Temperature-induced spectral weight transfer in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$: a conventional view

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In contrast with the recent photoemission observations by Shen et al. of anomalous temperature-induced momentum-dependent spectral weight transfer in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, we find that in the same material, in spite of the unusual spectral lineshape change between superconducting and normal states, the integrated spectral weight displays minimum variation as a function of temperature, which is in agreement with the sum rule of angle-resolved photoemission: the integrated spectral weight is proportional to the momentum density, $n(k)$.

PACS numbers: 71.25.Hc, 74.25.Jb, 74.72.Hs, 79.60.Bm

One of the many ways in which high temperature superconductors differ from previously studied materials is that their spectra measured by angle-resolved photoemission are strongly temperature dependent. This dependence has been attributed to strong electron-electron interactions, which are the dominant scattering mechanism for electrons in these materials. Much has been learned from studying the spectral lineshapes. We have shown that, under suitable experimental conditions, the intensity measured in an angle-resolved photoemission (ARPES) experiment is given by

$$I(k, \omega) = I_0(k)f(\omega)A(k, \omega),$$

where $k$, the in-plane momentum, gives the location in the 2D Brillouin zone, and $\omega$ is the energy of the initial state measured relative to the chemical potential. Experimentally $\omega$ is measured relative to the Fermi level of a good metal like Pt or Au in electrical contact with the sample. $I_0(k)$ includes all the kinematical factors and the dipole matrix element (squared). It depends, in addition to $k$, on the incident photon energy and polarization. $I_0$ determines the overall intensity of the measured spectra through the dipole selection rules obeyed by the matrix elements, and does not affect the spectral lineshape.

The spectral lineshape ($\omega$ dependence) and its $T$ dependence, at the low frequencies and temperatures of interest to us, are entirely controlled by $f(\omega)A(k, \omega)$. Here $A(k, \omega)$ is the initial state or “photo-hole” spectral function $A(k, \omega) = (-1/\pi)\text{Im}G(k, \omega + i0^+)$, and the Fermi function $f(\omega) = 1/\text{exp}(\omega/kT) + 1$ ensures that we are only looking at the occupied part of this spectral function. Furthermore, the ARPES intensity obeys the sum rule such that the integral of a single spectral peak is proportional to the momentum distribution, $n(k)$

$$\int_{-\infty}^{+\infty} d\omega f(\omega)A(k, \omega) = n(k).$$

An experimental example from the high-$T_c$ superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) can be found in Ref. 3. We have shown that, in spite of the unusual spectral lineshape changes exhibited by Bi2212 with temperature, the integrated spectral weight still satisfies the sum rule (2), such that the integrated weight at, or far away from, the Fermi surface ($k_F$) is temperature independent. This work has found that as the temperature is changed from above to below $T_c$ (approximately 90 K), lineshape changes occur over an energy scale of order $4\Delta_0$, where $\Delta_0$ is the maximum value of the superconducting gap. In general, one does not expect spectral changes to occur over an energy range which is orders of magnitude larger than $4\Delta_0$, unless there is an intervening structural phase transition. Such phase transitions have not been observed in clean Bi2212.

However, a recent photoemission study on Bi2212 by Shen et al. reported anomalous temperature-induced momentum-dependent changes between ARPES spectra in the superconducting and normal states. The reported effect is rather drastic, with spectral changes occurring over an energy range as large as the bandwidth, ~ 300 meV, much larger than the maximum superconducting gap, $\Delta_0$, (~30 - 40 meV). Also, spectral weight is found to be transferred over a sizable momentum vector, 0.45$\pi$, which is much larger than the conventional thermal effect, $\max(kT, \Delta_0)/v_F$, where $v_F$ is the Fermi velocity. According to Ref. 3, this is due to the presence of fluctuating stripes which have charge- and spin-order periodicities of (0.45$\pi$, 0).

The topic of spin and charge stripes and their role in high temperature superconductors is of current interest. There is some evidence that spin and charge stripes ex-
exist in the high-$T_c$ superconductor $La_{2-x}Sr_xCuO_4$ doped with Nd. For Bi2212, Ref.\textsuperscript{[6]} would represent the strongest evidence yet for the presence of charge stripes in this material. Thus it is important to rule out other possible explanations for such an unusual result. In this paper we wish to point out that there are experimental artifacts that can produce the effect observed by Shen et al., and that these must be first ruled out in order to strengthen the case for the observation of stripes by ARPES. Here we show that there are two possible effects which can lead to the results reported in Ref.\textsuperscript{[6]}, namely a change in emission angle in the experiment, and sample aging. After discussing the source for these artifacts, we propose experiments designed to check for their presence, and in the first case, how to account for it.

Our experiments were performed at the Synchrotron Radiation Center, Wisconsin, using a high resolution 4-meter normal incidence monochromator. The high quality single crystals Bi2212, grown by the traveling solvent floating zone method, have low defect densities with very long structural coherence lengths. Also, a crucial requirement is the presence of a flat surface after cleaving, as we discuss in detail below.

We start by showing the normal behavior of the spectral weight transfer with temperature. In Fig. 1 we show, as an example, a slightly underdoped ($T_c = 89$K) sample which was a very flat surface and was measured from high temperature ($\sim$300K) to low temperature (14K) in a short period of time (less than 3 hours) in a good vacuum ($\sim$5x10$^{-11}$) to ensure the absence of surface contamination. Fig. 1a displays spectra along (0,0) to ($\pi$, 0) at different temperatures. First, the broad normal state peak evolves into a sharp peak, dip and broad peak (hump) in the superconducting state. This has been previously described in detail,\textsuperscript{[1]} and occurs as a result of a rapid variation with $\omega$ of the electron damping in the superconducting state. Second, spectra show identical high-binding-energy features (broad peaks and tails) beyond binding energies of 4$\Delta_0$. No anomalous weight transfer is observed, as shown in Fig. 1b, which plots the area under each spectra (from -0.6 eV to 0.1 eV) as a function of momentum. The areas of the two states are the same for each $k$ point within the experimental uncertainty. The fact that most experiments, under carefully controlled experimental conditions, show spectra which are "well-behaved" immediately throws suspicion on unusual results, such as those shown in Fig. 2 (and those of Ref.\textsuperscript{[6]}).

In Fig. 2 we show ARPES spectra of a slightly overdoped Bi2212 sample ($T_c = 87$K) along (0,0) to ($\pi$,0), extending to the second Brillouin Zone with a high density of $k$ points. Solid curves are for the normal state at 105K, dotted ones are for the superconducting state at 13K. It is clear from Fig. 2 that, unlike the case of Fig. 1, the spectra are quite different between normal and superconducting states. The overall spectral weight changes between the two temperatures. The change is most noticeable at small momenta, where the dispersion is strongest (see spectra between (0.37,0)$\pi/a$ and (0.56,0)$\pi/a$). The self-energy is not expected to change significantly at such high binding energies with an increase in temperature of only $\sim$100 K. The change is quantified in Fig. 2b, which shows a plot of the integrated intensity of the data in Fig. 2a. Note that this observation is exactly what is described in Ref.\textsuperscript{[6]}. We should point out that we use a different normalization procedure from that of Ref.\textsuperscript{[6]}. Our data are simply normalized to the photon flux by normalizing each spectra to the same second order intensity well above the Fermi energy. Therefore our spectra are plotted as being proportional to electrons per photon. The use of this single normalization procedure, and an artifact to be described below, result in discrepancies at high binding energy between the two states. The same problem is present in Ref.\textsuperscript{[6]}, but there the authors use an additional normalization (different for each $k$ point) to match the high binding energy tails of the two states. This procedure is highly undesirable, since it rescales the spectra in unknown ways and is a sign of potential experimental problems, as discussed below.

That an artifact is responsible for the unusual spectral weight transfer is confirmed by a closer inspection of the data in Fig. 2. If, instead of comparing spectra in the normal and superconducting states at nominally the same momenta, we instead translate the normal state spectra by ($0.09\pi/a$, 0) with respect to the superconducting spectra (equivalent to a two-degree change of the emission angle along $k_x$), then not only do most of the broad features now agree, but the high-binding-energy tails also match (see Fig. 3a) – in agreement with the behavior of most of our data. By plotting the integrated spectral weight (from -0.6 eV to 0.1 eV) as a function of momentum (Fig. 3b), one can clearly see this effect: by a simple shift in $k_x$ of 0.09$\pi/a$, one obtains a much better agreement of the integrated weight between the two states, akin to the spectra shown in Fig. 1.

This immediately suggests a possible cause for the experimental artifact, a possible experimental check, and a method for correcting the data. This particular case of large scale spectral weight transfer is caused by sample movement, which necessarily occurs in the experiment. As the sample temperature is changed from the normal to the superconducting regime, the sample changes position because of the thermal expansion of the long cryostat on which the sample is mounted.\textsuperscript{[13]} During an experimental run, the sample position must be continuously adjusted to account for such movements. Such position changes can shift emission angle, especially when the sample surface is not flat. Fortunately, given a sufficiently high number of spectra, this effect can be easily corrected for, as shown in Fig. 3a.

The second type of effect, sample aging, unfortunately, cannot be easily corrected for. Sample aging also produces similar large scale changes in the data.\textsuperscript{[13]} This effect is more pronounced in a lower vacuum, as shown in Fig. 4, where the chamber pressure is $\sim$4x10$^{-10}$, almost one order of magnitude worse than the one in Fig. 1. Fig.
ure 4 shows ARPES spectra at the most dispersive region along (0,0) to (π,0) for a slightly overdoped Bi2212 sample (T_c = 88K). Dotted curves are for the superconducting state at 50K and solid ones correspond to the normal state at 100K. The sample was cleaved and measured at 50K, then heated to 100K. Notice that the 100K spectra shift considerably towards the Fermi energy, similar to the previous case, where the shift of more aged spectra is always towards lower binding energy, unlike in the previous case, where the direction of shift is determined by temperature.

We have measured several samples with various doping levels to check for the presence of a weight transfer. We find the effects discussed in Fig. 2 and Fig. 4 only when the samples have a non-flat surface or they visibly age, or when there is an instability in the synchrotron beam. Therefore, it is reasonable to conclude, at least in our case, that the anomalous weight transfer is an experimental artifact. This conclusion strongly suggests that the artifacts described here need to be ruled out in the case of the samples used by Shen et al in order to strengthen the case for an anomalous spectral weight transfer in Zn-doped samples.

Several possible experiments suggests themselves to this effect. One must first ensure that the sample position remains constant during temperature changes, which can easily be accomplished to high precision using existing optical techniques, such as theodolites or laser interferometers. One must also ensure that the cleaved surfaces are optically flat, which, again, can be accomplished in situ with laser reflectometry. The data can also be checked for internal consistency. A plot of the integrated intensity vs momenta, such as those shown in Figs 2b and 3b, will indicate the presence of an artifact. But most importantly, if the anomalous weight transfer is indeed due to the presence of stripes which shift the spectra by a given momentum transfer Q, one should check that the spectral weight is periodic in Q. In our case, as clearly indicated by Fig. 3b, it is not periodic, and therefore the effect cannot be ascribed to an additional periodicity introduced by stripes.

This work was supported the National Science Foundation DMR 9624048, and DMR 91-20000 through the Science and Technology Center for Superconductivity, and by the U. S. Dept. of Energy, Basic Energy Sciences, under contract W-31-109-ENG-38. The Synchrotron Radiation Center is supported by NSF grant DMR-9212658.

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FIG. 1. (a). Temperature-dependent ARPES spectra in the (0,0) to (π,0) direction from a slightly underdoped Bi2212 with T_c = 89K. For each momentum, there are three curves measured at different temperatures, dashed curves are from 192K to 141K, solid ones from 137K to 81K, thick dotted ones from 76K to 15K. (b). The corresponding integrated spectral weight of the spectra in (a).

FIG. 2. a) ARPES spectra along (0,0) to (π,0) in the normal state at 105K (solid curves) and the superconducting state at 13K (dashed curves) from a slightly overdoped Bi2212 sample with T_c = 87K; b) Plot of the differences of the integrated intensities of the normal and superconducting states as a function of angle for the data in (a).

FIG. 3. (a). Same ARPES data as in Fig. 2, but with the normal state shifted by 0.09π/a in the k_x direction, which corresponds to two-degree emission angle change. (b). Integrated areas as a function of momentum, k_x. Note the discrepancy between normal state areas (dotted line with empty circles) and superconducting ones (solid line with asterisks) can be corrected by a small shift of normal state data (dashed line with filled circles).

FIG. 4. ARPES spectra at the most dispersive region along (0,0) to (π,0) in the normal state at 100K (solid curves) and the superconducting state at 50K (dashed curves) from a slightly overdoped Bi2212 sample with T_c = 88K.
Intensity (arb. units)

Energy (eV)

Area (arb. units)

(a) (b)

192 - 141K
137 - 81K
76 - 15K
