PHYSICAL REVIEW B **74**, 174516 (2006)

Intraband optical spectral weight in the presence of a van Hove singularity: Application to $Bi_2Sr_2CaCu_2O_{8+\delta}$

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(Received 26 June 2006; revised manuscript received 7 September 2006; published 22 November 2006)

The Kubo single-band sum rule is used to determine the optical spectral weight of a tight-binding band with farther than nearest-neighbor hopping. We find for a wide range of parameters and doping concentrations that the change due to superconductivity at low temperature can be either negative or positive. In contrast, the kinetic energy change is always negative. We use an angle-resolved-photoemission-spectroscopy-determined tight-binding parametrization of $Bi_2Sr_2CaCu_2O_{8+\delta}$ to investigate whether this can account for recent observations of a positive change in the spectral weight due to the onset of superconductivity. With this band structure we find that in the relevant doping regime a straightforward BCS calculation of the optical spectral weight cannot account for the experimental observations.

DOI: 10.1103/PhysRevB.74.174516 PACS number(s): 74.25.Gz, 74.20.Fg, 74.72.−h, 79.60.−i

I. INTRODUCTION

Recent optical experiments on several high-T_c cuprates at optimal and low doping levels[1–4] have shown an increase in the low-frequency spectral weight when the system goes superconducting. These observations are at odds with the simplest expectation based on BCS theory,[5–7] where the kinetic energy is expected to increase in the superconducting state; however, they conform with the general notion of "kinetic-energy-driven" superconductivity.[8] Since the optical spectral weight is just the negative of the kinetic energy for a single band with nearest-neighbor hopping only, a *decrease* in spectral weight is expected to occur below the superconducting transition temperature. Several alterations to the standard BCS picture have been proposed, the most minor of which involve an alteration to the boson spectrum when the system goes superconducting.[9–12]

More recent measurements[13,14] have shown a continuous evolution with doping from "non-BCS-like" (low doping) to "BCS-like" (high doping) behavior; an understanding of this doping dependence has been suggested in Refs. 14–17 based on strong electron-electron correlations and in Refs. 18–20 based on the doping dependence of a transition driven by pairing versus phase coherence.

While all these proposals remain interesting possibilities to explain the observations, the purpose of this paper is to revisit the question of what "BCS-like" behavior is, by taking into account band structure details. It is important to do this, since our intuition is based on the behavior of the kinetic energy which (as we illustrate below) always increases in the superconducting state. However, the optical spectral weight for a single band is given by[21,22]

$$W(T) = \frac{2\hbar^2}{\pi e^2}\int_0^{+\infty} d\nu\, \mathrm{Re}[\sigma_{xx}(\nu)] = \frac{2}{N}\sum_k \frac{\partial^2 \epsilon_k}{\partial k_x^2} n_k, \qquad (1)$$

whereas the negative of the band kinetic energy is given by a somewhat different expression; in the simplest case, it is given by

$$-\langle K\rangle = -\frac{2}{N}\sum_k \epsilon_k n_k, \qquad (2)$$

where ϵ_k is the tight-binding dispersion (which takes into account already Hartree-Fock-type corrections) and n_k is the single-spin momentum distribution function (we take the lattice spacing to be unity). The sum over k is over the first Brillouin zone and, in the case with bilayer splitting (see below), includes a summation over the two split bands. Note that this is *not* the total kinetic energy of all the electrons, but just the kinetic energy of the electrons in the given tight-binding band(s); furthermore, *only* in the case of nearest-neighbor hopping is W proportional to $-\langle K\rangle$. In the presence of more complicated interactions, the expectation value of the kinetic energy has more complicated terms.

We first review the expectation for the kinetic energy, based on Eq. (2), since this correspondence has been used to build intuition concerning the optical spectral weight. First, what happens when the system goes superconducting? The momentum distribution function changes as discussed previously[7]—it goes from a Fermi-like distribution function (in the absence of strong correlations) to a distribution smeared by the presence of a superconducting order parameter. For an order parameter with d-wave symmetry, the momentum distribution is no longer a function of the band structure energy ϵ_k alone. For example, for a BCS order parameter with simple nearest-neighbor pairing form, $\Delta_k = \Delta(\cos k_x - \cos k_y)/2$; then, as k varies from (0,0) to $(\pi,0)$, the magnitude of the order parameter changes from zero to Δ. On the other hand, as k varies along the diagonal (from the bottom of the band to the top), the order parameter is zero (and constant). In any event, even at zero temperature, BCS-like superconductivity *raises* the kinetic energy of the electrons [see Fig. 1(b) of Ref. 7]. This is as expected, since for noninteracting electrons the normal state at zero temperature corresponds to a state with the lowest possible kinetic energy. Therefore, any modification to this state (for example, because of a superconducting instability) can only increase the kinetic energy expectation value.

The question, partially answered in Refs. 7 and 14 is, does this behavior remain at all electron densities? Furthermore, with farther than nearest-neighbor hopping, does the spectral weight [given by Eq. (1)] also follow the same trend as the negative of the kinetic energy? Perhaps not surprisingly, we find that the spectral weight does not qualitatively follow the kinetic energy near a van Hove singularity. However, as will be discussed further below, we find that for the band structure and doping regime thought to be applicable in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO),[24] the spectral weight should decrease in the superconducting state relative to the normal state. That is, correlations, phase fluctuations, scattering rate collapse, or some other scenario is required to understand the "anomalous" behavior. We will also address the temperature dependence in the normal state; in some ways, this is a more easily measured quantity than the change below T_c.

In the next section we examine the optical spectral weight for a model with nearest-neighbor hopping only. This simple band structure yields an optical spectral weight that is directly proportional to the expectation value of the negative of the kinetic energy. We examine the behavior of the optical spectral weight as a function of electron density. Note that we will use the symbol n to denote electron density; for a single band, this quantity will span values from 0 to 2. It will be used when systematic investigations of the spectral weight for a given band structure are carried out. When comparing with experiments in the cuprates, we will use the symbol δ to denote doping away from half-filling—i.e., $n=1$. Thus, $\delta=1-n$ and the regime of experimental interest is roughly $0<\delta<0.25$. We use the phrase "hole doping" to refer specifically to the value of δ.

Following this section we introduce next-nearest-neighbor hopping into the band structure (t-t' model). This moves the van Hove singularity away from half filling and also causes the spectral weight to deviate from the kinetic energy; hence, both will be plotted in the ensuing plots. We find already in this simple extension significant departures from the "standard BCS" description based solely on the kinetic energy.

Finally, following Ref. 24, we also introduce a next-next-nearest-neighbor hopping and a bilayer splitting term; these are required for a quantitatively accurate description of the angle-resolved photoemission spectroscopy (ARPES) results. We find that these terms have significant effects on the optical sum rule. First, the van Hove singularity is split into two singularities; second, the first of these occurs at a much lower hole doping level than in the t-t' model.

As discussed in the summary, the end result is that (i) the change in the optical spectral weight due to superconductivity can be either positive or negative, depending on the band structure and electron density, and (ii) if a parametrization of the band structure is adopted from ARPES studies, then the optical spectral weight *decreases* in the superconducting state. The observed *increase* for optimal and underdoped samples then requires additional ingredients. Some possibilities are briefly mentioned.

II. NEAREST-NEIGHBOR HOPPING ONLY

For nearest-neighbor hopping only, the band structure is given by

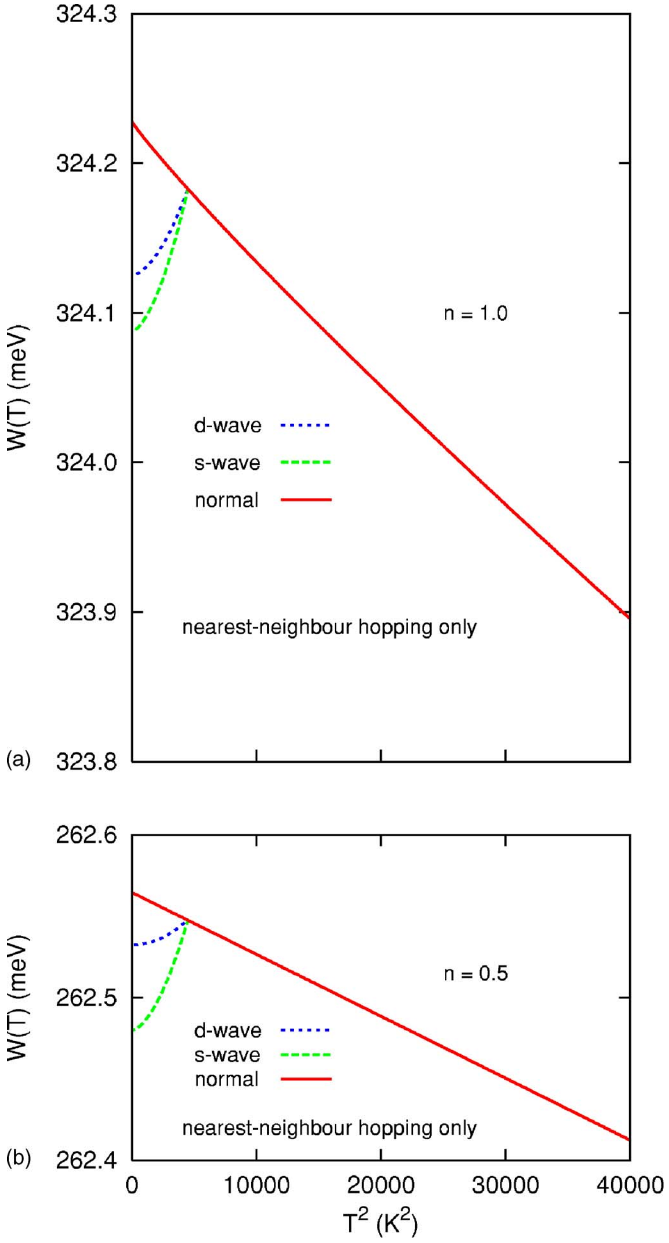

FIG. 1. (Color online) Spectral weight vs T^2 for (a) half-filling and (b) $n=0.5$. The normal state is given by the solid red curve, and the superconducting state with d-wave (s-wave) symmetry by the short-dashed blue (dashed green) curve. In both cases the normal-state result is almost linear in T^2 and the superconducting state shows a decrease in the spectral weight (increase in the kinetic energy) as expected. We used $t=0.4$ eV and BCS values for order parameters, etc., with $T_c=69$ K.

$$\epsilon_k^{nn} = -2t(\cos k_x + \cos k_y) \tag{3}$$

and we have that $2W=-\langle K\rangle$ in two dimensions. In Fig. 1 we show plots of the spectral weight versus T^2 for two representative electron densities $n=1$ and $n=0.5$. The first places the Fermi level right on the van Hove singularity, while the second is well removed from all van Hove singularities. These are computed through the usual procedure: first, even in the normal state, the chemical potential must be determined at each temperature to ensure that the electron density remains constant as a function of temperature. This is the common procedure, though it is true that in complicated systems for which one is using some "low-energy" tight-binding Hamiltonian to describe the excitations that it is not immediately obvious that the electron number density should remain fixed as a function of temperature; nonetheless, we adopt this procedure here. In Eq. (1) the chemical potential enters the momentum distribution function, which, in the normal state, is replaced by the Fermi-Dirac distribution function, $n_k \rightarrow f(\epsilon_k - \mu)$. In the superconducting state, we simply adopt a model temperature dependence for the order parameter, following Ref. 7. This has been tested for both s-wave and d-wave symmetries by comparing to fully self-consistent solutions to BCS equations with separable potentials.[7] One still has to determine the chemical potential self-consistently for each temperature, which is done by solving the number equation in the superconducting state for a fixed chemical potential and order parameter, and iterating until the desired number density is achieved. We use the standard BCS expression

$$n = 1 - \frac{1}{N}\sum_k \frac{\epsilon_k - \mu}{E_k}[1 - 2f(E_k)], \tag{4}$$

where $E_k \equiv \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}$ and Δ_k can take on both s-wave and d-wave forms. In the normal state this expression reduces to the simple Fermi function; even above T_c, however, iteration for the correct value of the chemical potential is required. Interestingly, if one (incorrectly) adopts the same chemical potential as a function of temperature, then the effects discussed here become more pronounced [for example, in Fig. 6(c) below, the variation above T_c and the reversal below T_c is stronger].

The value of the zero-temperature order parameter is fixed by the weak-coupling BCS values, $2\Delta_0 = \eta k_B T_c$ where $\eta = 4.2(3.5)$ for the d-wave (s-wave) case. Further details are provided in Ref. 7. For the electron densities studied in the first part of this paper, we simply take $T_c = 69$ K for all electron densities. In Sec. IV we will adopt T_c values as observed from experiment.

Both plots in Fig. 1 show somewhat linear behavior with T^2, though in Fig. 1(a) there is some noticeable upward curvature due to the van Hove singularity which is present at the Fermi level for this electron density. The decrease in spectral weight at the transition is more pronounced for s-wave symmetry (dashed green curves) than for d-wave symmetry (dotted blue curves). The normal-state results show a decreasing value with increasing temperature, indicative of an increasing kinetic energy. This is a "textbook" example of the temperature dependence of the spectral weight through a superconducting transition.[5–7]

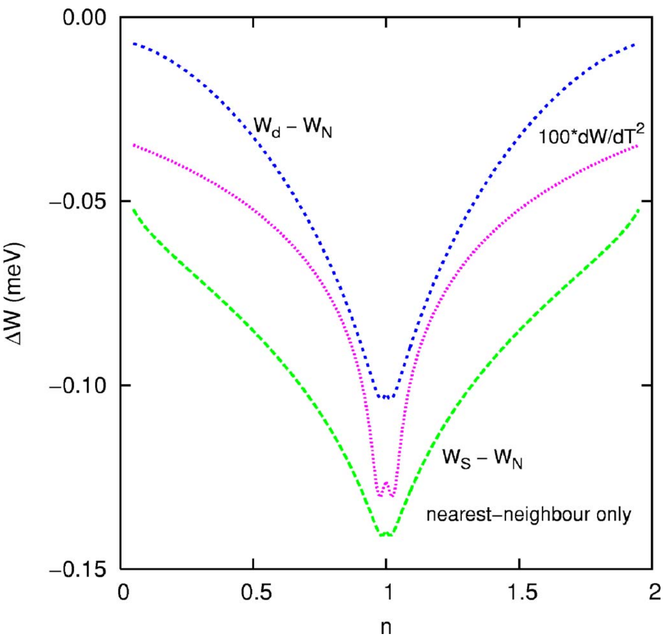

FIG. 2. (Color online) The difference ($W_d - W_N$) in the spectral weight between the superconducting state with d-wave symmetry and the normal state at zero temperature vs doping (dotted blue curve). The dashed green curve shows the same quantity for s-wave symmetry, and the pink points indicate the slope (with respect to T^2) of the spectral weight near T_c. All three quantities are always negative and show an enhancement near half-filling due to the van Hove singularity. In fact, the pink points are almost a perfect inverted image of the density of states [see the minus sign in Eq. (8)], except for the small density regime near half-filling, where the van Hove singularity makes the Sommerfeld expansion invalid.

In Fig. 2 we examine both the spectral weight difference ($W_s - W_N$ and $W_d - W_N$ for s- and d-wave symmetry, respectively—N here stands for "normal") at zero temperature, and the slope of $W(T)$ with respect to T^2 at T_c versus electron density n. These plots make evident several important points. First, the van Hove singularity clearly plays a role; it enhances the overall magnitude of the effect, whether we examine the difference between the superconducting and normal state at zero temperature or the slope at T_c. In fact the latter tracks the former, indicating that both are related to one another. One can understand this qualitatively by the observation that in both cases (warming up or going superconducting) the momentum distribution function broadens, though for different reasons.[7] The most important point to learn from this plot is that the difference is always negative, indicating that, for nearest-neighbor hopping only, the opening of a gap does indeed increase the kinetic energy and decrease the spectral weight in a superconductor.

III. NEXT-NEAREST-NEIGHBOR HOPPING

When next-nearest-neighbor hopping is included in the band structure, one obtains the so-called t-t' model. This model has band structure

$$\epsilon_k^{nnn} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y \tag{5}$$

and goes a long way towards understanding the Fermi surface of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), as determined by ARPES,[23,24] at least for the doping levels studied. On the theoretical side, the presence of t' shifts the van Hove singularity to an energy given by $\mu = -4t'$. For the sake of this study one can study all electron densities; however, one must bear in mind that most experiments on BSCCO are at doping levels such that the van Hove singularity is not crossed; i.e.,

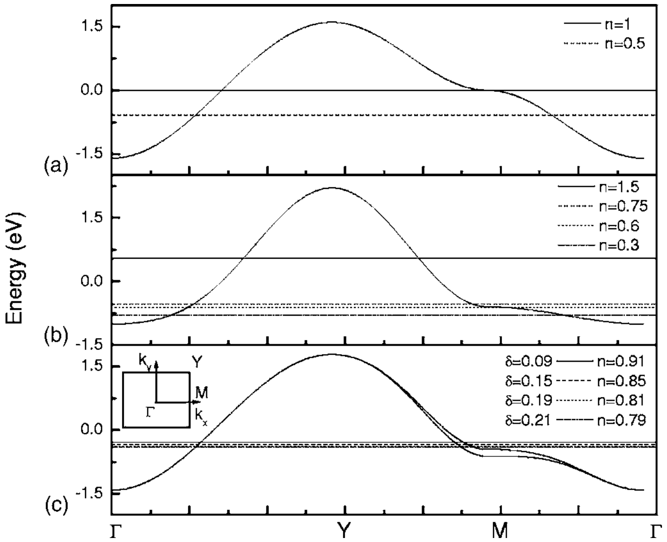

FIG. 3. Illustrative plots of the band structure for (a) nearest-neighbor hopping only, (b) the t-t' model, and (c) parametrization of Kordyuk *et al.* (Ref. 24) of the band structure with bilayer splitting. The van Hove singularities occur where the band dispersion flattens.

the Fermi surfaces are always hole like. We will also study (see next section) a band structure more pertinent to BSCCO,[23,24] which uses a next-next-nearest-neighbor hopping amplitude in addition:

$$\epsilon_{k\pm} = \epsilon_k^{nnn} - 2t''(\cos 2k_x + \cos 2k_y) \pm t_\perp(\cos k_x - \cos k_y)^2/4, \tag{6}$$

which we will refer to as the t-t'-t'' model. Note that we allow for a bilayer splitting term as well, following Kordyuk *et al.*[24] However, they actually adjust hopping parameters for each doping, while we simply adopt the ones used for their overdoped sample: $t=0.40$ eV, $t'=0.090$ eV, $t''=0.045$ eV, and $t_\perp=0.082$ eV. Illustrative plots of the band structures are shown in Fig. 3.

Returning now to the t-t' model, the van Hove singularity occurs at an electron density $n=0.60$—i.e., a hole doping (away from half-filling) of $\delta=1-n=0.4$. As mentioned above, this high level of doping is never realized in samples of BSCCO.[25] In any event, we are interested in the more generic behavior of the spectral weight, given a reasonably representative band structure for the cuprates.

In Fig. 4 we show a summary of the doping dependence of the various quantities with the t-t' band structure. In both Figs. 4(a) and 4(b) we have plotted the density of states at the Fermi level as a function of doping (this is possible for a doping-independent band) to illustrate where the van Hove singularity is. The remarkable feature in Fig. 4(a), for electron densities below the van Hove singularity, is that the spectral weight change in the superconducting state is positive. Similarly, in Fig. 4(b) the actual slope of the spectral weight above T_c is positive. Note that our intuition about the kinetic energy change remains correct; it is indeed negative, for all electron densities, for both s-wave and d-wave symmetries. Moreover, the slope is also everywhere negative,

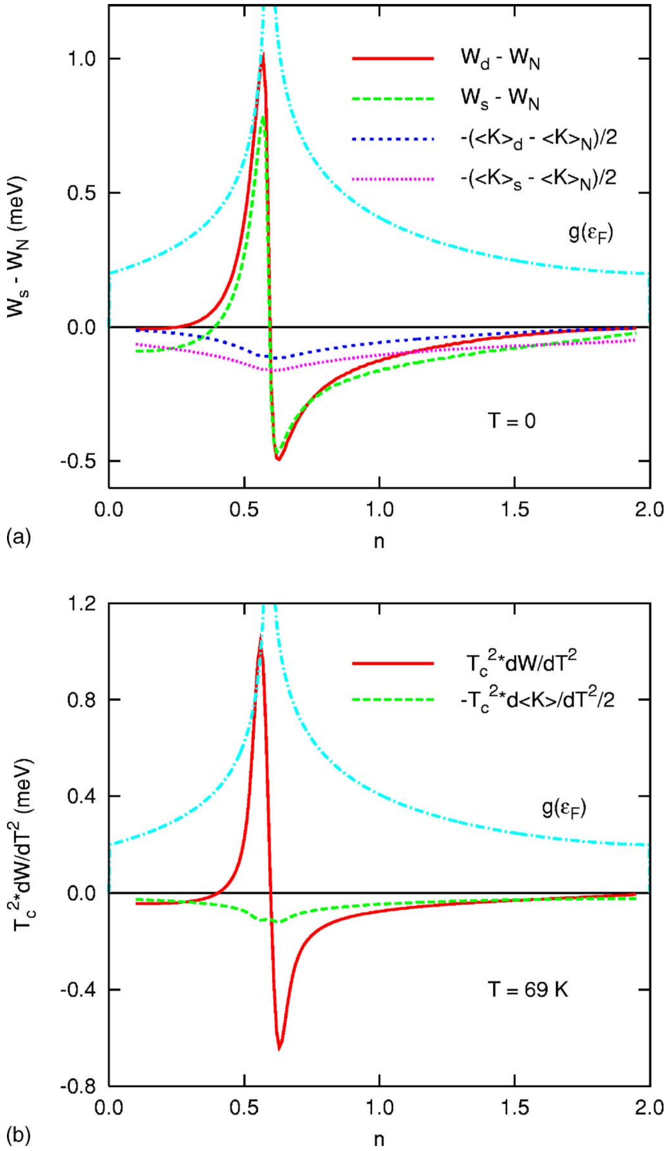

FIG. 4. (Color online) (a) The difference $(W_d - W_N)$ in the spectral weight between the superconducting state with d-wave symmetry and the normal state at zero temperature vs doping (solid red curve), for the t-t' band structure, with $t=0.4$ eV and $t'=0.09$ eV. The dashed green curve shows the same quantity for s-wave symmetry. Both exhibit positive values to the left of the van Hove singularity (the density of states at the Fermi level is indicated, as a function of doping, by the dot-dashed cyan curve). The negative of the kinetic energy for d-wave (blue short-dashed curve) and for s-wave (dotted pink curve) symmetry behaves as expected, always negative, and peaks (in absolute value) at the van Hove singularity. (b) The normal-state slope (taken at $T_c=69$ K) of the spectral weight vs doping (solid red curve). The dashed green curve shows the same quantity for the negative of the kinetic energy. These behave in very similar fashion to the differences (taken at zero temperature) shown in (a).

which establishes a definite correlation between the slope above T_c and the change at $T=0$. Note that in Ref. 7 (see Fig. 4 of that reference) the doping parameters were such that the optical sum rule and the negative of the kinetic energy were qualitatively (and even quantitatively) similar.[26] Here, in the vicinity of the van Hove singularity we encounter a regime where these two properties are markedly different from one another.

How do we understand this strange dependence near the van Hove singularity? It is easiest to focus on the temperature dependence in the normal state. One should first review the simple argument for why the slope for the negative of the kinetic energy is expected to *always* be negative, no matter what the band structure. This quantity is defined as

$$-\langle K\rangle = -2\int_{-\infty}^{+\infty} d\epsilon\,\epsilon g(\epsilon) f(\epsilon-\mu), \tag{7}$$

where $g(\epsilon)\equiv\frac{1}{N}\Sigma_k\delta(\epsilon-\epsilon_k)$ is the single-spin, single-particle density of states for electrons with band dispersion ϵ_k. One can perform a Sommerfeld expansion, which yields two terms, one of which is eliminated by performing the analogous expansion for the electron density, with the requirement that the density remain constant as a function of temperature.[27] The result is[27]

$$-\langle K\rangle = -\langle K\rangle_{T=0} - \frac{\pi^2}{3}(k_B T)^2 g(\epsilon_F), \tag{8}$$

where, it is now clear that, regardless of the Fermi level, the temperature correction is always negative. This means that the kinetic energy ($\langle K\rangle$) always increases as the temperature increases, a statement which is physically obvious.

With the spectral weight

$$W \equiv \frac{2}{N}\sum_k \frac{\partial^2\epsilon_k}{\partial k_x^2} f(\epsilon_k-\mu), \tag{9}$$

there is no simple cancellation, as occurs in the kinetic energy. If one defines the quantity

$$g_{xx}(\epsilon) \equiv \frac{1}{N}\sum_k \frac{\partial^2\epsilon_k}{\partial k_x^2}\delta(\epsilon-\epsilon_k), \tag{10}$$

then the Sommerfeld expansion can be applied to $W(T)$ as was done for the kinetic energy. The result is

$$W(T) = W(0) + \frac{\pi^2}{3}\frac{(k_B T)^2}{8t}\phi(\epsilon_F), \tag{11}$$

where

$$\phi(\epsilon_F) = 8t\left\{\frac{g_{xx}'(\epsilon_F)g(\epsilon_F) - g'(\epsilon_F)g_{xx}(\epsilon_F)}{g(\epsilon_F)}\right\}. \tag{12}$$

Using $g_{xx}(\epsilon_F)=-\epsilon_F g(\epsilon_F)$, which is correct for nearest-neighbor hopping only, one finds $\phi(\epsilon_F)=-8tg(\epsilon_F)$ and one recovers the previous result, given by Eq. (8) for the optical spectral weight as well as for the kinetic energy. Otherwise, the sign of the correction is dependent on the quantity within the braces. This quantity involves a difference between two terms, both of which contain singularities. This quantity is plotted in Fig. 5 for the t-t' model for various values of t', along with the corresponding one for the kinetic energy, which, by Eq. (8), is $-8tg(\epsilon_F)$. It is evident that as t' increases, a larger anomaly over a wider range of electron densities is expected. For more complicated band structures, an assortment of Fermi energies (i.e., electron concentrations) will exist for which the slope (and the change in the superconducting state) is "anomalous"—i.e., positive.

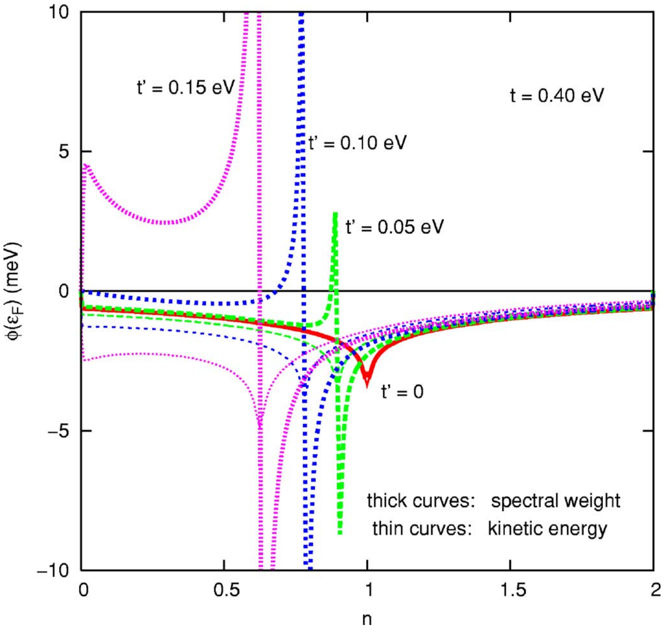

FIG. 5. (Color online) The finite-temperature correction to the optical spectral weight (thick curves), for various values of t', as indicated. Also plotted is the analogous quantity for the kinetic energy [which, by Eq. (8), is just $-8tg(\epsilon_F)$]. Note that the latter is always negative, while the spectral weight becomes positive for a finite electron concentration for electron (hole) densities below (above) the van Hove singularity. The magnitude of the anomalous region increases with increasing t'.

In Fig. 6 we show some specific examples of the temperature dependence of the optical spectral weight for a variety of electron concentrations. These results clearly show the progression from the "standard" result shown for $n=1.5$ (top frame) to the highly anomalous result shown for $n=0.6$ (third frame). Note the variation of the vertical scale: there is the obvious progression of lower spectral weight with decreasing electron density. However, the magnitude of both the slope and the change due to superconductivity also experiences a large increase for the two electron densities near the van Hove singularity ($n=0.75$ and $n=0.6$). For example, the absolute value of the slope in the second frame ($n=0.75$) is approximately a factor of 5 higher than that in the first frame ($n=1.5$). Similarly at $n=0.6$ the slope is much higher than at $n=0.3$, particularly at low temperatures. The reason is evident from Fig. 5: this enhancement occurs in the vicinity of the van Hove singularity. Note that the results of Fig. 6 are displayed for $t'=0.15$ eV. In this case, Fig. 5 shows that there is an extended range of electron densities for which a positive slope (and positive change below T_c) occurs. Using $t'=0.10$ eV, for example, would result in a very narrow range of electron densities for which the optical spectral weight has behavior opposite to that of the negative of the kinetic energy (see Fig. 5, blue dashed curves).

In summary, in the case of the simple next-nearest-neighbor model considered, the anomalous region always oc-

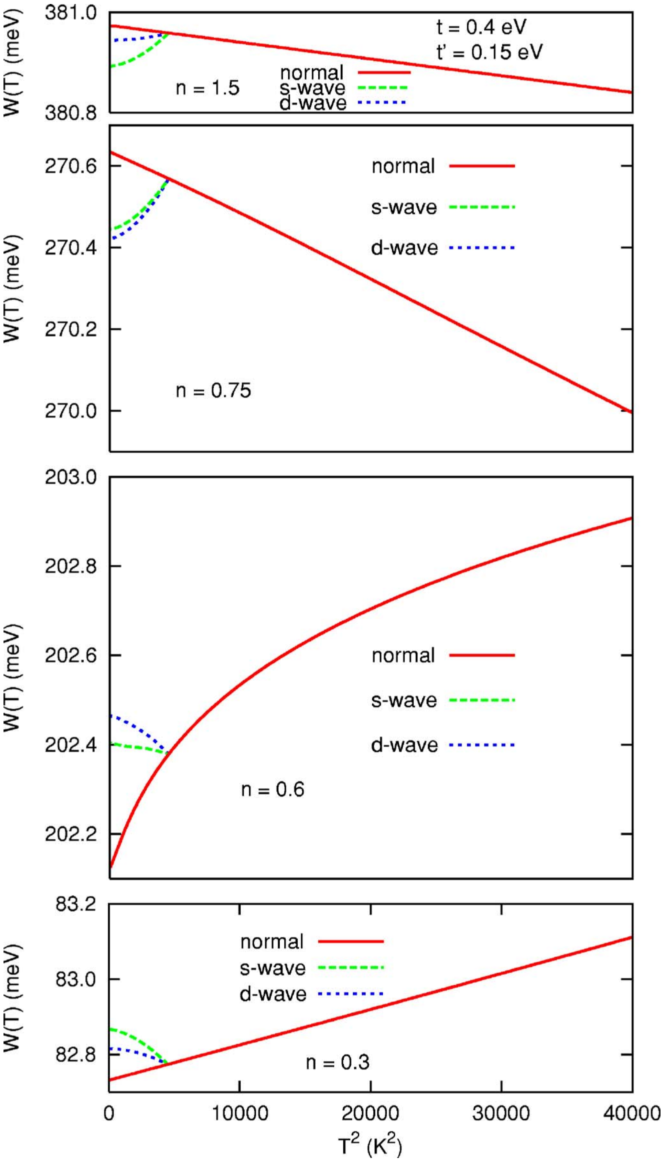

FIG. 6. (Color online) Spectral weight for four representative densities for the t-t' model (see Fig. 5). The progression from top to bottom is from high electron concentration to low electron concentration. Note the qualitative change from negative slope (lower-superconducting vs normal-state difference) to positive slope (higher-superconducting vs normal-state difference) as the electron concentration changes such that the chemical potential sweeps through the van Hove singularity.

curs at electron concentrations *below* the van Hove singularity. In many of the high-temperature superconducting cuprates, this electron concentration is not experimentally achieved. Certainly in the experiments that report a positive ("anomalous") optical spectral weight change in BSCCO, this regime is believed to be irrelevant. Hence, while this investigation of the behavior of the optical spectral weight using the t-t' model certainly plays havoc with our intuition (which motivated the experiments in the first place), it apparently does not provide an explanation of the experimental results.[28] This is further explored in the next section.

IV. BILAYER SPLITTING

It is evident that the characteristics of the optical spectral weight will be very dependent on the band structure and the doping level. A complete investigation of parameter space, with an accompanying catalog of optical spectral weight behavior, would undoubtedly reveal a wide assortment of results. Perhaps a more useful procedure at this point would be to adopt the band structure proposed for a particular compound (BSCCO), as prescribed by some other experiment (ARPES), and determine the behavior of the optical spectral weight in this case. As discussed in the previous section, we will adopt the parameters used in Ref. 24 to fit their ARPES results; these include a bilayer splitting term, which, as will now be discussed, can result in even more unusual doping dependence. Their determined structure was given in the previous section by Eq. (6) with parameters listed below this equation. We will adopt these parameters for all electron concentrations (i.e., hole doping) for simplicity.

Figure 7 shows the optical spectral weight as a function of temperature for the four doping levels considered in the experiments.[14,29] It is clear that with the band structure determined from ARPES,[24] the optical spectral weight cannot be explained by the simple BCS model adopted here.

However, very recently, very overdoped BSCCO samples have been produced;[30] ARPES measurements[30] have determined that the chemical potential moves through the first van Hove singularity. Thus, it is instructive to examine the consequences of this BCS model for higher hole doping concentrations (lower electron densities). In Fig. 8 the doping dependence of the optical spectral weight slope is shown as a function of electron concentration n for the hole-doped region (with respect to half-filling). This figure uses the band structure parameters from Kordyuk *et al.*,[24] so the crossing of the first van Hove singularity occurs at a higher hole doping (about $\delta \approx 0.28$) than reported in Ref. 30. Leaving this detail aside for the moment, it is clear from Fig. 8 that a dramatic change is expected in the optical spectral weight anomaly for this doping. In Fig. 9 we show the temperature dependence for some hole doping concentrations near this region, as indicated by the open squares in Fig. 8. Both the normal-state and superconducting-state behaviors show a transition as one crosses the van Hove singularity. It would be most interesting to measure the optical spectral weight in this doping regime. Such measurements would provide a good indication of whether or not the van Hove singularity is relevant in these materials.

Returning to the samples whose optical properties have already been measured, Figs. 7 and 8 make clear that, taking the ARPES-determined band structure seriously, then the observed doping dependence of the optical spectral weight change below T_c (Refs. 4, 13, and 14) *cannot* be explained by BCS theory. In this respect the observations may be indicative of physics beyond BCS theory. This remains true even if the hole doping is shifted by a small amount—that is, if the measured samples actually have hole concentrations that are larger than $0.09 < \delta < 0.21$; then, the spectral weight anomaly calculated here has almost the opposite doping dependence compared with experiment.[14]

On the other hand, the band structure is a parametrization and is reliant on a very surface sensitive probe. As an ex-

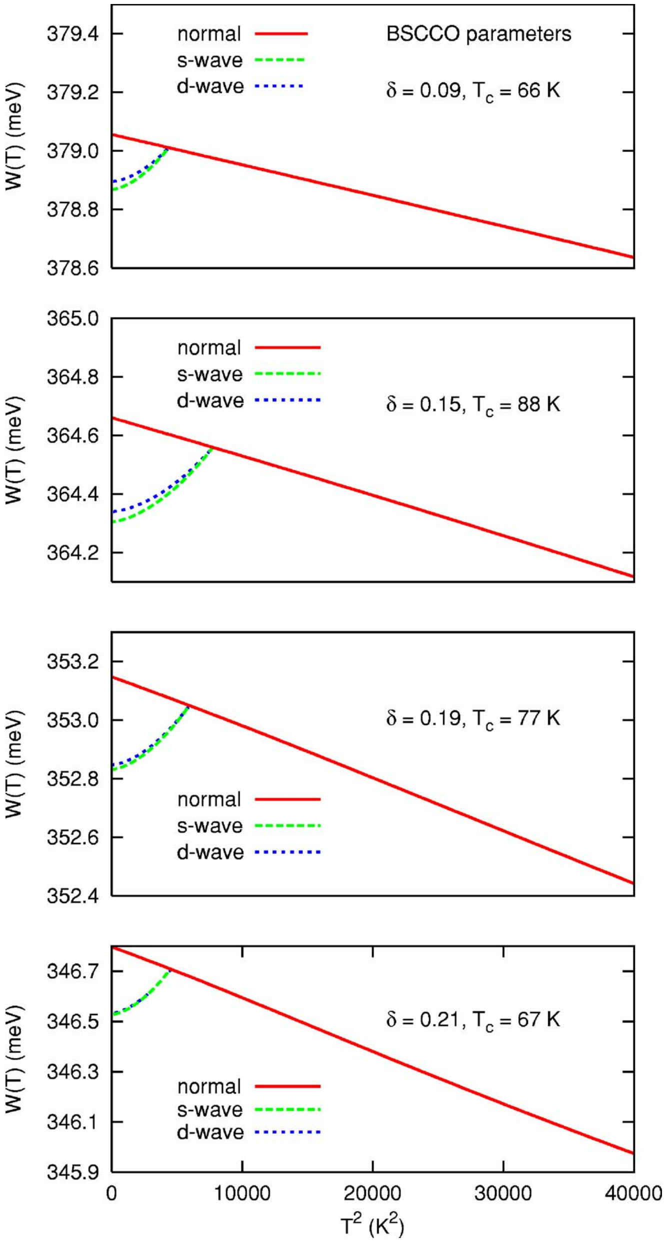

FIG. 7. (Color online) Spectral weight for the four hole doping concentrations (along with their measured T_c's) considered in the experiments (Ref. 14). These calculations use the ARPES-determined band structure parameters from Ref. 24, including the bilayer splitting. Slopes are always negative, and the change at T_c is also always negative. Note that in this case the *s*-wave order parameter gives roughly the same value as the *d*-wave parameter.

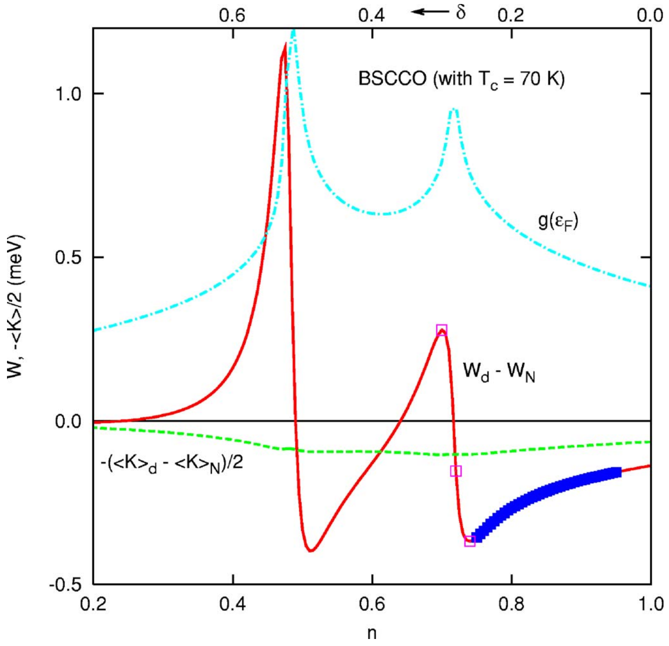

FIG. 8. (Color online) Spectral weight difference (solid red curve) as a function of electron concentration for the band structure determined by ARPES (Ref. 24). For simplicity we put T_c=70 K for all electron densities. The normal-state slope shows very similar behavior. Also plotted is the negative of the change in the kinetic energy (dashed green curve) and the density of states at the Fermi level (dot-dashed cyan curve), for reference. Note that "anomalies" in the spectral weight occur at the two van Hove singularities, while the change in kinetic energy is simply gently modulated by the density of states. Also shown with solid blue symbols is the hole doping regime of relevance to the BSCCO experiments in Ref. 14 and considered in the previous figure. For clarity only *d*-wave results are shown. The three open squares show the doping concentrations considered in the next figure, of possible relevance for overdoped samples with chemical potential that crosses the van Hove singularity (Ref. 30).

ample of what we consider a remote possibility, Fig. 8 indicates that if the doping levels for BSCCO are *not* as indicated, but rather lie in the regime *between* the two van Hove singularities (i.e., approximately between $n=0.5$ and $n=0.7$), then the results will be very different. Then "underdoped" would have a positive change below T_c (near $n\approx 0.7$) while "overdoped" would exhibit a negative change (compatible with experiment and with expectations based on the negative of the kinetic energy) (near $n\approx 0.6$). The corresponding slope above T_c would, however, be *inconsistent* with experiment (not shown), but the slope is a purely normal-state property and, like all other normal state properties, undoubtedly requires electron correlations for a proper understanding. We view this possibility as remote, however, since many studies have established this band structure and the low-doping scenario.

A more reasonable explanation comes from including effects considered in Ref. 7, along with the band structure of Kordyuk *et al.* The proposal there was to include the effect first observed in microwave measurements,[31,32] that the inelastic scattering rate decreases significantly below T_c. This has the effect of shifting the blue points in Fig. 8, for example, upwards. Thus, the anomaly below T_c would agree with experiment,[13,14] including a crossover from a positive change for underdoped samples to a negative change for overdoped samples. Furthermore, the slope above T_c would always be negative, as observed. Finally, the magnitude of the slope would increase as the anomaly becomes more BCS like, also in agreement with experiment. This was also found in C-DMFT calculations,[14] and further theoretical work and experiments would be required, however, to disentangle band

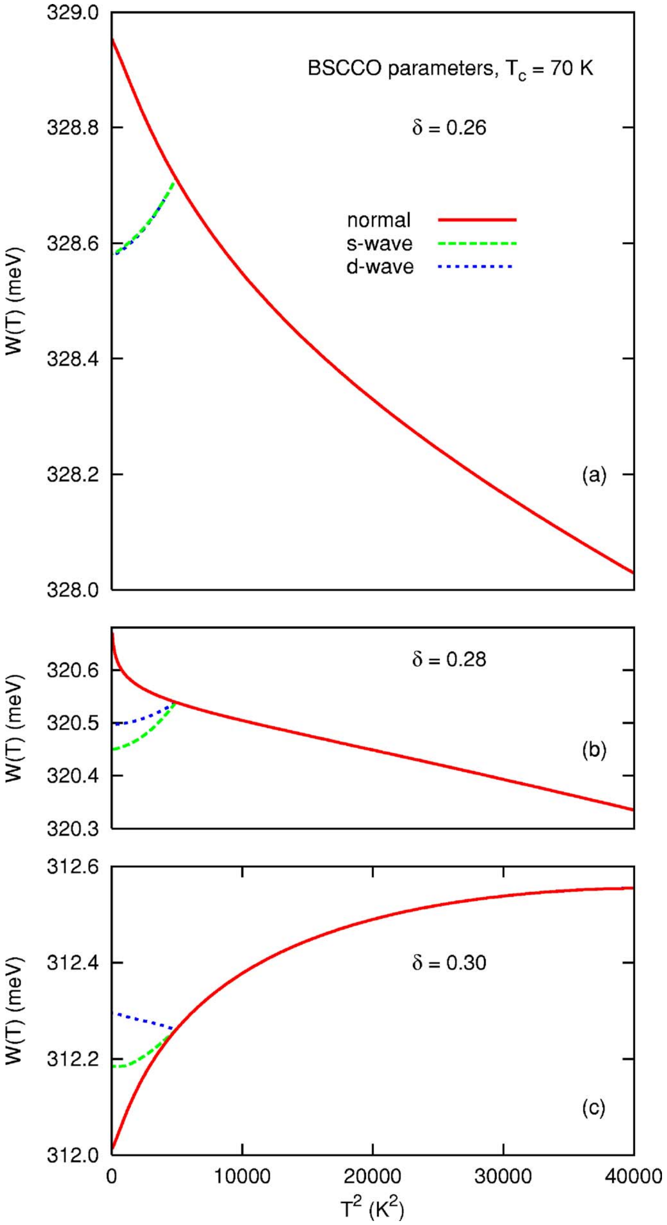

FIG. 9. (Color online) Spectral weight for three hole doping concentrations that move the chemical potential across the first van Hove singularity (see Fig. 8). Note the dramatic change that occurs as one dopes across the van Hove singularity (see text).

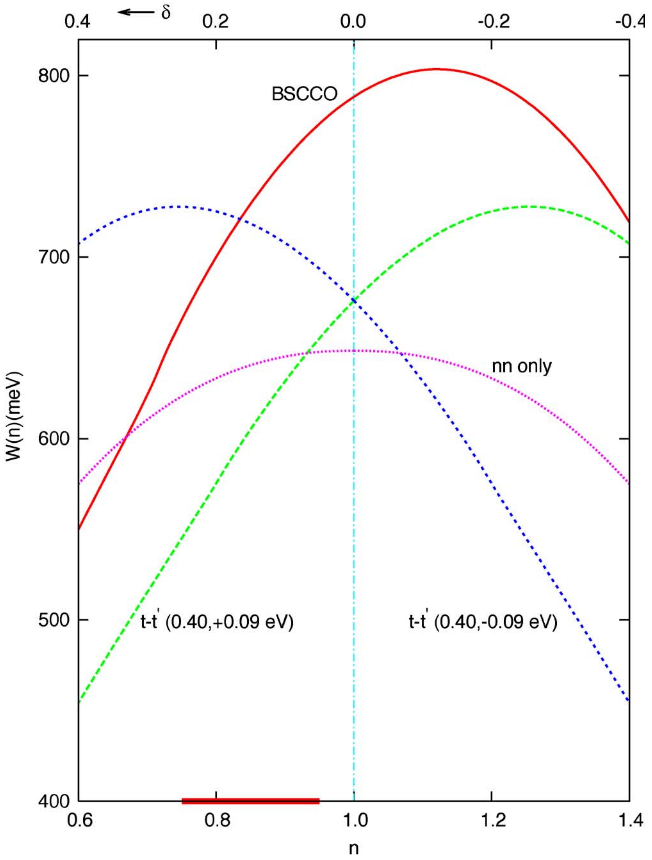

FIG. 10. (Color online) Spectral weight at zero temperature in the normal state vs electron concentration for four different band structures: that applicable to BSCCO (solid red curve), the *t*-t' model with t=0.40 eV and t'=0.09 eV (long-dashed green curve) and with t'=−0.09 eV (short-dashed blue curve), and the nearest-neighbor hopping only model, with t=0.40 eV. The three models that are physically relevant to the hole-doped cuprates (LSCO and BSCCO) have non-negative next nearest-neighbor hopping (t') and show a spectral weight that *decreases* with increasing hole doping δ over the relevant hole doping regime (see thick solid red line along the bottom axis). See text for further discussion.

structure effects from strong correlation effects. For example, the phenomenology of a collapsed scattering rate is generally indicative of an electronic scattering mechanism being responsible for superconductivity, so the C-DMFT calculations may be reconstructing the same phenomenology; it would be interesting to examine the interplay between strong correlation and band structure effects in these calculations. (To our knowledge calculations at this level have not been carried out with more detailed underlying band structures.) We should also remark that very early on Norman and Pépin[9] found that using a frequency-dependent scattering rate extracted from optical data gave rise to a crossover as a function of doping very similar to what has been observed in experiment. Further work is required to distinguish between these various scenarios.

Finally, one can ask about the doping dependence of the magnitude of the optical spectral weight. In Fig. 10 we show the doping dependence of the spectral weight for various band structures: that applicable to BSCCO (solid red curve), the *t*-t' model with t=0.40 eV and t'=0.09 eV (long-dashed green curve) and t'=−0.09 eV (short-dashed blue curve), and the nearest-neighbor hopping only model, with t =0.40 eV. The magnitudes are not important, but the trends with respect to hole doping (relevant region is indicated by the thick solid red line along the doping axis) are indicative of the "base" hole dependence—i.e., without any interactions included. Comparison with experiment indicates discrepancies; for BSCCO, experiment indicates a slight increase as δ increases (see Fig. 9 in Ref. 14), whereas our result shows a significant decrease. For LSCO, the $t-t'$ model with positive t' is applicable, so we again find a decrease with increasing δ (long-dashed green curve) while experiment finds an increase (see Fig. 2 in Ref. 16). Again, the success of DMFT and C-DMFT calculations at reproducing these trends (see Refs. 14 and 16) should be reassessed with improved underlying band structures in the calculations. If strong correlations and/or phase coherence scenarios are required for an understanding of the high-T_c oxides, then quantitative agreement with these experiments will undoubtedly require the correct band structure.

V. SUMMARY

The primary result of this paper is the revelation that the single-band optical spectral weight may behave very differently from the kinetic energy, both in the normal state and in the superconducting state. This occurs when one uses a band structure more complicated than one involving nearest-neighbour (NN) hopping only, since, with NN hopping only, the two are identical. Thus, one cannot use the phrase "BCS-like" behavior for the optical spectral weight, but one can continue to use that phrase for the kinetic energy.

This means that a wide variety of dependence on doping is in principle possible, due to band structure effects alone. This has a significant impact on the interpretation of experimental results, as doping dependence due to correlation effects, for instance, would have to be separated out either experimentally or theoretically.

On the other hand, if one accepts the band structure for, say, BSCCO, as determined by ARPES, then the spectral weight observations[1–4,13,14] remain anomalous—i.e., cannot be explained by BCS theory alone. We have advanced a couple of possibilities, and many others have been proposed in the literature: doping levels may be shifted slightly compared to what we think they are, in which case strong correlations well beyond BCS theory are required to explain the observed trend with doping.[14–20] A much stronger shift in doping actually reproduces the observed trends in the superconducting anomaly, but not in the normal-state behavior. Finally, including a scattering rate collapse below T_c also qualitatively accounts[7] for the data.

Note added. Recently, we became aware of the paper by Cásek *et al.*,[33] where band structure dependent effects on the optical sum rule are also discussed.

ACKNOWLEDGMENTS

F.M. greatly appreciates the hospitality of the Department of Condensed Matter Physics at the University of Geneva, where this research was performed. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), by ICORE (Alberta), by the Canadian Institute for Advanced Research (CIAR), and by the University of Geneva. This work was also supported by the Swiss National Science Foundation through the National Center of Competence in Research, Materials with Novel Electronic Properties (MaNEP).

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