Collective modes and the superconducting-state spectral function of $Bi_2Sr_2CaCu_2O_8$

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Photoemission spectra of the high-temperature superconductor $Bi_2Sr_2CaCu_2O_8$ near $(\pi,0)$ show a dramatic change when cooling below T_c: the broad peak in the normal state turns into a sharp low-energy peak followed by a higher binding-energy hump. Recent experiments find that this low-energy peak persists over a significant range in momentum space. We show in this paper that these data are well described by a simple model of electrons interacting with a collective mode that appears only below T_c. [S0163-1829(98)51318-5]

Angle resolved photoemission spectroscopy (ARPES) has become one of the key tools used to elucidate the physics of high temperature superconductors. It has produced a number of important observations concerning the nature of the normal and superconducting phases. Examples are the existence of a large Fermi surface, and an anisotropic energy gap in the superconducting and pseudogap phases.[1] The most interesting aspect of the ARPES data, though, is the unusual nature of the spectral lineshape and how this lineshape changes as a function of doping, momentum, and temperature. Perhaps the most profound example in this regard is the temperature dependence of the lineshape near the $(\pi,0)$ point in $Bi_2Sr_2CaCu_2O_8$ (Bi2212). A very broad normal-state spectrum evolves quite rapidly below T_c into a resolution limited quasiparticle peak, followed at higher binding energies by a dip then a hump, after which the spectrum is equivalent to that in the normal state.[2–4] Similar effects have been seen in tunneling spectra, where it has been found that all of these spectral features (peak, dip, and hump) scale with the superconducting gap.[5] This implies that the electron self-energy has a dramatic change below T_c.

In a recent paper, our group has shown that the low energy peak persists over a surprisingly large range in momentum space along the $(\pi,0)$-(0,0) and $(\pi,0)$-(π,π) directions.[6] As argued in that paper, this result can be connected to the change in lineshape with temperature noted above. The idea is that the dip in the spectrum at $(\pi,0)$ implies that the imaginary part of the self-energy, $\mathrm{Im}\Sigma$, has a steplike drop from a large value at binding energies larger than the dip to a small value for smaller energies. This step behavior has recently been verified by us by a direct extraction of Σ from the data. By Kramers-Kronig transformation, then, $\mathrm{Re}\Sigma$ will have a strong peak at the dip energy. The consequence of this is that there will always be a low energy quasiparticle pole trapped on the lower-binding energy side of the dip energy, even when the normal-state binding energy is quite large. It is this effect which we believe leads to the persistent peak.

This raises the question of what kind of microscopic picture can lead to such behavior. As discussed in our paper,[6] a step edge in $\mathrm{Im}\Sigma$ is equivalent to the problem of an electron interacting with a sharp (dispersionless) mode. This model has been worked out in detail in the classic literature of strong-coupling superconductors, where the mode is an Einstein phonon.[7] In the current case, though, the effect of the mode only appears below T_c, and therefore implies a collective mode of electronic origin. Still, the mathematics is largely equivalent. What we show in this paper is that this simple model gives a good quantitative fit to the data.

We begin by discussing self-energy effects in superconductors. For now, we ignore the complication of momentum dependence. The lowest-order contribution to electron-electron scattering is represented by the Feynman diagram shown in the inset of Fig. 1. In the superconducting state, each internal line will be gapped by Δ. This implies that the scattering will be suppressed for $|\omega|<3\Delta$.[8] This explains the presence of a sharp resolution-limited quasiparticle peak at low temperatures. What is not so obvious is whether this in addition explains the strong spectral dip. Explicit calculations show only a weak diplike feature.[9] To understand this in detail, we equate the bubble plus interaction lines (Fig. 1 inset) to an ''α^2F'' as in standard strong-coupling literature.[7] In a marginal Fermi liquid (MFL) at $T=0$, $\alpha^2F(\Omega)$ is simply a constant in Ω. The effect of the gap is to

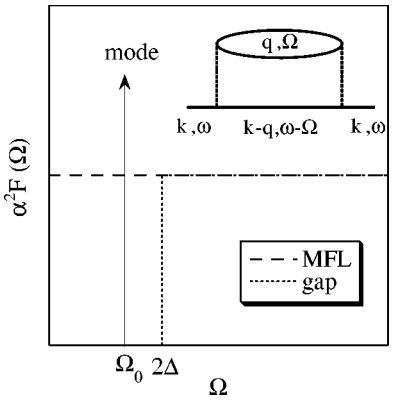

FIG. 1. α^2F for three models, MFL (dashed line), gapped MFL (dotted line), and gapped MFL plus mode (dotted line plus δ function). Inset: Feynman diagram for the lowest-order contribution to Σ from electron-electron scattering.

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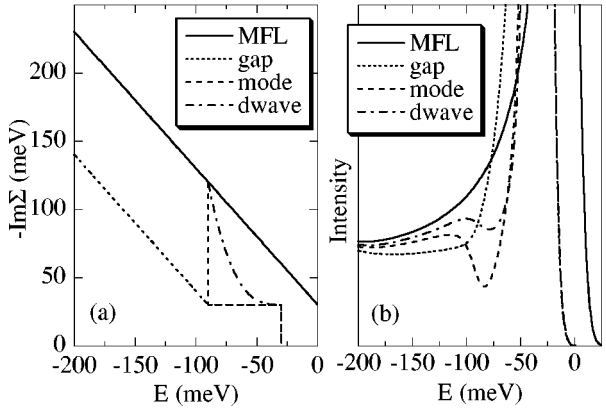

FIG. 2. (a) ImΣ for MFL (solid line), gapped MFL (dotted line), gapped MFL plus mode (dashed line), and simple *d*-wave model (dashed-dotted line). Parameters are $\alpha=1$, $\omega_c=200$ meV, $\Delta=30$ meV (0 for MFL), $\Omega_0=2\Delta$, and $\Gamma_0=30$ meV. (b) Spectral functions (times a Fermi function with $T=14$ K convolved with a resolution Gaussian of $\sigma=7.5$ meV) for these four cases ($\epsilon=-34$ meV).

force α^2F to zero for $\Omega<2\Delta$. The question then arises where the gapped weight goes. It could be distributed to higher energies, but in light of the above discussion, we might expect it to appear as a collective mode inside of the 2Δ gap. For instance, this indeed occurs in fluctuation-exchange calculations where the bubble represents spin fluctuations,[10] in which case a sharp mode will appear if the condition $1-U\chi_0(\mathbf{q},\Omega)=0$ is satisfied for $\Omega<2\Delta$. These three cases (MFL, gapped MFL, and gapped MFL plus mode) are illustrated in Fig. 1.

Σ is easy to obtain analytically[7] if we ignore the complication of the superconducting density of states from the $\mathbf{k}-\mathbf{q}$ line of Fig. 1 and just replace this by a step function at Δ. The resulting ImΣ for the gapped MFL and gapped MFL plus mode models are shown in Fig. 2(a) in comparison to the normal-state MFL. Note that structure in α^2F at Ω appears in Σ at $|\omega|=\Omega+\Delta$ due to the gap in the $\mathbf{k}-\mathbf{q}$ line. Moreover, the MFL plus mode is simply the normal-state MFL cut off at 3Δ (this is obtained under the assumption that all the gapped weight in α^2F shows up in the mode). In contrast, the gapped MFL decays linearly to zero at 3Δ. This gapped MFL form is not changed that much if one actually solves the strong-coupling equations for Σ and Δ.[9] (For an *s*-wave gap, the linear behavior of ImΣ is replaced by a square-root behavior).

The spectral function is given by[7]

$$A(\omega)=\frac{1}{\pi}\mathrm{Im}\frac{Z\omega+\epsilon}{Z^2(\omega^2-\Delta^2)-\epsilon^2}, \tag{1}$$

with (a complex) $Z(\omega)=1-\Sigma(\omega)/\omega$. These are shown in Fig. 2(b) and were convolved with a Gaussian of $\sigma=7.5$ meV, typical of high resolution ARPES, with a constant ImΣ (Γ_0) added for $|\omega|>\Delta$ to reduce the size of the quasiparticle peak. We note that there is no dip as such for the gapped MFL model, whereas the addition of the mode causes a significant dip. The latter behavior is consistent with experiment. Moreover, the mode model has the additional advantage that ImΣ recovers back to the normal-state value by 3Δ, which is also in agreement with experiment in that the normal and superconducting state spectra agree beyond 90 meV.[6]

We contrast this behavior with that expected for a simple *d*-wave model. To a first approximation, this can be obtained by replacing the step drop in ImΣ in the MFL plus mode model with $(|\omega|-\Delta)^3$ for $|\omega|<3\Delta$.[11] This is shown in Fig. 2(a) as well, with the resulting spectrum in Fig. 2(b). Only a weak dip appears. Moreover, we have analyzed models with the exponent 3 replaced by some n and have found that n must be large to obtain a dip as strong as seen in experiment. Therefore, the upshot is that at the least, something similar to a step is required in ImΣ to be consistent with experiment.

In principle, we could take the above MFL plus mode model and fit experiment with it. In this paper, though, we consider a simpler model. There are several reasons for this. First, the MFL model has a number of adjustable parameters associated with it. There is the coupling constant (α), the cutoff frequency (ω_c), and the mode energy (which is not in general 2Δ). Moreover, the spectrum for $\mathbf{k}$ points near the $(\pi,0)$ point does not appear to be MFL-like in nature. We have found that the normal-state Bi2212 spectrum is fit very well by a Lorentzian plus a constant in an energy range less than 0.5 eV. This is also true for Bi2201 spectrum where the normal state can be accessed to much lower temperatures. The constant term represents the so-called ''background'' contribution, and is essentially equivalent to spectrum for $k>k_F$, where it is also seen that the background gets gapped by Δ in the superconducting state. There are several possibilities for what the background could be due to, and in fact could be a combination of all of these: (1) incoherent part of A, (2) inelastic secondaries, (3) emission from the BiO layers, (4) diffraction of the photoelectrons by the surface BiO layer, etc. Since this has little to do with the peak/dip/hump structure, we choose to subtract this off, but note the caveat that this is an incomplete description if part of the background is intrinsic. Finally, the Lorentzian simplification allows us to directly obtain the dispersion $\epsilon_{\mathbf{k}}$ from tight binding fits to the normal-state peak positions.[4]

In the resulting Lorentzian model, the normal state Σ is purely an imaginary constant, and α^2F is a mode at zero energy. In the superconducting state, this mode gets pushed back to some energy within 2Δ. This model is artificial in the sense that all the self-energy is being generated by the mode. That is why we went through the above discussion motivating the mode more properly as a rearrangement of α^2F due to the superconducting gap. In practice, though, the results are very similar to the MFL plus mode model, and has the further advantage of having the several parameters of that model collapse to just the mode strength (Γ_1) and mode position (Ω_0) of the Lorentzian model. Moreover, analytic results can still be obtained for Σ when the superconducting density of states for the $\mathbf{k}-\mathbf{q}$ line of Fig. 1 is taken into account. The result is

$$\begin{aligned}-\mathrm{Im}\Sigma(\omega)&=\Gamma_0N(|\omega|)+\Gamma_1N(|\omega|-\Omega_0),\quad |\omega|>\Omega_0+\Delta\\&=\Gamma_0N(|\omega|),\quad \Delta<|\omega|<\Omega_0+\Delta\\&=0,\quad |\omega|<\Delta,\end{aligned} \tag{2}$$

where $N(\omega)=\omega/\sqrt{\omega^2-\Delta^2}$ is the BCS density of states, and

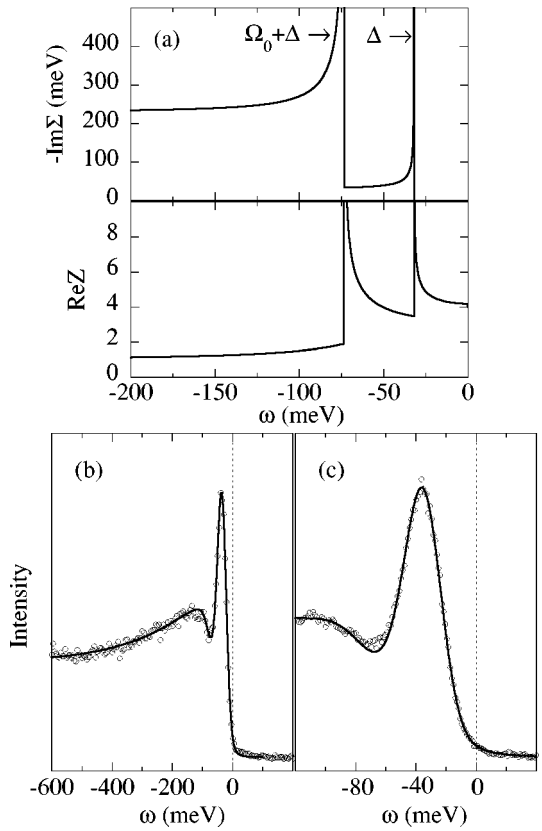

FIG. 3. (a) ImΣ and ReZ at $(\pi,0)$ from Eqs. (2) and (3) ($\Gamma_1=200$ meV, $\Gamma_0=30$ meV, $\Delta=32$ meV, $\Omega_0=1.3\Delta$). Comparison of the data at $(\pi,0)$ for (b) wide and (c) narrow energy scans with calculations based on Eqs. (1)–(3), with an added step edge background contribution.

$$\pi \mathrm{Re}\Sigma(\omega)=\Gamma_0 N(-\omega)\ln[|-\omega+\sqrt{\omega^2-\Delta^2}|/\Delta] + \Gamma_1 N(\Omega_0-\omega) \times \ln[|\Omega_0-\omega+\sqrt{(\omega-\Omega_0)^2-\Delta^2}|/\Delta] - \{\omega\rightarrow-\omega\}, \quad (3)$$

where it has again been assumed that Δ is a real constant in frequency. An s-wave density of states has been used to obtain an analytic result. A d-wave density of states will not be that different. The advantage of an analytic result is that it is useful when having to take spectra and convolve with resolution to compare to experiment. Our results are not very sensitive to Γ_0 (30 meV), included again to damp the quasiparticle peak. (A more realistic damping of the peak would require making Δ complex.) We use the same set of parameters for all $\mathbf{k}$ ($\Gamma_1=200$ meV), and therefore assume a d-wave gap $\Delta_{\mathbf{k}}=\Delta_{max}(\cos(k_x a)-\cos(k_y a))/2$ in Eqs. (1)–(3) with $\Delta_{max}=32$ meV. The best agreement with experiment is found by choosing the mode energy $\Omega_0=1.3\Delta_{\mathbf{k}}$, so that the spectral dip for $(\pi,0)$ is at $2.3\Delta_{max}$.[12]

The resulting real [Eq. (3)] and imaginary [Eq. (2)] parts of Σ at $(\pi,0)$ are shown in Fig. 3(a). Note the singular behaviors at Δ due to the Γ_0 term and at $\Omega_0+\Delta$ due to the Γ_1 term. In both cases, step drops in ImΣ would also give singularities in ReΣ. The advantage of peaks in ImΣ (due to the density of states) is that it makes the dip deeper in better agreement with experiment. In Figs. 3(b) and 3(c), we show a comparison of the resulting spectral function (convolved with the experimental energy and momentum resolution) to experimental data at $(\pi,0)$ for both wide and narrow energy scans, where a step edge background with a gap of Δ is added to the calculated spectrum as discussed above. The resulting agreement is excellent.

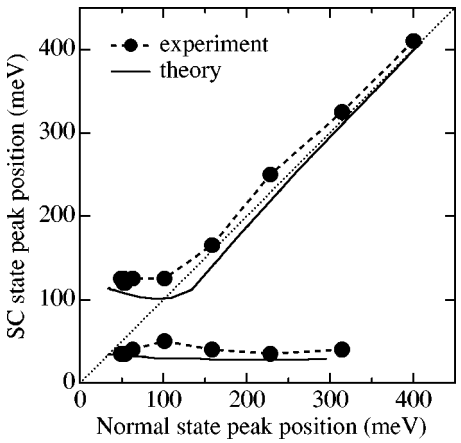

FIG. 4. Positions (meV) of the sharp peak (lower set) and the broad hump (upper set) in the superconducting state versus normal-state peak position along $(\pi,0)$-(0,0). Solid points connected by a dashed line are the experimental data (Ref. 6), the solid lines are obtained from the calculations, and the dotted line represents the normal-state dispersion.

To better appreciate these results, the positions of the sharp peak and the higher binding energy hump obtained from the calculations are plotted relative to the normal-state binding energy $\epsilon_{\mathbf{k}}$ along the (0,0)-$(\pi,0)$ direction, and compared to those obtained from the experimental data of Ref. 6 in Fig. 4. This plot is very similar to that obtained for electrons interacting with an Einstein mode.[7] The calculations reproduce the dispersionless nature of the low-frequency peak, as well as its lack of visibility for $\mathbf{k}$ vectors close enough to (0,0). The dispersionless behavior is due to several factors: (1) the weakness of the dispersion $\epsilon_{\mathbf{k}}$ near $(\pi,0)$, (2) the lowering of $\Omega_0\sim\Delta_{\mathbf{k}}$ as one moves towards (0,0), and (3) the influence of both ReΣ and Δ. The last is a new effect worth commenting on. The real part of the self-energy implies a mass enhancement ($Z>1$) in the superconducting state relative to the normal state, which acts to push spectral weight towards E_F. On the other hand, Δ itself pushes spectral weight away from E_F. Thus the dispersion is dramatically flattened relative to the normal state.

In the above calculations, it was assumed that the mode frequency was proportional to $\Delta_{\mathbf{k}}$. This was the easiest way we found to properly simulate the loss of the experimental low-frequency peak as one disperses towards (0,0). In reality, Ω_0 is a function of $\mathbf{q}$ in the diagram of Fig. 1, not $\mathbf{k}$. Moreover, it was our assumption of independence of Ω_0 on $\mathbf{q}$ that allowed us to obtain a step drop in ImΣ, leading to the spectral dip. Without some microscopic theory, only qualitative observations can be made at this stage concerning the true dependence of Σ on momentum $\mathbf{k}$.[13] Assuming an artificial limit where only $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$ contributes, we would replace $\Gamma_1 N(\omega+\Omega_0)$ in Eq. (2) by $g^2_{k,k+Q}A_{k+Q}(\omega+\Omega_0)$ (for $\omega<0$), where g is the interaction vertex. Using a qua-

siparticle pole approximation for A when solving Eqs. (2) and (3), this would imply a dip in the spectrum at $|\omega| = E_{k+Q} + \Omega_0$ where $E_k^2 = \epsilon_k^2/(\mathrm{Re}Z_k)^2 + \Delta_k^2$, and a persistent low-frequency peak if Z is large enough. The coupling of $\mathbf{k}$ and $\mathbf{k}+\mathbf{Q}$ in the self-energy equations also implies that if a low-frequency peak exists for $\mathbf{k}$, then one also exists for $\mathbf{k}+\mathbf{Q}$. This is just the effect observed in the data along $(\pi,0)$-(π,π),[6] in that a low-frequency peak exists for about the same momentum range as that along $(\pi,0)$-$(0,0)$. It remains to be seen whether such simple momentum dependent models give as good a fit to the spectra as the dispersionless model presented here.

Finally, it is interesting to note that the mode energy we infer from the data is 41 meV, equivalent (probably fortuitously) to a resonant mode energy observed in $YBa_2Cu_3O_7$ by neutron scattering data[14] at $\mathbf{Q}=(\pi,\pi)$. The models proposed for this mode are similar to the model discussed in this paper.[15] So far, neutron-scattering data on Bi2212 have yet to see a similar structure,[16] although these experiments were done on a rod of aligned small crystals. Our results here would imply that such experiments on large single crystals would be of interest.

In conclusion, we have shown that a simple model of an electron interacting with a collective mode in the superconducting state gives a quantitative description of the unusual spectral lineshape seen by ARPES data in the superconducting state of Bi2212. This implies that electron-electron scattering plays a dominant role in high-temperature superconductors, and is in support of an electron-electron origin for the pairing.

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