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Phenomenology of the low-energy spectral function in high-T_c superconductors

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We introduce a simple phenomenological form for the self-energy which allows us to extract important information from angle-resolved photoemission data on the high-T_c superconductor $Bi_2Sr_2CaCu_2O_8$ for binding energies of order the spectral gap. First, we find a rapid suppression of the single particle scattering rate below T_c for *all* doping levels. Second, we find that in the overdoped materials the gap Δ at all **k** points on the Fermi surface has significant temperature dependence and vanishes near T_c. In contrast, in the underdoped samples such behavior is found only at **k** points close to the diagonal. Near $(\pi,0)$, Δ is essentially T independent in the underdoped samples. The filling-in of the pseudogap with increasing T is described by a broadening proportional to $T-T_c$, which is naturally explained by pairing correlations above T_c. [S0163-1829(98)52218-7]

Angle-resolved photoemission spectroscopy (ARPES) has played a major role in developing our understanding of the high-T_c superconductors. The momentum and frequency resolved information contained in the one-particle spectral function[1] probed by ARPES provides critical insights difficult to obtain from other techniques. However, an important open problem in interpreting ARPES data for binding energies of order the gap is the absence of simple representations of the spectral line shape, analogous to the Drude formula for optical studies.

In this paper, we take a step in this direction by introducing a simple phenomenological form for the self-energy which captures much of the important low frequency information contained in the ARPES data for the normal, superconducting, and pseudogap phases of high-T_c superconductors. We first test this on ARPES data at $\mathbf{k}_F$ for overdoped $Bi_2Sr_2CaCu_2O_8$ (Bi2212), from which we determine the T dependence of the superconducting (SC) gap and the one-particle scattering rate, the latter found to decrease rapidly in the SC state, leading to the appearance of sharp quasiparticles at low temperatures.

We then turn to underdoped Bi2212, where a highly anisotropic pseudogap is known to persist well above T_c.[2–4] The magnitude of this gap and its smooth evolution through T_c establish a strong connection between the normal-state pseudogap and the SC gap below T_c, and suggest that the pseudogap arises from pairing correlations in a state without long-range phase coherence.[5] Here, we use our simple self-energy to gain insight into the ARPES line shape in the pseudogap regime. We find that near $(\pi,0)$ Δ is T independent, and the pseudogap fills in due to a T-dependent broadening which is naturally explained by pairing correlations above T_c.

Finally, we use our analysis to shed more light on the very recent surprising result that the pseudogap at different **k** points turns off at different temperatures, leading to gapless arcs above T_c which expand in length until the entire Fermi surface is recovered at T^*.[6] We show below that the T dependence of the underdoped line shape away from $(\pi,0)$ is rather different, with the vanishing of the pseudogap controlled instead by a T-dependent Δ.

The data analyzed below have been reported earlier.[3,4,6] The ARPES intensity $I(\mathbf{k},\omega)$ is proportional to $f(\omega)A(\mathbf{k},\omega)$, where f is the Fermi function and A the spectral function.[1] Recently, we have proposed a method[6] which allows us to eliminate the effect of f from ARPES data and focus directly on A. In brief, using the mild assumption of particle-hole symmetry $A(-\epsilon_{\mathbf{k}},-\omega)=A(\epsilon_{\mathbf{k}},\omega)$ for small $|\omega|$ and within the small **k** window centered at $\mathbf{k}_F$, one can show that the symmetrized intensity $I(\omega)+I(-\omega)$ at $\mathbf{k}_F$ is simply the spectral function (convolved with the resolution).[7] Results obtained from symmetrized data agree with those obtained from the leading edge of the raw data.[6] Here, we use the symmetrized data for two reasons: it is a useful visual aid, and (due to absence of Fermi cutoff) it allows more stringent comparisons to the fits. We have checked that the fits discussed below agree equally well with the raw data.

We begin with the overdoped samples, where there are no strong pseudogap effects. The simplest self-energy which can describe the data at all T is

$$\Sigma(\mathbf{k},\omega)=-i\Gamma_1+\Delta^2/[(\omega+i0^+)+\epsilon(\mathbf{k})]. \qquad (1)$$

Here Γ_1 is a single-particle scattering rate taken, for simplicity, to be an ω-independent constant. It is effectively an average of the (actual ω-dependent) Σ'' over the frequency range of the fit. The second term is the BCS self-energy

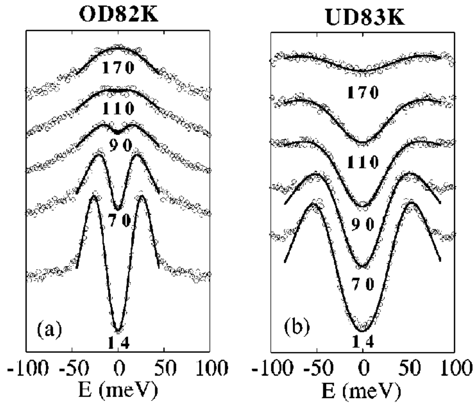

FIG. 1. Symmetrized data for (a) a $T_c=82$ K overdoped sample and (b) a $T_c=83$ K underdoped sample at the $(\pi,0)-(\pi,\pi)$ Fermi crossing at five temperatures, compared to the model fits described in the text.

(corresponding to the diagonal term of the Nambu-Gorkov propagator), where Δ is the SC gap, and $\epsilon(\mathbf{k})$ the dispersion (with $\epsilon(\mathbf{k}_F)=0$). We emphasize that this is a minimal model; modeling the full ω dependence of the self-energy will involve more than Γ_1 and Δ.

In Fig. 1(a), we show symmetrized data for an overdoped $T_c=82$ K sample at $\mathbf{k}_F$ along $(\pi,0)-(\pi,\pi)$ together with the fits obtained as follows. Using Eq. (1) we calculate the spectral function $\pi A(\mathbf{k},\omega)=\Sigma''(\mathbf{k},\omega)/[(\omega-\epsilon_{\mathbf{k}}-\Sigma'(\mathbf{k},\omega))^2+\Sigma''(\mathbf{k},\omega)^2]$, convolve it with the experimental resolution, and fit to symmetrized data. The fit is restricted to a range of ± 45 meV given the small gap in the overdoped case and the sharpness of the quasiparticle peaks below T_c. We find that Eq. 1 describes the data quite well.[8]

The T variation of the fit parameters Δ and Γ_1 are shown in Fig. 2(a). $\Delta(T)$ decreases with T, and although small at T_c, it only vanishes above T_c, indicating the possibility of a weak pseudogap. This effect is sample dependent, in that in several overdoped samples we have looked at, the gap vanishes closer to T_c. We caution that the error bars shown in Fig. 2(a) are based on the rms error of the fits, but do not take into account experimental errors in μ and $\mathbf{k}_F$.

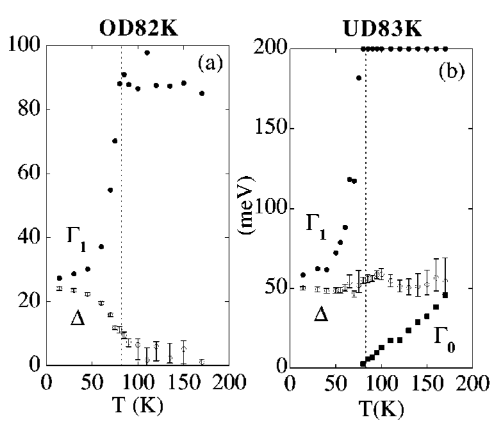

FIG. 2. Δ (open circles), Γ_1 (solid circles), and Γ_0 (solid squares) versus T at the $(\pi,0)-(\pi,\pi)$ Fermi crossing for (a) a $T_c=82$ K overdoped sample and (b) a $T_c=83$ K underdoped sample. The dashed line marks T_c. The error bars for Δ are based on a 10% increase in the rms error of the fits.

$\Gamma_1(T)$ is found to be relatively T independent in the normal state. In comparing this to optical conductivity data, it must be kept in mind that Γ_1 is an average of the true Σ'' near $(\pi,0)$ over the ω range of the fit, whereas $1/\tau_{tr}$ is a zone average weighted by velocity factors which also differs from Σ'' due to different thermal factors. Despite this, it is interesting to note that optical conductivity work has also found a relative lack of T dependence to $1/\tau_{tr}(\omega)$ for $\omega>2\Delta$.[9] Below T_c, we see that Γ_1 decreases very rapidly, and can be perfectly fit to the form $a+bT^6$.[10] This rapid drop in linewidth leading to sharp quasiparticle peaks at low T, which can be seen directly in the ARPES data, is consistent with SC state microwave and thermal conductivity[11] measurements, and implies that electron-electron interactions are responsible for Γ_1.[1,8] Note the clear break in Γ_1 at T_c, despite the fact Δ has not quite vanished. We have seen similar behavior to that described above for a variety of overdoped samples at several $\mathbf{k}$ points.

We next turn to the more interesting underdoped case. We find that near $(\pi,0)$ the self-energy (1) cannot give an adequate description of the data, in that it does not properly describe the pseudogap and its unusual ''filling in'' above T_c. Theoretically, we cannot have a divergence in $\Sigma(\mathbf{k}_F,\omega=0)$ in a state without broken symmetry. A simple modification of the BCS self-energy rectifies both these problems:

$$\Sigma(\mathbf{k},\omega)=-i\Gamma_1+\Delta^2/[\omega+\epsilon(\mathbf{k})+i\Gamma_0]. \qquad (2)$$

The new term $\Gamma_0(T)$ should be viewed as the inverse pair lifetime; below T_c, where the pairs have infinite lifetime, $\Gamma_0=0$, and Eq. (2) reduces to Eq. (1). The theoretical motivation for Eq. (2) is given in the Appendix. We stress that this three parameter form is again a minimal representation of the pseudogap self-energy. Since it is not obviously a unique representation, it is very important to see what one learns from the fits.

In Fig. 1(b), we show symmetrized data at the $(\pi,0)-(\pi,\pi)$ Fermi crossing for a $T_c=83$ K underdoped sample. Below T_c we see quasiparticle peaks. Above T_c these peaks disappear but there is still a large suppression of spectral weight around $\omega=0$. As T is raised further, the pseudogap fills in (rather than closing) leading to a flat spectrum at a temperature of T^* (200 K). The self-energy (2) gives a good fit to the data. These fits were done below T_c over a larger energy range (± 75 meV) than in the overdoped case because of the larger SC gap. The range above T_c was increased to ± 85 meV so as to properly describe the pseudogap depression.

In Fig. 2(b), we show the T dependence of the fit parameters. We find a number of surprises. First, Δ is independent of T within error bars. Similar behavior has been inferred from specific heat[12] and tunneling[13] data. This T independence is in total contrast to the behavior of the overdoped 82 K sample with almost identical T_c at the same $\mathbf{k}$ point. In addition, for the underdoped sample, the gap evolves smoothly through T_c.

The single-particle scattering rate $\Gamma_1(T)$ for the underdoped sample is found to be qualitatively similar to the overdoped case. It is consistent with being T independent above T_c, but with a value over twice as large as the overdoped case (allowing Γ_1 to vary above T_c does not improve the

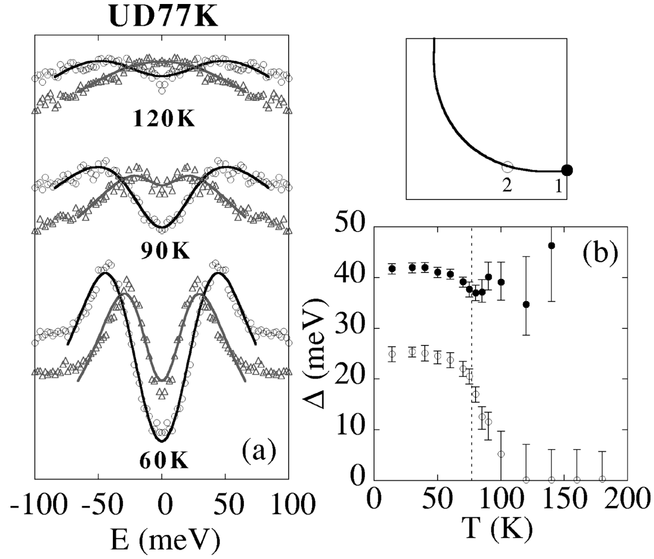

FIG. 3. (a) Symmetrized data for a $T_c=77$ K underdoped sample for three temperatures at (open circles) $\mathbf{k}_F$ point 1 in the zone inset, and at (open triangles) $\mathbf{k}_F$ point 2, compared to the model fits. (b) $\Delta(T)$ for these two **k** points (filled and open circles), with T_c marked by the dashed line.

RMS error of the fits). Second, we see the same rapid decrease in Γ_1 below T_c as in the overdoped case.[10] Note again the clear break at T_c.

The most interesting result is $\Gamma_0(T)$. We find $\Gamma_0=0$ below T_c and proportional to $T-T_c$ above. This behavior is robust, and is seen in all the fits that we have tried. Moreover, a nonzero Γ_0 is needed above T_c to obtain a proper fit to the data (its effect cannot be reproduced by varying the other parameters). The fact that this T dependence is exactly what one expects of an inverse pair lifetime (with a prefactor about twice the weak coupling BCS value; see the Appendix), is a nontrivial check on the validity of the physics underlying Eq. (2). Further, we observe from Fig. 2 that T^* corresponds to where $\Delta(T)\sim\Gamma_0(T)$. This condition can be understood from the small ω expansion of Eq. (2).[14]

We note, in passing, that both ARPES (Refs. 15 and 16) and tunneling measurements[17] indicate that the low temperature SC gap $\Delta(0)$ in Bi2212 increases as the doping is reduced. This increase closely tracks that of the T^* values determined from ARPES.[16] This is further evidence linking T^* to the onset of pairing.

The next important question is whether the T dependence near $(\pi,0)$ described above exists at other $\mathbf{k}_F$ points. To answer this, we have looked at T-dependent data for a number of underdoped samples at two different **k** vectors.[6] All data at the $(\pi,0)-(\pi,\pi)$ Fermi crossing give results similar to those for the 83 K sample. However at the second **k** point, about halfway between the first and the d-wave node along the $(0,0)-(\pi,\pi)$ direction, we see quite different behavior. We demonstrate this in Fig. 3(a) where symmetrized data for a 77 K underdoped sample are shown. For the first **k** point, one clearly sees the gap fill in above T_c, with little evidence for any T dependence of the position of the spectral feature defining the gap edge, just as for the 83 K sample. In contrast, at the second **k** point, the gap is clearly closing, indicating a strong T dependence of Δ. Similar behavior is seen in other underdoped samples with T_c between 75 and 85 K.

In Fig. 3(b), we show the T dependence of Δ obtained from fits (over a range of ± 66 meV) at the second **k** point for the 77 K sample. Δ is found to be strongly T dependent, being roughly constant below T_c, then dropping smoothly to zero above. The strong T dependence of Δ makes it difficult to unambiguously determine Γ_0 from the fits at this **k** point.[18] On theoretical grounds, we expect that, here too, there is a nonzero Γ_0, and the closing of the pseudogap is again determined by $\Delta(T)\sim\Gamma_0(T)$, however this condition is satisfied by the rapid drop in $\Delta(T)$, rather than the rise in $\Gamma_0(T)$. For completeness, we also show $\Delta(T)$ for this sample at the $(\pi,0)-(\pi,\pi)$ Fermi crossing, which has a similar behavior to that of the 83 K sample.

We see that these results give further evidence for the unusual **k** dependences first noted in Ref. 6. Strong pairing correlations are seen over a very wide T range near $(\pi,0)$, but these effects are less pronounced and persist over a smaller T range as one moves closer to the diagonal. This is clearly tied to the strong **k** dependence of the effective interaction and the unusual (anomalously broad and nondispersive) nature of electronic states near $(\pi,0)$. Some of these features are captured in recent theoretical studies of the pseudogap.[19–21]

To summarize, we have introduced a simple phenomenological self-energy expression which helps us to analyze ARPES data and gain insight into the T dependences of important parameters like the gap and the one-particle scattering rate. Perhaps the most interesting new result concerns the modeling of the pseudogap data in the underdoped cuprates, where we found a new lifetime effect above T_c proportional to $T-T_c$. We argue that this is naturally explained as an effect of pairing correlations above T_c on the one-particle spectral function. In fact, this qualitative observation argues against nonpairing theories of the pseudogap, in that a term proportional to $T-T_c$ does not naturally appear in such theories. A second important result concerns the differences between the pseudogap behavior in different parts of **k** space. Near $(\pi,0)$ we found a constant $\Delta(T)$ with ''filling in'' of spectral weight with increasing T. Away from this region, the pseudogap closes rather than fills in. These observations impose very important constraints for the microscopic theory of high-T_c cuprates.

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APPENDIX

The simplest way to motivate the second term of Eq. (2) is as follows. The BCS Σ of Eq. (1) may be seen as arising from a bare Green's function G_0 dressed by a pair ''susceptibility'' of the form $\Delta_{\mathbf{k}}^2\delta(\mathbf{q})\delta(\omega)$ representing static long-range order. If the pairs have a finite inverse lifetime Γ_0, then $\delta(\omega)$ is broadened into a Lorentzian, leading to Eq. (2).

We next sketch a more formal derivation, valid in the regime of ''small fluctuations,''[22] which gives further insight into the form of $\Gamma_0(T)$. The lowest-order graph is G_0 dressed by the fluctuation pair propagator L: $\Sigma(\mathbf{k},\epsilon_n)=-T\Sigma_\nu\int(d\mathbf{q})L(\mathbf{q},\omega_\nu)G_0(\mathbf{q}-\mathbf{k},\omega_\nu-\epsilon_n)$. Here $L^{-1}(\mathbf{q},\omega_\nu)=N_0(\varepsilon+\alpha|\omega_\nu|+q^2\xi_0^2)$ with $\varepsilon\simeq(T-T_c)/T_c$, $\alpha=\pi/8T_c$, the coherence length $\xi_0\sim v_F/T_c$, and N_0 is the density of states. ϵ_n and ω_ν are Fermi and Bose frequencies, respectively, and $\int(d\mathbf{q})=\int d^Dq/(2\pi)^D$. Evaluating Σ_ν using standard contour integration, we obtain $\Sigma(\mathbf{k},\epsilon_n)=(T/N_0)\int(d\mathbf{q})F_1(\mathbf{q})F_2(\mathbf{q})$. Here $F_1(\mathbf{q})=1/[\varepsilon+q^2\xi_0^2]$ is sharply peaked in q with a scale $\xi_0^{-1}\sqrt{\varepsilon}$. Before analytic continuation $|i\epsilon_n|\geqslant\pi T$, and thus the q variation of $F_2(\mathbf{q})=1/[i\epsilon_n+i8T_c(\varepsilon+q^2\xi_0^2)/\pi+\epsilon(\mathbf{q}-\mathbf{k})]$ is on the much larger scale of ξ_0^{-1}. Thus we make the approximation $\Sigma\simeq F_2(0)(T/N_0)\int d(\mathbf{q})F_1(\mathbf{q})$. Finally, doing the Bose sum in $\langle|\Delta(\mathbf{r},t)|^2\rangle=T\Sigma_\nu\int(d\mathbf{q})L(\mathbf{q},\omega_\nu)$, we get the ''fluctuating'' gap $\langle|\Delta|^2\rangle=(T/N_0)\int(d\mathbf{q})F_1(\mathbf{q})$. Substituting this in Σ, and setting $i\epsilon_n\rightarrow\omega+i0^+$, we obtain the second term in Eq. (2) with $\Gamma_0(T)=8(T-T_c)/\pi$.

In $D=0$ dimensions, which may be relevant in the vicinity of the dispersionless $(\pi,0)$ point, we do not need to make the approximation of pulling $F_2(0)$ out of the q integration, which justifies the result even for arbitrarily small ω. In any case, we emphasize that the above derivation is used here only to motivate the form of Eq. (2), which is then used for fits in a more general context.

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[7] Spectra analyzed below were normalized to the constant signal above the Fermi energy, which was then subtracted off. No other background subtractions were made since we are focusing on low energy data.

[8] The deviations beyond about 40 meV at low T are due to the strong ω dependence of the SC state self-energy for $\omega>2\Delta$; see M. R. Norman *et al.*, Phys. Rev. Lett. **79**, 3506 (1997); M. R. Norman and H. Ding, preceding paper, Phys. Rev. B **57**, R11 089 (1998). To consider these higher binding energy effects will require a more general ansatz than the one presented here with correspondingly more parameters.

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