic spectral function based on measured neutron spin susceptibility (triangles) with the derivative of the optical conductivity $W(\omega)$ (equation (18)). (b) $W(\omega)$ derived from the experimental data for the conductivity of an optimally doped YBa$_2$Cu$_3$O$_{6.95}$ single crystal with $a$-axis polarization (solid curve) and for an underdoped, untwinned YBa$_2$Cu$_3$O$_{6.6}$ single crystal (dashed line). The results bear considerable resemblance to the theoretical curve and gives strong evidence for coupling to the spin resonance in the superconducting state at 5 K. In the lower frame of figure 25 the results for $W(\omega)$ in YBa$_2$Cu$_3$O$_{6.95}$ (solid curve) are compared with results for underdoped sample of YBa$_2$Cu$_3$O$_{6.6}$ (dashed curve) which shows that the resonance seen in optics moves to lower frequency with underdoping. In later work Schachinger and Carbotte (2000) further applied their method to other systems. From the second derivative of the measured optical conductivity in the superconducting state they conclude that YBa$_2$Cu$_4$O$_8$ (Y124) ($T_c = 82$ K), Tl$_2$Ba$_2$CuO$_{6+\delta}$ ($T_c = 90$ K), and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ ($T_c = 90$ K) should have spin-one resonances at 38 meV, 43 meV and 46 meV, respectively, while overdoped Tl$_2$Ba$_2$CuO$_{6+\delta}$ ($T_c = 23$ K) should have none. After their work, a resonance in Tl$_2$Ba$_2$CuO$_{6+\delta}$ with ($T_c = 90$ K) was indeed measured (He et al 2002) at 47 meV but with a rather small resolution limited width. In figure 26 we show results obtained by Schachinger and Carbotte (2000) for the case of Y124 with $T_c = 82$ K. What is shown in the lower frame are the experimental results of Puchkov et al (1996) at 300 K (light solid) in the normal state for the optical scattering rate which is a fit (light dashed line) in Eliashberg calculations of the conductivity with input spectral density given by a simple spin-fluctuation form (MMP),

$$I^2\chi(\omega) = I^2_s \frac{\omega}{\omega^2 + \omega_{sf}^2},$$

(20)
cut off at $\omega_c \approx 300-400$ meV (Millis et al 1990) and $\omega_{sf} = 80$ meV referred to as an MMP form. The heavy solid black curve is the experimental results at $T = 10$ K in the superconducting state. These experimental results were then processed to get the second derivative $W(\omega)$ and only its resonant piece which peaked at 38 meV (resonance) + 24 meV (gap) = 62 meV was retained and used to modify the MMP
form found at $T_c$ by replacing its value below 38 meV by the resonance peak which was interpreted as a spin resonance contribution. The result was the heavy dashed curve for the calculated superconducting state optical scattering rate of figure 26 (lower frame) which agrees well with the data (heavy solid curve). The second derivative curve obtained from the theoretical data is shown as the dashed curve in the upper frame which agrees well with the experimental data (solid curve) in the resonance energy region up to 62 meV and with the ($T = 10 \text{ K}$) input spectral density (solid squares) for $I^2\chi(\omega)$. It is important to realize that no reference to neutron scattering data is made in this comparison which proceeds entirely on the basis of charge dynamic data based on optics.

While the second derivative method has been quite useful in the analysis of the optical data, in view of its obvious limitations it seems worthwhile to look at the possibility of having an alternate method which does not suffer from unwanted and unphysical negative tails in $I^2\chi(\omega)$, although it should be noted that Abanov \textit{et al} \textnormal{(2001)} have made use of this negative tail to extract the superconducting gap. One can start with a model problem, namely the inversion of the equation

$$
\frac{1}{\tau^{op}(\omega, T)} = \int_0^\infty d\Omega I^2(\Omega)\chi(\Omega) K(\omega, \Omega, T)
$$

with the kernel $K(\omega, \Omega, T)$ given by the thermal factor in the square brackets of equation \textnormal{(12)} (times $\pi/\omega$) to recover the spectral density $\alpha^2(\Omega)F(\Omega)$ from a finite temperature optical scattering rate $1/\tau^{op}(\omega)$. Dordevic \textit{et al} \textnormal{(2005)} have considered the so-called singular value decomposition (SVD) method and Schachinger \textit{et al} \textnormal{(2006)} considered in addition a maximum entropy scheme and offer comparisons between the two methods. In figure 27 we reproduce a comparison from this last reference. In each frame the input $\alpha^2(\Omega)F(\Omega)$ is given as the shaded curve while the solid, dashed, dotted and dashed–dotted curves give results of the inversion of equation \textnormal{(21)} for $T = 0.3 \text{ K}$, 1 K, 10 K and 50 K, respectively, with computed data for $1/\tau^{op}(\omega, T)$ calculated from (approximate) equation \textnormal{(12)}. The top frame uses the second derivative method, the middle is for SVD and the bottom frame the maximum entropy case, denoted by ME$(\omega)$. All show thermal smearing as $T$ is increased with the double peak moving towards a single peak structure. The SVD curve shows considerable unwanted oscillations and produces negative values for the spectral density. This is not allowed in the maximum entropy case which is a better choice. In figure 28 we show additional inversion results but with two differences. First a spectrum, more appropriate for the normal state when a spin-fluctuation mechanism applies with $I^2\chi(\Omega)$ given by equation \textnormal{(20)}. The second difference is that now the scattering rate on the left-hand side of equation \textnormal{(21)} is based on results obtained from full numerical solutions of the Eliashberg equations and the Kubo formula. As before, the shaded curve is the input $I^2\chi(\Omega)$ and the others the results of the inversion at different temperatures. Note that the SVD solutions (middle frame) have extra wiggles, which are not part of the input $I^2\chi(\Omega)$, and these are absent in the top and bottom frames. While the results in the top frame show a temperature smearing of the peak around $o_d$ and a small shift in this peak towards higher energies not part of the input data, the differences are not large. The same is true for the bottom frame where an MEM is used. As previously commented, it is the entire function $I^2\chi(\Omega)$ which determines the size of the critical temperature in a d-wave Eliashberg superconductor so that the small differences just mentioned as $T$ is increased are not of major concern, at least for this purpose. We will return to the issue later however when we look at the experimental results.

We have seen that the function $I^2\chi(\Omega)$ can be found by the inversion of the optical scattering rate, but it is the real
part of the optical self-energy that is most closely related to the renormalized quasiparticle dispersion curves measured in ARPES. We begin with a discussion of data on $\Sigma^{\text{OP}}(\omega)$ with an eye to a qualitative comparison with ARPES. In figure 29 we show results for $1/\tau^{\text{OP}}(\omega)$ or $-2\Sigma^{\text{OP}}(\omega)$, in the left column and the corresponding real part $-2\Sigma^{\text{OP}}(\omega)$ in the right column from Hwang et al (2004). From top to bottom we go from underdoped to overdoped samples of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, as indicated in the caption and various $\lambda$s in the spin-fluctuation formulation controls the $\Sigma^{\text{OP}}(\omega)$ just above $T_c$ in the normal state. The difference, shown as blue triangles in the left frame, shows that there is an extra peak in the superconducting as compared with the normal state. The peak varies in energy with doping, becoming weaker as one goes from underdoped to overdoped. This agrees with the data of Johnson et al (2001) also shown for ease of reference in the right-hand column. The temperature and doping dependence of the peak seen in optical characteristics can be taken as further support for the interpretation given to this peak by Johnson et al (2001), as related to spin fluctuations.

We point out however that this peak is far too weak to completely saturate the optical self-energy and consequently corresponds to only a small part of the total $I^2\chi(\Omega)$ which, it should be noted, is the quantity most relevant to the glue which causes the superconductivity. We can sharpen this argument by looking not at the self-energy or scattering rates themselves but at the underlying spectra $I^2\chi(\Omega)$ obtained through maximum entropy inversion of the optical data.

This is shown in figure 31 for three samples of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, OPT96A, OD82B and OD60G, from top to bottom, left-hand column, at various temperatures reproduced from Hwang et al (2007b). As we expect from our previous discussion of the corresponding real part of the self-energy, a peak is seen in $I^2\chi(\Omega)$ around 60 meV in the OPT96A sample. This peak is reduced in height as $T$ increases and shifts to higher energies. Also, as the doping increases, the peak loses amplitude and shifts somewhat in frequency. In the overdoped sample OD60G it has almost disappeared. More importantly, the overall magnitude of the spectral density is reduced in the overdoped regime as compared with underdoped. These trends are quantified in figure 32, where we show the energy of the peak position as a function of critical temperature value in the top frame. For our samples $\Omega_\text{peak} \cong 8.0k_B T_c$. Noting that above the peak there is a valley which is particularly prominent at optimum doping (top frame of figure 31, we can also define an area associated with it as we can for the peak. As temperature or doping is increased this valley gets progressively filled in as the peak size reduces and the peak energy moves to higher values. These trends with temperature are qualitatively captured in the phenomenological analysis of Prelovšek and Sega (2006) of the temperature evolution of the magnetic collective mode which they describe using a memory function approach. They also contrast their results with those obtained in a more conventional formalism based on the random phase approximation for the spin susceptibility. In the middle frame of figure 32 we show the peak area (red hexagons) as well as the area of the valley (green diamonds). Both quantities drop towards zero, as $T_c$ is reduced. Similarly the authors define a value of the mass enhancement $\lambda$ associated with the background (blue hexagons) which extends to very high values of energy as well as a mass enhancement associated with the peak (red squares). While the $\lambda$ associated with the peaks is rapidly dropping towards a zero value for $T_c \sim 50$ K, the background $\lambda$ is not. It does decrease with decreasing value of $T_c$ but remains significantly above unity for $T_c \sim 50$ K. It is this $\lambda$ which in the spin-fluctuation formulation controls the size of $T_c$ and not the value of $\lambda$ associated with the peaks seen only in the superconducting state at low temperatures. Returning to the right-hand column of figure 31, we show in frame (d) the temperature dependence found for the peak position in the OPT96A sample. It moves from 60 meV in the superconducting state at 27 K to nearly 100 meV at room
Figure 29. The optical self-energy of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ from Hwang et al (2004). ((a)–(d)) The doping and temperature-dependent optical scattering rate, $1/\tau(\omega)$ at four doping levels. (a) $T_c = 67$ K (underdoped); (b) 96 K (optimally doped); (c) 82 K (overdoped); (d) 60 K (overdoped). ((e)–(h)) The real part of the optical self-energy. The slope of $-2\Sigma^R_1(\omega)$ near $\omega = 0$ is proportional to the mass enhancement factor, and decreases as the doping increases, consistent with other studies. We note the weakening of the feature at 700 cm$^{-1}$ in both sets of curves as the doping level increases.

temperature. At the same time the shape of the spectrum has changed from a sharp peak, around 60 meV followed by a valley which is then followed by a second very broad peak at 200–300 meV, to a simple background which looks much more like the MMP spectrum of equation (20) of spin-fluctuation theory. Below $T_c$, in the superconducting state, the evolution of the peak looks more like a simple reduction of the area under it, while above $T_c$ it also shows a tendency to move. The $T = 300$ K spectra for each of the three samples are compared in frame (e). Each look like MMP forms and are all comparable in size. The temperature evolution just outlined for Bi-2212 is very similar to that for the odd component of the spin susceptibility seen in a sample of YBa$_2$Cu$_3$O$_{6+\delta}$ with $T_c = 52$ K reproduced in frame (f) from the inelastic neutron scattering (Bourges et al 1997, 1999, Fong et al 2000).

We remind the reader that the superconductivity state spectra of figure 31 were obtained using a maximum entropy inversion technique based on a generalization to the superconducting state of our equations (12) and (21) as
developed by Schachinger et al (2006). At zero temperature the appropriate kernel which replaced the kernel $K(\omega, \Omega, T)$ in equation (21) is

$$K_{sc}(\omega, \Omega) = \frac{2\pi}{\omega} \left( (\omega - \Omega)\theta(\omega + 2\Delta_0(\phi) - \Omega) \right)$$

$$\times E \left( \sqrt{1 - \frac{4\Delta_0^2(\phi)}{(\omega - \Omega)^2}} \right),$$

(22)

where the bracket $\langle \rangle$ indicates an integration over angles $\phi$, $\Delta_0(\phi)$ is the d-wave superconducting gap and $E(\omega)$ is the elliptic integral. This form is used to get a first estimate of $I^2\chi(\Omega)$ in the superconducting state. In a final calculation, the spectral density obtained is further modified slightly through a least squares fit to the experimental scattering rates of the full Kubo formula results obtained from the d-wave Eliashberg equations. These are given in Schachinger et al (2006) where the procedure is further described.
Figure 31. The bosonic spectral density $I^2\chi(\Omega)$ of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ as determined by a maximum entropy inversion of the optical scattering rate at three doping levels (OPT96A $T_c = 96$ K, OD82B $T_c = 82$ K and OD60G $T_c = 60$ K). From Hwang et al (2007b).

Copyright 2007 by the American Physical Society. At room temperature all samples exhibit a broad continuum background shown in (e). On lowering the temperature, the broad background peak in the 300 K spectrum evolves into a low-energy peak with a deep valley above it. The spectral weight gained in the peak is roughly balanced by the spectral weight loss in the valley in all three samples. With increasing doping the intensity of the peak and intensity lost in the valley are significantly weakened (see figure 32(b)). (d) shows the temperature dependence of the frequency of the peak maximum in OPT96A marked by a star. (f) shows the local magnetic susceptibility of underdoped YBa$_2$Cu$_3$O$_{6+x}$ from neutron scattering. We note a qualitatively similar temperature evolution to (a).

A more recent application of the MaxEnt inversion is reproduced in figure 33 for the one-layer mercury compound Hg1201 from Yang et al (2009). The top frame shows the experimentally measured scattering rate at a series of temperatures while the bottom frame displays the bosonic spectral function for the eight values of temperature as labelled in the top frame. At low temperatures in the superconducting state we see a prominent low energy peak around 56 meV, which is followed by a valley and then by a second broad region of spectral weight extending to high energies. Subsequent to the optical work, Yu et al (2010) found a spin resonance in inelastic neutron scattering studies at $\Omega_R = 56$ meV in excellent agreement with the above data. This surprisingly high frequency for the neutron resonance was confirmed subsequently by van Heumen et al (2009). The energy of the lower peak $\Omega_r$, while almost constant in the superconducting state, begins to move to higher energy as $T$ rises towards room temperature as seen in this inset to the frame (solid blue.
Figure 32. $T_c$-dependent properties of the peak and the valley in the bosonic spectral function of figure 31 from Hwang et al (2007b). The central peak frequency is proportional to $T_c$, i.e. $\omega_{\text{peak}} = 8.0 k_B T_c$. The peak and valley are closely connected, have a very similar $T_c$ dependence and vanish at the same $T_c = 50$ K. The coupling constant $\lambda_{\text{peak}}$ and $\lambda_{\text{BG}}$ (background). $\lambda_{\text{peak}}$ vanishes at the same $T_c$ as the peak and valley. Copyright 2007 by the American Physical Society.

Figure 33. Top frame: the optical scattering rate $1/\tau_{\text{op}} (T, \omega)$ for Hg1201 versus $\omega$ for 8 temperatures (light curves). The wider curves are our maximum entropy reconstructions. Bottom frame: the electron–boson spectral function $I^2 \chi (\Omega)$ versus $\Omega$. The inset gives the peak position (blue triangles) left scales as a function of temperature and the red squares give the corresponding peak amplitude. Reprinted with permission from Yang et al (2009). Copyright 2009 by the American Physical Society.
The temperature evolution found in the data represents a real extrinsic temperature shift towards higher energies, much of though maximum entropy inversions do incorporate some based on the actual optical data found for Bi-2212 OPT96A,\textsuperscript{22} \(\Delta = 22.4 \text{ meV}\).

Figure 34. The optical self-energy of Hg1201. Reprinted with permission from Yang et al.\textsuperscript{28} Copyright 2009 by the American Physical Society. The inset shows theoretical results based on numerical solutions of the generalized Eliashberg equations (solid blue, superconducting and dashed black, normal state). The electron–boson exchange spectral density used is shown as the dashed–dotted blue curve. The superconducting gap value is from the Kubo formula and full Eliashberg equations. The temperature and frequency-dependent optical scattering rate thus obtained are then inverted using an unbiased and also a biased technique. This leads, respectively, to the blue pentagon and green diamond results for peak position, width, height and area (clockwise from top left) shown in figure 35. It is clear that biased or unbiased results are quite similar with greatest differences seen for peak height. Since \(I^2\chi(\Omega)\) was never changed with temperature, the significant temperature dependence seen for the width and height of the peak around 60 meV in the spectral density used is due to the maximum entropy inversion itself. It is not in the input spectral density. Nevertheless, when these results are compared with the red hexagon symbols of figure 35 which represent inversion based on the actual optical data found for Bi-2212 OPT96A, we see that the real data show much more evolution with temperature than do the numerical simulations. Thus, even though maximum entropy inversions do incorporate some extrinsic temperature shift towards higher energies, much of the temperature evolution found in the data represents a real shift in the spectral function itself.

A closer comparison between optics and the spin susceptibility measured in inelastic neutron scattering can be made in La\(_{2−x}\)Sr\(_x\)CuO\(_4\) as reported by Hwang et al.\textsuperscript{29} As we have already described, the electron–boson spectral density is a function associated with all the transitions of the electrons at or around the Fermi energy from an occupied state to all the possible final states, again on and around the Fermi energy to the unoccupied states through the exchange of a boson to which momentum has been transferred. These transitions provide an average over all the bosons defined in the Brillouin zone and as such the resulting spectral density should retain an identifiable similarity in shape to the local i.e. momentum-averaged spin susceptibility. Vignolle et al.\textsuperscript{4} have given results for the local spin susceptibility in La\(_{2−x}\)Sr\(_x\)CuO\(_4\) and find a peak centred around 18 meV and another near 40–70 meV as well as smaller features extending as high as 150 meV. Optical data are also available in La\(_{1.83}\)Sr\(_{0.17}\)CuO\(_4\) (Gao et al.\textsuperscript{22}, close in doping to the sample investigated by neutron scattering La\(_{1.84}\)Sr\(_{0.16}\)CuO\(_4\) which has a \(T_c = 38.5 \text{ K}\), and for which neutron scattering results are reproduced in the inset of the middle frame of figure 36. The results for \(I^2\chi(\Omega)\) obtained for optics appear in the main frame of the middle panel of this same figure for several temperatures identified in the top frame. In the top frame, we also show the data for the optical scattering as well as the theoretical results obtained from the Kubo formula and Eliashberg equations with \(I^2\chi(\Omega)\) retrieved from a maximum entropy fit (middle frame). First, we note that \(I^2\chi(\Omega)\) at 30 and 50 K do not differ much and both show distinct peaks emphasized by the solid black arrows at the energy seen in the neutron data. As the temperature is increased the \(I^2\chi(\Omega)\) obtained from optics evolve towards a single peak structure. The low energy peak at 15 meV is now gone as is the sharp peak at 44 meV which is replaced by a single much broader peak around 60 meV. This evolution in temperature is in qualitative agreement with the neutron data shown in the inset at 300 K (open circles) where we see the peak at 15 meV at 12 K (solid squares) has completely disappeared. This striking resemblance of the optically derived \(I^2\chi(\Omega)\) and the local susceptibility is taken as evidence that the spin fluctuations play an important role in the many-body renormalizations in La\(_{2−x}\)Sr\(_x\)CuO\(_4\). In the lower frame of figure 36 we show the results for the real part of the optical self-energy in which the two-peak structure at 15 and 44 meV are clearly seen in the quantity without analysis. This is expected from theory as shown in the inset of the lower frame of the figure leaving little doubt that there are peaks at these energies in the electron–boson spectral density \(I^2\chi(\Omega)\).

A somewhat different approach to inversion of normal state optical data has been presented by van Heumen et al.\textsuperscript{30} They work with equation (13) for the conductivity in the normal state at a finite temperature and use a least squares fit to data based on a histogram form for the spectral density \(\alpha^2\Phi(\Omega)\). In this way they obtain the results produced in figure 37. Several different families of cuprates as labelled in the figure are considered in and each case at several temperatures. In particular, we focus on their data for Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) OpD88 which might be compared with the data from Hwang et al.\textsuperscript{31} shown in the left-hand upper frame (a) of figure 31. Both spectra have a large peak around 50–60 meV followed by a valley and then a second peak providing a long high-energy tail or background. At 100 K the peak height is of order 1 in both sets of results. The main difference between the two spectra is the evolution with a temperature between 100 and 300 K. While Hwang et al.\textsuperscript{31} find a clear evolution towards a broad spectrum with a
Figure 35. Comparison of fitting parameters obtained from the actual measured optical data and the simulated optical scattering rate calculated from the Kubo formula and full Eliashberg equations (see text).

A single peak that has moved towards 100 meV, van Heumen et al (2009) find much less change with temperature and note that the peak at 50–60 meV remains largely unchanged and is robust. As can be seen in figure 29 both the optical scattering rate (left-hand column) and the corresponding real part of the optical self-energy (right-hand column) become rather smooth and unstructured with increasing temperature, and consequently an accurate determination of the underlying spectral density becomes harder. As we saw in figure 27, temperature tends to smear out some of the features of the recovered spectral density whether one uses a second derivative technique, singular value decomposition or maximum entropy. Another point of agreement between the data in figures 31 and 37 on Bi-2212 is that in both sets of data the mass enhancement factor associated with the peak is reduced with increasing doping while the background is more constant. Returning to the middle column in figure 37, we note that in Hg1201 OpD07 van Heumen et al (2009) find that $\alpha^2 F(\Omega)$ has very much the same shape as for Bi-2212 OpD88: a large peak around 50–60 meV, a dip, followed by a second step which provides a background extending to higher energies of 300 meV. This agrees qualitatively with the findings of Yang et al (2009).

In the work described so far on optics no attempt has been made to account explicitly for the opening of a pseudogap which is known to exist in underdoped cuprates (Timusk and Statt 1999, Norman et al 2005). In particular, equation (13) holds only under the assumption of an infinite band approximation with a constant bare band density of states. Formula (21) with kernel $K(\omega, \Omega, T)$ of equation (12), while it accounts for finite temperature effects, does not include the possibility of an energy-dependent dressed electronic density of states. The study of effects of an energy-dependent density of states $\tilde{N}(\epsilon)$ on normal and superconducting state properties has a long history, in particular in relation to the A15 compounds as described by Mitrović et al (1983a, 1983b). More recent work has been aimed at understanding the influence of these finite band effects on the quasiparticle self-energy (Doğan and Marsiglio 2003, Cappelluti and Pietronero 2003) and optical properties (Knigavko et al 2004, Knigavko and Carbotte 2005, 2006). Following the work of Allen (1971, 1976), Mitrović and Fiorucci (1985) derived an approximate formula which is a generalization of equation (11) to include energy dependence in the effective renormalized electronic density of state defined by $\tilde{N}(\epsilon)$. Following this work Sharapov and Carbotte (2005) generalized it further by including both temperature dependence, as in the work of Shulga et al (1991), and energy-dependent electronic density of state, as in the work of Mitrović and Fiorucci (1985), to yield

$$
\tau^{\text{op}}(\omega, T) = \frac{\pi}{2} \int_{\Omega_0} d\Omega \int_{-\infty}^{\infty} dz [\tilde{N}(\omega - \Omega) + \tilde{N}(\omega + \Omega)]
\times [\tilde{n}_B(\Omega) + 1 - f(\omega - \Omega)][f(\omega - \Omega) - f(\omega + \Omega)],
$$

(23)

where $\tilde{N}$ is the fully renormalized frequency-dependent density of states. For a constant density of states this
formula reduces to equation (12) and at zero temperature it simplifies to

$$\frac{1}{\tau^{\text{e}}(\omega, T = 0)} = \frac{2\pi}{\omega} \int_0^\omega d\Omega_2 \Omega_2 F(\Omega) \times \int_0^{\omega-\Omega} dz \left[ \tilde{N}(z) + \tilde{N}(-z) \right],$$

which is the equation given by Mitrović and Fiorucci (1985). Consider scattering by a single boson mode \(\Omega_E\), for \(\omega < \Omega_E\) the scattering rate is zero and for \(\omega > \Omega_E\) is given by

$$\frac{1}{\tau^{\text{e}}(\omega, T = 0)} = \frac{2\pi}{\omega} \int_0^{\omega-\Omega_E} dz \tilde{N}(z),$$

where for simplicity we have taken a model where \(\tilde{N}(z)\) is symmetric about the Fermi energy. It follows directly from equation (25) that a full gap \(\Delta_{pg}\) in \(\tilde{N}(z)\), for example, will look like the case of a constant density of states but with a boson mode set at \(\Omega_E + \Delta_{pg}\). Thus the analysis of boson structure needs to account for pseudogap effects in the underdoped cuprates. Hwang et al (2006) have considered the case of the \(a\)-axis conductivity of de-twinned Ortho-II \(\text{YBa}_2\text{Cu}_3\text{O}_{6.5}\). Their results for the optical scattering rate at a number of temperatures are shown in figure 38. The two vertical arrows at 400 and 850 cm\(^{-1}\) indicate regions where the scattering rate undergoes a faster than average increase with frequency. To analyse these data Hwang et al (2006) use the approximate formula equation (23) and allow for the existence of a pseudogap of size 350 cm\(^{-1}\) estimated from the \(c\)-axis infrared conductivity (Homes et al 1993) and tunnelling (Kugler et al 2001). For the electron–boson spectral density they take a Gaussian peak and an MMP (equation (20)) background. The position of the Gaussian and its width are taken from known neutron scattering data of Stock et al (2005) for the local \((q\text{ integrated})\) spin susceptibility. The parameters of the MMP form are obtained from a fit to the 295 K optical data without the Gaussian peak.

The remaining parameters of the model are determined through a least squares fit to the data as are the height of the Gaussian and the depth of the pseudogap depression below the Fermi energy. Reasonable values are obtained for both of these parameters with the depth ranging from 40% of the value at low temperatures to only 17% at room temperature. In figure 39 we show the \(I^2\chi(\Omega)\) obtained in this way for the eight values of temperature labelled. In the inset we show the inelastic neutron scattering results for \(T = 6\) K on which the model for the Gaussian part of \(I^2\chi(\omega)\) is based. In figure 40 we show the results for the area under the Gaussian peak obtained from the least squares fit as a function of temperature. These values compare with the energy-integrated amplitude of the neutron data (upright triangles) and an area estimated from the peak in the second derivative function \(W(\omega)\) obtained directly from data on \(\sigma(\omega)\) according to equation (18), open diamonds with crosses. The agreement between these points is good and is taken as an indication that the optical data of Ortho-II \(\text{YBa}_2\text{Cu}_3\text{O}_{6.5}\) are consistent with the neutron data and the existence of a sharp peak in the local spin susceptibility at 248 cm\(^{-1}\). This also serves to show that the pseudogap should be accounted for in studies of boson structure.

In figure 41 we summarize the results obtained from optical measurements for the peak energy \(\Omega_c\) as a function of critical temperature. The black dashed line is a guide to the eye and corresponds to \(\Omega_c = 6.3k_BT_c\). This value is close to that obtained for the spin-one resonance in inelastic neutron scattering which is \(\Omega_{res} = 5.4k_BT_c\) and is shown as the dotted curve in the figure. A universal relationship between magnetic resonance and superconducting gap is also stressed in a recent paper by Yu et al (2009).

Wang et al (2002) have used optics to study the effect of a complete substitution of \(^{16}\text{O}\) with \(^{18}\text{O}\) in an underdoped sample of \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) with \(T_c = 67.6\) K for \(^{16}\text{O}\) and \(T_c = 66.7\) K for \(^{18}\text{O}\). Analysis of the shift in energy of the reflectance shoulder around 400–500 cm\(^{-1}\) leads these authors to conclude that the feature cannot be due to a copper-oxygen phonon stretching mode and that it is largely electronic in origin. The observation is consistent with the evidence presented in this review that
phonon effects are small and can perhaps only be seen with probes that emphasize the nodal direction where the magnetic contribution is smaller. This would make such effects unlikely to show up in optics which is a momentum averaged probe.

4. Tunnelling

Tunnelling spectroscopy was used in BCS superconductors soon after its discovery by Giaever in 1960. It showed that there was a gap at the Fermi level when the superconducting state, as shown in figure 42, was formed and after some refinements subtle changes in the tunnelling conductance at higher energies were used to yield the spectrum of excitations responsible for superconducting pairing (Giaever 1960, McMillan and Rowell 1965, Scalapino 1969, Carbotte 1990).
Figure 40. Temperature dependence of the amplitude of the sharp bosonic mode in Ortho-II YBCO. The crossed open diamonds and the closed hexagons are from fitting a scattering rate to the model of the optical data of Hwang et al (2006), including a sharp mode and a background. ‘Eq. 4’ in the rubric refers to an equation in Hwang et al (2006). The triangles show the energy-integrated amplitude of the neutron mode (Stock et al 2005).

In superconductor–insulator–normal metal (S–I–N) tunnelling an oxide layer separates the normal metal and a superconductor as shown in figure 42(a). In scanning tunnelling microscopy (STM) the normal metal is a sharp tip and a vacuum space separates the tip and the surface of the sample. With the tip and the sample at the same voltage, their Fermi levels line up and no current can flow in either direction since the filled states on the left are on the same level with filled states on the right or no states in the gap. When a bias is applied, such that $V > \Delta$, as shown in figure 42(b), electrons can flow from the filled states in the superconductor to the empty states in the metal. When a bias of opposite polarity is applied the tunnelling current will flow in the opposite direction provided $V < \Delta$. The inset shows the current as a function of bias. In this simple example, with a constant density of states the current will be proportional to the amount of overlap between the filled and the empty states and will rise linearly with bias. In a more complicated situation the current will be proportional to the integral of the joint density of states of the two sides of the junction. The conductance defined as $dI/dV$ at zero temperature will be proportional to the density of states $N(\omega)$ where

$$N(\omega) = \sum_{k, BZ} A(k, \omega).$$  

While there are issues associated with the precise form of the tunnelling matrix element, the current–voltage characteristic of the junction is related to the carrier spectral density averaged over all momenta $k$ in the Brillouin zone as well as appropriate thermal factors.

Figure 41. The optical resonance frequency $\Omega_1$ as a function of the superconducting transition temperature $T_c$. Reprinted with permission from Yang et al (2009). Copyright 2009 by the American Physical Society. The points refer to various superconducting cuprate families at different doping levels. A linear relationship is found to hold over nearly an order of magnitude in $T_c$. In STS it is the local density of states at an atomically resolved site that is measured and involves an S–I–N junction. In break junction experiments, the junction is formed by mechanically breaking a crystal and then allowing the resulting crack to close to form a thin well-defined insulating barrier. In this case, it is the spatial average of equation (26) which is directly involved and a superconducting–insulating–superconducting (S–I–S) junction is formed. Zasadzinski et al (2001, 2003, 2006) and Ozyuzer et al (2000) have considered both STM and break junctions of overdoped samples of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ with a gap of 10.5 meV and critical temperatures of 56 K as well as nearly optimally doped samples with a gap of 28 meV. After appropriate normalizations by a state-conserving background, representative of a normal state, the conductance of the highly overdoped sample is deduced and shown in the main frame of figure 43 (dots). The solid curve is a d-wave Eliashberg fit to the data with a gap $\Delta = 10.5$ meV. The inset shows results for three other break junctions with gaps in the range 17–19 meV and a $T_c$ of the order of 60 K. The spectral density $\alpha^2 F(\Omega)$ which provides the fit (solid black curves) is shown in figure 44, also shown for comparison is the $\alpha^2 F(\Omega)$ (#1) obtained for the nearly optimally doped sample with $\Delta = 28$ meV. Both spectra exhibit the same characteristic shape with a well-defined peak at $\approx 20$ meV and a broad tail beyond extending to higher energies. A comparison with spectra obtained from optics and shown in figure 31 reveals the same general trends. For optimally doped Bi-2212 with $T_c = 96$ K the peak in the spectral density is closer to 60 meV, but Schachinger and
Figure 42. When a normal metal (N) and a superconductor (S) are separated by an insulating or vacuum barrier (I) no current can flow as shown in (a) since filled states in the metal are faced with either states that are filled in the superconductor or no states in the gap. When a bias $V_0$ is applied, filled states in the superconductor face empty states in the metal and electrons can flow from the superconductor into these states provided the bias exceeds the gap value, $V_0 > \Delta$. As the bias increases the number of states rises linearly if the joint density of states is constant.

Figure 43. S–I–S break junction tunnelling conductance adapted from Zasadzinski et al (2006) (dots) and d-wave Eliashberg fit (solid line) for a junction of overdoped Bi-2212 with $\Delta = 10.5$ meV. The inset shows series of junctions from the same study with $T_c = 60$ K.

Carbotte (2000) found that in a second Bi-2212 sample with a lower $T_c$ of 90 K from the optical data of Puchkov et al (1996), the peak was instead at 43 meV. The same value was found by Schachinger et al (2006) based on data in Bi-2212 by Tu et al (2002). To improve the quality of the sample the material used in figure 31 had some Y doping and some of the differences in the recovered spectra could be related to sample dependence. Another reason for differences between optical and tunnelling spectra is certainly related to different relationships between the underlying spectral densities and the experimental data. The transport spectral densities weigh backward scattering more strongly than forward scattering as these deplete the current more efficiently while quasiparticle lifetime weighs both processes equally. It should be noted, however, that a very different picture emerges in the tunnelling work of Shim et al (2008) on films of La$_{1.84}$Sr$_{0.16}$CuO$_4$. These authors identify 11 minima in their second derivative data for current versus voltage and find that these match precisely the published Raman data on phonons.
Figure 45. ((a) and (b)) Spectra taken at two different atomic locations on an overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ sample ($T_c = 68$ K, OV68) at various temperatures adapted from Pasupathy et al (2008). The gaps in the spectra close at different temperatures leading to a temperature-independent background conductance at high temperatures. (c) Histogram of pairing gap values measured in the OV68 sample. The inset shows a typical pairing gap map (300 Å) obtained at 30 K. ((d) and (e)) Same as (a) and (b) but for an optimally doped sample ($T_c = 93$ K, OPT). The background remains temperature dependent well above $T_c$. (f) Same as (e) but for the OPT sample.

STM has revealed important gap inhomogeneities on the atomic scale. In figure 45 we show the results of Pasupathy et al (2008) at two different atomic locations in an overdoped Bi-2212 sample with $T_c = 68$ K ((a) and (b)) and optimally doped with $T_c = 93$ K ((d) and (e)) at various temperatures. Note that the current–voltage characteristics are asymmetric between positive and negative biases. To analyse the data in terms of a boson structure they normalize their data to the

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normal state above $T_c$. Frames (c) and (f) give, respectively, the gap distribution histogram found in each of the samples and the inset shows gap maps on a 300 Å square patch. The normalized conductances, denoted $R = \left[ dI/dV \right]_{n}/\left[ dI/dV \right]_{s}$, are shown in figure 46(a). All exhibit a peak–dip–hump structure. When the dip energy is referred to the gap, i.e. $V - \Delta$ is used on the horizontal axis rather than $V$, as shown in frame (b) all the dips align and fall around 35 meV. Also the dip size is uncorrelated with the size of the gap (see frame (c)) in contrast to what is expected of a conventional strong coupling superconductor where the gap and the size of the bosonic dip would be correlated. Another closely related STM study is that of Lee et al. (2006). These authors identify the boson energy involved from the second derivative $d^2I/dV^2$ imaging measurements and obtain a constant value of $\Omega = 52$ meV independent of doping. This is shown in figure 47 which is reproduced from their work. The top frame (a) shows a histogram of the local gap variation for five samples characterized by the mean gap value for each sample as indicated in the figure. The lower frame (b) gives the histogram of boson energies obtained in each case. All are very similar and peak around 52 meV. This leads the authors to conclude that the boson involved is a phonon. This view is further reinforced in the work as the peak energy is found to scale with the inverse square root of the oxygen isotope mass on $^{16}$O $\rightarrow$ $^{18}$O substitution. A possible explanation is that the phonon is an oxygen vibration created during inelastic tunnelling of the charge carriers through the region between CuO$_2$ layers (Pilgram et al. 2006, Hwang et al. 2007c, Scalapino 2006).

The work of Jenkins et al. (2009) provides additional insight into the effects just described. These authors have made a detailed study of the effect of a boson mode of energy $\Omega_1$ peaked in the Brillouin zone around momentum $(\pi, \pi)$ on the average density of states for a d-wave superconductor with general tight binding band structure including the possibility that a van Hove singularity may fall near the Fermi energy. They consider an optimally doped ($T_c = 109$ K) and an overdoped ($T_c = 108$ K) of Bi-2223. Both show large boson structures and have large values of the critical temperature. The cleaved surfaces have supermodulations of $\cong 5a$ and the authors introduce an angle $\phi$ to characterize this periodicity. In figure 48 we reproduce the results for their optimally doped sample of Bi-2223. The conductance $dI/dV$ is shown in frame (a) for many values of the phase $\phi$. Frame (b) gives the distribution of gaps $\Delta_p$ as a function of $\phi$ (the yellow curve is the average gap for a given $\phi$). The gaps display periodicity with $\phi$ as expected from the supermodulation on the cleaved surface of the sample. In frame (c) we show average spectra all having the same gap value $\Delta_p$ equal to the difference $(\Delta_{+p} - \Delta_{-p})/2$ where $\Delta_{+p}$ and $\Delta_{-p}$ are the energy of the positive and the negative bias coherence peaks. The solid curves through the data are fits obtained from calculations of the density of states including a boson at $\Omega_1$ and momentum

Figure 46. (a) The low temperature ($T = 30$ K) conductance ratio plotted for several different gaps adapted from Pasupathy et al (2008). The conductance ratios deviate systematically from the d-wave model (thin lines) and go below unity over a range of voltages (50–80 mV) indicating strong coupling to bosonic modes. (b) The positive bias conductance ratios referenced to the local gap at different locations showing a common dip–hump feature. The heavy line is the average of all the locations. The inset shows gap referenced conductance ratios for negative bias. (c) The rms deviation of the conductance ratios from the d-wave model for positive (blue) and negative (red) bias over the energy range 20–120 mV, which shows no correlation with the size of the gap.
dashed line the minimum in the $d^2I/dV^2$ spectrum as was used by Lee et al (2006) to locate their phonon at 52 meV in Bi-2212. While the dip energy decreases from 39 to 35 meV corresponding in this case to a CME $\Omega_2$, decrease from 34 to 24 meV, the position of the dashed line is almost independent of the gap value and is at ≈57 meV close to the value of 52 meV quoted above. Another recent study by Das et al (2008) has further confirmed in hole-doped NbBa$_2$Cu$_3$O$_{7-\delta}$ that the gap and the CMEs are anticorrelated favouring more a spin fluctuation rather than a phonon explanation.

5. Raman spectroscopy

There have been attempts to include inelastic scattering in the calculations of the Raman response of d-wave superconductors. Jiang and Carbotte (1996) and Branch and Carbotte (2000) based their work on a generalization of BCS theory of the nearly antiferromagnetic Fermi liquid model (Branch and Carbotte 1995) which included d-wave but no dynamics. Attempts to extract the inelastic contribution from Raman spectra have also appeared, among them the work of Gallais et al (2006) and Grilli et al (2009). Muschler et al (2010) write the Raman cross section for polarization $\mu$ as

$$\text{Im } \chi_{\mu}(\Omega) = \frac{\Omega \Gamma_\mu(\Omega)}{(\Omega + \lambda_\mu(\Omega))^2 + \Gamma^2_\mu(\Omega)}$$

(27)

and following the work of Sharapov and Carbotte (2005) show that the Raman scattering rate $\Gamma_\mu(\Omega)$ can be written in an identical form to our equation (12) for the optical conductivity but with $\alpha^2F(\Omega)$ replaced by an appropriate electron–boson spectral density $I^2_{\mu}X(\Omega)$ which is dependent on the Raman polarization $\mu$. One can introduce an angular-dependent version of this function as $I^2_{\mu}X(\Omega, \theta)$. Within a continuum model for the electronic structure the function entering the usual spectral density would correspond to a straight angular average while for Raman there would be a further $\cos^2(2\theta)$ weighting for $B_{1g}$ and $\sin^2(2\theta)$ for $B_{2g}$ in the integral over angles. This provides new information on the spectral density. The weighting for $B_{1g}$ favours the antinodal direction while for $B_{2g}$ it favours the nodal direction.

In figure 50 we reproduce the results obtained by Muschler et al (2010) for an optimally doped sample of Bi-2212 with $T_c = 94.5$ K. The $B_{1g}$ (antinodal) spectrum has a large peak around 30 meV followed by a dip and then a second peak centred around 300 meV. As the temperature is increased there is a clear evolution in the spectra with the reduction in amplitude of the lower peak and its movement towards higher energy filling in the dip region. This distribution is very close to the optically derived spectrum found in Schachinger et al (2006) for a comparable sample of Bi-2212 measured by Tu et al (2002) with a peak around 40 meV and overall very similar shape (frame (c)). For the $B_{2g}$ (nodal direction) spectrum, the peak around 30 meV remains but is smaller in magnitude than for $B_{1g}$ 3% of the area under the curve as opposed to 23% in $B_{1g}$, but as it has the same energy is probably of the same origin. Both could be associated with scattering about ($\pi, \pi$) which would favour antinodal as opposed to nodal direction scattering.
from one point in the Fermi surface to another again on the Fermi surface. It is instructive to compare the $B_{2g}$ spectrum with that obtained from nodal direction ARPES described in the previous section (see figure 18(a)) and reproduced in the lower right-hand frame (d). This spectrum looks a lot like $B_{2g}$ but with a very important difference, it has a prominent peak at 65 meV, a much higher energy than found in the other case. It could be that this peak is related to scattering from a different boson, perhaps a phonon with scattering confined to the region of the nodal direction and so not sufficiently important in the Raman and optical cases because of averaging away from the nodal regions in momentum space. This possibility is supported by the recent work of Schachinger et al (2009) and further elaborated upon by Schachinger and Carbotte (2010). The recent isotope effect experiments of Iwasawa et al (2008) described in the previous section on ARPES can be understood on the assumption that only the sharp peak above the background in the $I^2 \chi(\Omega)$ shown in the lower right-hand frame of figure 50 is shifted in substituting $^{16}$O by $^{18}$O and this involves only 10% of the area under the total spectral density, or a mass enhancement $\lambda$ of about 0.2.

In maximum entropy inversion one needs to specify an initial starting value for the spectral density. In the unbiased inversion mode this is taken as flat, while in the biased mode the next lowest temperature converged solution for $I^2 \chi(\Omega)$ is used as the starting value for the next higher temperature run. The results for the biased mode are presented in the top two frames of figure 51 and these are to be compared with the top frames of figure 50 obtained by unbiased inversion. We note that these methods give very similar results except for one important difference. The unbiased mode shows more temperature evolution than does the biased case. This does not translate into important differences for the value of mass enhancement and its evolution with temperature. This is seen in the bottom frame of figure 51 where we plot $\lambda$ as a function of $T$. The differences do, however, have an impact on the possible interpretation of the boson spectral density. For phonons one would expect little $T$ dependence of the peak frequencies and also little broadening, while for spin fluctuation the opposite holds. In that regard, the unbiased maximum entropy results differ from those obtained by least squares fit of the formula for $I^2 \chi(\Omega)$ as shown in figure 37. This alternative method shows less temperature evolution than the unbiased MEM. The exact source of this difference is not fully understood. In maximum entropy noise always leads to some smearing of the resulting distributions. An alternate interpretation of boson structure seen in Raman has been
Figure 49. STM conductance spectra of Bi-2223 \( (T_c = 111 \text{ K}) \) at \( T = 2 \text{ K} \). Reprinted with permission from de Castro et al (2008). Copyright 2008 by the American Physical Society. Each curve is an average of several spectra taken at different locations on the same sample, all having the indicated peak-to-peak \( \Delta p \). The energy \( \Omega_{\text{dip}} \) is the energy difference between the dip minimum (dot) and the peak maximum at negative bias, relative to which voltages are measured.

Figure 50. The electron–boson spectral density (dimensionless) as a function of energy \( \omega \) in meV from B1g (a) and B2g (b) Raman data from Muschler et al (2010). We show in (c) the results (Schachinger et al 2006) obtained from optical data (Tu et al 2002) and in (d) a result (Schachinger and Carbotte 2008) obtained from nodal direction ARPES (Zhang et al 2008a).

6. Summary and conclusion

The experiments presented in this review, primarily ARPES and optical conductivity, of the hole-doped high-temperature superconductors, lead us to the strong conclusion that the mobile charge carriers are scattered by a spectrum of bosonic presented very recently by Caprara et al (2010). Their data are for the La\(_{2-x}\)Sr\(_x\)CuO\(_4\) family and an aim of their work is to unravel the nature of the glue responsible for pairing. They do not provide inversions of their data. Instead they proceed with calculations of Raman response for B1g and B2g symmetry which they then compare with experiments. The calculations employ the equivalent of a Shulga et al (1991) approximation adapted to the Raman cross section as opposed to optics. Separate spectral densities are introduced for spin and charge fluctuations with different characteristic wave vectors \( q_s \sim (\pi, \pi) \) for spins and \( q_c \sim (\pm \pi/2, 0, \pm \pi/2) \) for charges with each having its own dynamics and collective modes (boson). While the spin fluctuations correspond to the proximity of the antiferromagnetic state, the charge fluctuations correspond to the tendency towards stripes or checkerboard order. They find guidance from a selection rule in momentum space which emphasizes the spin in B1g and charge in B2g symmetry. At any doping they can separate each contribution and thus get additional information on the relative contribution of each process which goes beyond what has been provided in the main part of this review.
Figure 51. (a) The electron–boson spectral density $I^2 \chi(\omega)$ (dimensionless) as a function of energy $\omega$ in meV from B$_{1g}$ Raman scattering rates using a biased maximum entropy inversion as described in the text from Muschler et al (2010). (b) The same as (a) but now for B$_{2g}$ symmetry. (c) and (d) compare the temperature dependences of the mass enhancement parameter $\lambda$ obtained from biased and unbiased inversion of the B$_{1g}$ and B$_{2g}$ Raman scattering rates, respectively.

excitations. Although these two techniques are quite different they yield similar results. Confirming tunnelling and Raman experiments have also been published. An early comparison between ARPES and optics was made by Kaminski et al (2000). As figure 52 shows the quasiparticle lifetime, as measured by the ARPES MDC widths, tracks in both magnitude and structure the free carrier lifetime as determined from the optical conductivity in the same material (Bi-2212). This convergence of ARPES and optical self-energies has been confirmed in many additional experiments as we have shown in this review. For example, figure 30 shows this for the real part of the quasiparticle self-energy. But such comparisons are of limited use since, on theoretical grounds, one expects to see somewhat different results for the two techniques (Hwang et al 2007a). First ARPES looks at single particle excitations while optics deals with particle–hole pairs and the self-energies associated with the two processes are not the same. Also ARPES is momentum resolved whereas the optical self-energy is a weighted average over the Fermi surface. In both cases there are momentum-dependent matrix elements that have to be taken into account. More accurate experiments may identify these differences in the future.

Nevertheless, there is a remarkably uniform bosonic spectrum that emerges from the various experiments. At low temperatures the spectrum has a peak whose frequency varies from 15 to 75 meV depending on the material and doping level. This frequency is generally proportional to the superconducting transition temperature $T_c$ as shown in figure 41, but is totally absent in some materials with very low transition temperatures. The amplitude of the peak is strongly dependent on both temperature and doping. It is the strongest at low temperatures in the superconducting state but weakens at higher temperatures. In some cases, such as the optimally doped YBCO, it vanishes at $T_c$ but in other cases persists into the normal state such as underdoped YBCO. In addition to the peak there is a continuum in all the samples extending to 200–400 meV as shown in figure 18. The continuum seems to be fairly temperature independent but develops a gap at low
temperatures. The peak appears to be in the middle of this gap as shown in figures 31 and 33.

We next address the question of the origin of the bosonic spectrum. The main candidates for this are spin fluctuations and phonons. While there seems to be a consensus among the ARPES groups that the spectrum is magnetic, arguments are made from time to time in favour of phonons. The case for the spin-fluctuation scenario is strong. First the bosonic function appears to change with temperature, the peak weakens as the temperature is increased and shifts in frequency to higher values. As figure 41 shows, the peak frequency is systematically related to the transition temperature of the superconductor. Further, the spectrum of fluctuations extends to energies of the order of 300 meV. None of these properties are expected for a phonon. Finally, where magnetic neutron spectra are available, the peak in the $q$-averaged susceptibility is close to the peak extracted from ARPES or optical conductivity spectra.

However, there remain compelling arguments for some role of phonons. In particular, as recent high-resolution ARPES data for nodal quasiparticles show there is an oxygen isotope effect on the low-frequency kink which is associated with the peak in the bosonic spectrum. This effect could be understood in terms of a phonon contribution at the 10% level to the self-energy of at least the nodal quasiparticles.

In summary, in our review of bosonic excitations in high-temperature superconductors, we have identified these excitations as spin fluctuations. They are responsible for the kinks in the ARPES dispersion curves and the spectral features in the optical conductivity. Their contribution is strong enough to account for the superconducting transition temperature $T_c$. But there remain several questions that need to be answered before we can claim to fully understand high-temperature superconductivity. What determines the nature of the magnetic fluctuation spectrum? For example, why is it so different in LSCO as compared with the three-layer mercury material? What is the role of the pseudogap? Is it a coincidence that near the doping level where the pseudogap vanishes, $p \approx 0.19-0.23$, the peak in the magnetic spectrum is replaced by a uniform featureless background? We look to future experiments, particularly magnetic neutron scattering, to address some of these issues.

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