Antiferromagnetically Induced Photoemission Band in the Cuprates

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Strong antiferromagnetic correlations in models of high critical temperature (high-T_c) cuprates produce quasiparticlelike features in photoemission (PES) calculations above the Fermi momentum $\mathbf{p}_F$ corresponding to weakly interacting electrons. This effect, discussed before by Kampf and Schrieffer [Phys. Rev. B **41**, 6399 (1990)], is analyzed here using computational techniques in strong coupling. It is concluded that weight above $\mathbf{p}_F$ should be observable in PES data for underdoped compounds, while in the overdoped regime it will be hidden in the experimental background. At optimal doping the signal is weak. The order of magnitude of our results is compatible with experimental data by Aebi *et al.* [Phys. Rev. Lett. **72**, 2757 (1994)] for $Bi_2Sr_2CaCu_2O_8$.

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The importance of antiferromagnetic (AF) correlations in the normal and superconducting states of the high-T_c cuprate materials is under much discussion. Studies of the strength of the AF correlation length ξ_{AF} in the normal state are crucial to test different theoretical scenarios. A key issue is how large ξ_{AF} should be to produce observable effects in experiments for the high-T_c compounds. NMR studies in the normal state of optimally doped $YBa_2Cu_3O_{6.94}$ (YBCO) suggest $\xi_{AF} \sim 2a$ [1]. Naively, this correlation seems too small to be of relevance. On the other hand, PES experimental results by Aebi *et al.* [2] on $Bi_2Sr_2CaCu_2O_8$ (Bi2212) seem to provide evidence for antiferromagnetically induced spectral weight above $\mathbf{p}_F$ ($\omega < 0$). Are these two results compatible?

To analyze Aebi *et al.*'s interpretation of their PES data, let us recall the intuitive physics involved. At half filling, the size of the Brillouin zone (BZ) is reduced by long-range AF order in the CuO_2 planes. This effect has implications for PES experiments, as discussed by Kampf and Schrieffer [3]. For example, along the diagonal $p_x = p_y = p$, and assuming long-range order, the quasiparticlelike peaks at momenta $\mathbf{p}_1 = (p, p)$ and $\mathbf{p}_2 = (\pi - p, \pi - p)$ should appear at the same energy, for any value of p. The coherent PES peaks observed *above* $\mathbf{p}_F$ are induced by strong correlations and do not exist for weakly interacting fermions [3].

How does this antiferromagnetically induced PES signal evolve as ξ_{AF} is reduced by hole doping? It is likely that its intensity will smoothly diminish when the system is doped away from half filling. Since in optimally doped Bi2212 ξ_{AF} in the CuO_2 planes should be similar to that of optimally doped YBCO (they should have the same in-plane hole density), a natural question arises: Can a small correlation length ($\sim 2a$) produce observable weight in PES experiments above $\mathbf{p}_F$ comparable to those reported by Aebi *et al.* [2]? On one hand, recent calculations [4] carried out in an AF background suggest that a short ξ_{AF} can have appreciable influence on some experimental quantities [like the flat bands near $\mathbf{p} = (\pi, 0)$ observed in Bi2212]. On the other hand, since the actual experimental PES signal for Bi2212 [Fig. 1(a)] is weak, concerns may arise about the interpretation of the data [as a reference, the PES weight above $\mathbf{p}_F$ induced by antiferromagnetism in experiments for the *insulating* layered copper oxide $Sr_2CuO_2Cl_2$ is

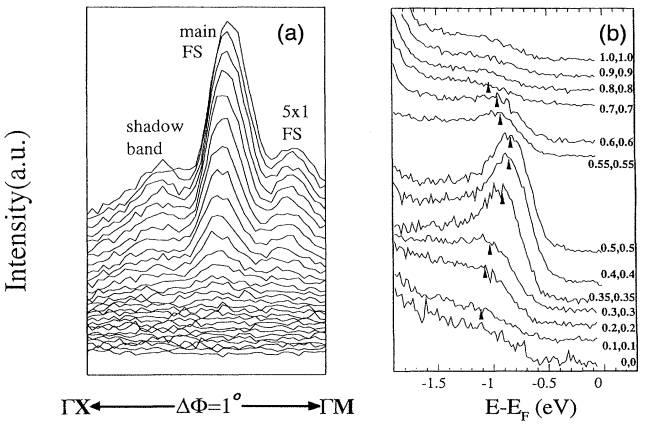

FIG. 1. (a) PES intensity in Bi2212, as reported by Osterwalder *et al.* (Ref. [2]). Their method produces PES intensity in a window of constant energy for all momenta, while conventional methods provide complete PES energy distribution curves at a few locations in the BZ. Each solid line corresponds to a fixed energy scan starting at the bottom at 0.3 eV above E_F, and arriving at the last top line at E_F. The spectra were measured at a polar angle of 39°, and for azimuthal angles spaced 1° apart beginning near the ΓM line and ending near the ΓX line. The "5 × 1" band is explained in the original text [2] in terms of structural modulations specific to Bi2212. The "shadow band" (Ref. [3]) is the feature under discussion. We thank P. Aebi and J. Osterwalder for providing us with these unpublished data. (b) PES intensity as a function of energy for $Sr_2CuO_2Cl_2$ taken from Wells *et al.* (Ref. [5]). The momenta are given in units of π and along the diagonal in the 2D square lattice convention.

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shown in Fig. 1(b)] [5]. Thus a theoretical *quantitative* calculation in strong coupling is needed to compare PES spectra and ξ_{AF} with experiments, and to decide whether Aebi *et al.*'s PES data are compatible with models of correlated electrons having PES weight above $\mathbf{p}_F$.

Here, this issue is explicitly addressed. PES spectra and spin correlations are calculated for electronic models expected to describe the CuO_2 planes. Consider first the standard two-dimensional (2D) one band Hubbard model simulated numerically using quantum Monte Carlo (QMC) techniques. To extract the dynamical spectral function $A(\mathbf{p},\omega)$ corresponding to the removal or addition of an electron with momentum $\mathbf{p}$, the maximum entropy (ME) technique was used [6]. We remark that using this low-resolution method we will not be able to distinguish between sharp quasiparticlelike peaks located at the top of the valence band, from the robust incoherent contribution to $A(\mathbf{p},\omega)$. Thus for the 2D Hubbard model only the strength of the spin correlations, and their influence on the integrated PES signal, will be addressed. This signal is calculated from the percentage of spectral weight below the chemical potential μ at momenta along the diagonal $p_x = p_y$ in the BZ with respect to the total intensity which for the Hubbard model satisfies $\int_{-\infty}^{+\infty} d\omega\, A(\mathbf{p},\omega) = 1$ at all dopings. The momentum dependence is crucial in our analysis.

The choice of coupling is important in our search for PES weight above $\mathbf{p}_F$. For example, working on an 8×8 cluster, at $U/t = 4$, half filling, and temperature $T = t/4$, the percentage of PES spectral weight at $\mathbf{p} = (3\pi/4, 3\pi/4)$, i.e., the next available momentum after $(\pi/2, \pi/2)$ on this cluster, is very small (less than 5% of the total), even though the spin correlations show clear indications of long-range order. Then, the actual value of the local moments is as important as the AF correlation length for the effect we are investigating. Since another feature induced by antiferromagnetism [7], namely, the "hole" pockets, is washed out by temperature effects in QMC simulations at $U/t = 4$, we consider this coupling to be too small for our purposes. Thus here the analysis was carried out at $U/t = 8$.

In Fig. 2, $A(\mathbf{p},\omega)$ at $T = t/2$ is shown [8]. We cannot reduce T due to sign problems, but nevertheless this temperature allows us to study the PES signal above $\mathbf{p}_F$ at different correlation lengths as the density is changed. At half filling, $\langle n\rangle = 1$, μ is located in the gap. The percentage of total PES spectral weight is shown for each momentum. A nonzero PES signal above the noninteracting Fermi momentum is clearly visible, and at $\mathbf{p} = (3\pi/4, 3\pi/4)$ it carries ~23% of the total weight. The result is similar if the temperature is reduced to $T = t/4$. Note that for a pure spin-1/2 antiferromagnet the weight at $\mathbf{p} = (\pi/4, \pi/4)$ and $\mathbf{p} = (3\pi/4, 3\pi/4)$ should be identical at this density, but for a Hubbard model at finite U/t spin-density-wave mean-field approximations

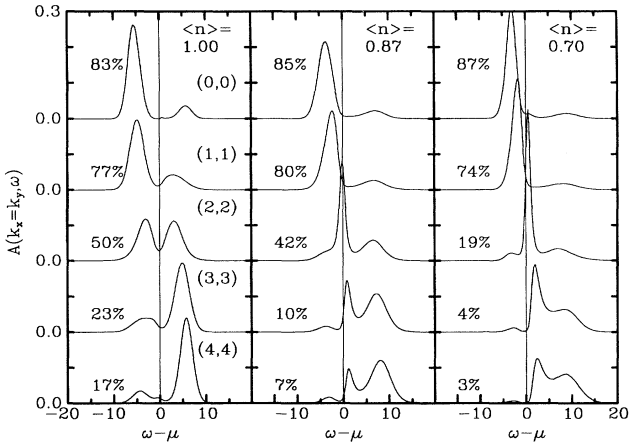

FIG. 2. $A(\mathbf{p},\omega)$, evaluated using QMC and ME techniques, for the 2D Hubbard model at $U/t = 8$, $T = t/2$ on an 8×8 cluster, at several densities $\langle n\rangle$. The momentum label varies along the diagonal in the BZ in units of $\pi/4$, and the percentages correspond to the integrated PES part of the spectral weight with respect to the total intensity (=1). The energy is in units of t.

[9] show a reduction of the intensity of the PES signal above $\mathbf{p}_F$ with respect to the Heisenberg limit [10]. Away from half filling, at $\langle n\rangle = 0.87$, the amount of weight at $\mathbf{p} = (3\pi/4, 3\pi/4)$ is reduced to ~10%, which is still visible in the scale of the figure. The height of the peak, as a percentage of the peak height at $\mathbf{p} = (\pi/2, \pi/2)$ and half filling, is about 15%.

At this point, it can be argued naively that the effect reported in Fig. 2 may only be evidence for the presence of the lower Hubbard band instead of antiferromagnetism. Actually, if the summation over momenta is carried out in Fig. 2 to construct the density of states away from half filling, it can be shown that aside from an expected redistribution of weight as the density changes, the two large bands in the spectrum are not much affected by doping. Thus, even at very low electronic densities where antiferromagnetism has clearly vanished, there is spectral weight below μ forming the lower Hubbard band. However, for $\langle n\rangle \sim 1$, i.e., with antiferromagnetism in the ground state, the weight below μ tends to be distributed evenly below and above $\mathbf{p}_F$, while for the case of $\langle n\rangle \sim 0.70$ when antiferromagnetism has virtually vanished the situation is much different with most of the PES weight located below $\mathbf{p}_F$. *Thus the momentum dependence of $A(\mathbf{p},\omega)$ is the key point to distinguish between an effect induced by AF correlations and an effect merely caused by the lower Hubbard band.*

To relate these results with experiments in Fig. 3(a) we show the numerically calculated spin correlations. At $\langle n\rangle = 1$, the correlation is robust (although it decays slowly to zero due to temperature effects), while at $\langle n\rangle = 0.70$, it is clearly very small. At an intermediate

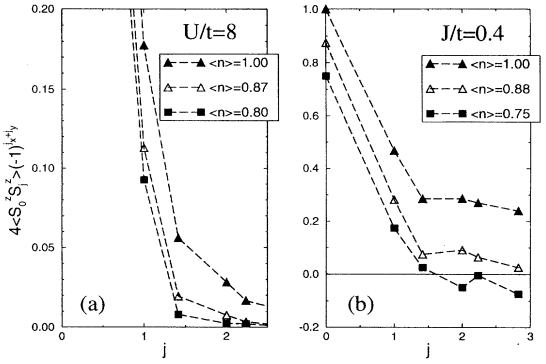

FIG. 3. (a) Spin-spin correlation $4\langle S^z_{\mathbf{0}} S^z_{\mathbf{j}}\rangle(-1)^{j_x+j_y}$ vs distance $j=|\mathbf{j}|$, where $\mathbf{j}=(j_x,j_y)$, for the 2D Hubbard model calculated using QMC at $T=t/2$, $U/t=8$, and several densities on an 8×8 cluster. (b) Spin-spin correlations as defined in (a), for the 2D t-J model calculated using ED techniques on a 4×4 cluster at several densities.

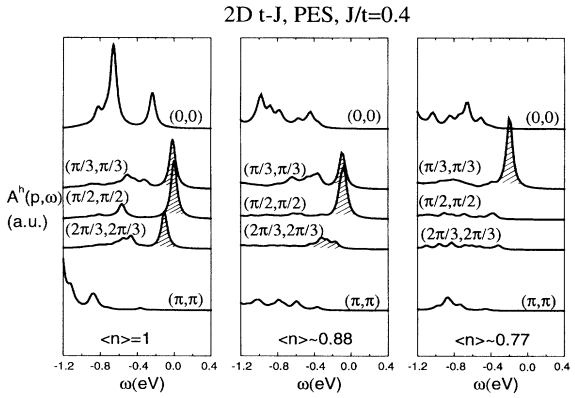

FIG. 4. PES $A(\mathbf{p},\omega)$ [denoted as $A^h(\mathbf{p},\omega)$] evaluated using ED techniques for the 2D t-J model, at $J/t=0.4$ on 4×4 and $\sqrt{18}\times\sqrt{18}$ clusters. The densities are shown in the figure. We assumed t = 0.4 eV, and provided a width $\delta=0.1t$ to the δ functions. The momenta are indicated, and the relevant peaks are shaded.

density $\langle n\rangle=0.87$, ξ_{AF} is between one and two lattice spacings, resembling the experimental situation in YBCO, and presumably also in Bi2212, since both are at optimal doping [11]. Comparing Figs. 2 and 3, it is clear that the QMC PES signal *above* $\mathbf{p}_F$ is *correlated* with the presence of antiferromagnetism in the spin correlations. Again, the momentum dependence of the spectral weight is crucial for our interpretation of the data. For this particular calculation we conclude that a doping of 25% holes makes the weight induced by antiferromagnetism almost negligible, while at 12% doping the effect is still observable [12]. Note that it is *not* necessary to have a large spin correlation length for the observation of weight above $\mathbf{p}_F$. $\xi_{\mathrm{AF}}\sim 2a$ seems to be enough.

Thus far our QMC analysis of the Hubbard model does not allow us to separate the actual sharp quasiparticlelike peak at the top of the valence band (which forms the band discussed in Refs. [2,3]) from the rest of the incoherent contribution at larger binding energies. To clarify this situation we need to study strongly correlated electrons with a technique that provides more accurate dynamical information than ME. For this purpose, we consider exact diagonalization (ED) techniques applied to the well-known 2D t-J Hamiltonian [13]. We expect the restriction to small clusters is not a problem in calculations where ξ_{AF} is small. To increase the momentum resolution along the diagonal in the BZ, we combined the results for the 16 and 18 site clusters.

In Fig. 4, the PES $A(\mathbf{p},\omega)$ spectrum is shown for the t-J model. $J/t=0.4$ was selected to model the cuprates, [13], but we checked that the results are similar in the range between $J/t=0.2$ and 0.8. As expected, at half filling the largest peak near the chemical potential (quasiparticle) is obtained at $\mathbf{p}=(\pi/2,\pi/2)$. Increasing the diagonal momentum away from it, a considerable amount of spectral weight induced by ξ_{AF} exists as was observed in early studies of the t-J model [14]. Moving away from half filling into the subspace of two holes (close to $\langle n\rangle\sim 0.88$) the dominant peak remains at $\mathbf{p}=(\pi/2,\pi/2)$ within our momentum resolution. At $(\pi/3,\pi/3)$ the quasiparticle strength is still large and coherent. At $\mathbf{p}=(2\pi/3,2\pi/3)$ the peak seems now broader in the scale used, although its integrated spectral weight remains close to that of $\mathbf{p}=(\pi/3,\pi/3)$. The height of the peak at $\mathbf{p}=(2\pi/3,2\pi/3)$ as a percentage of the largest peak located at $\mathbf{p}=(\pi/2,\pi/2)$ is (15-20)%, i.e., within the "observable" region [12]. Finally, at density $\langle n\rangle=0.77$, the result resembles that of a weakly interacting system with a Fermi momentum close to $\mathbf{p}=(\pi/3,\pi/3)$, above which the signal is too weak to be observable in PES experiments. Then, we believe that weight above $\mathbf{p}_F$ can be observed at $\langle n\rangle\sim 0.88$ but no longer at density $\langle n\rangle\sim 0.77$. To make contact with experiments consider again the spin correlations [Fig. 3(b)]. At half filling, ξ_{AF} is clearly larger than the lattice size. At $\langle n\rangle\sim 0.88$, a crude exponential fit of the spin correlation vs distance gives $\xi_{\mathrm{AF}}\sim 1.5a$ (similar to that of YBCO and Bi2212 at optimal doping), while at $\langle n\rangle\sim 0.77$, ξ_{AF} is less than one lattice spacing. Then, we conclude that for a real material with $\xi_{\mathrm{AF}}\sim 2a$ the antiferromagnetically generated PES weight, although weak, may still be observable above the background. In Fig. 5, $A(\mathbf{p},\omega)$ is shown at $\langle n\rangle\sim 0.88$ using an enlarged energy scale. The dispersion of the sharp peak (I) discussed before in Fig. 4 has a bandwidth of order J, while at higher energies a considerable amount of spectral weight is found contributing to the bulk of the valence band (II). Peak (I) may be smoothly connected to the bands discussed by Kampf and Schrieffer in weak coupling [3].

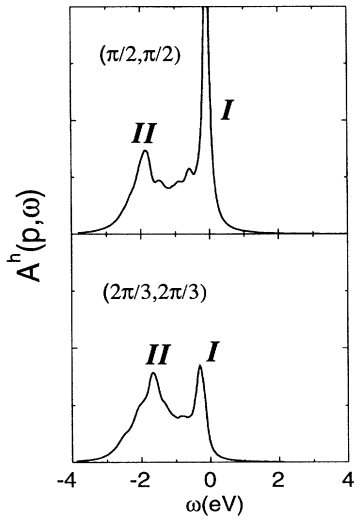

FIG. 5. $A^h(\mathbf{p},\omega)$ for the t-J model at $\langle n\rangle \sim 0.88$, $J/t = 0.4$, clusters of 16 and 18 sites, and expanding the energy scale used before in Fig. 4 to observe the two features structure. We use $\delta = 0.25t$ and $t = 0.4$ eV.

Summarizing, an analysis of the PES spectra in the 2D Hubbard and t-J models at several densities was reported. If these models reproduce the physics of the high-T_c compounds, then we conclude that antiferromagnetically induced photoemission weight should be observable even for materials with spin correlation lengths of only a couple of lattice spacings, as in Bi2212 at optimal doping. This is *compatible* with the experimental results of Fig. 1(a). However, we found that this regime is at the verge of observability and thus our results, based on rough models and order-of-magnitude estimations, cannot uniquely establish the validity of Aebi *et al.*'s interpretation of their experimental data. We have only shown that the strength of their signal and ours are similar, and thus there is compatibility between theory and experiments. We expect that the PES signal above $\mathbf{p}_F$ should no longer be visible above the large experimental background at dopings larger than optimal (~15%). To gather further evidence that the experimental signal is indeed caused by antiferromagnetism it is unavoidable to carry out PES experiments as a function of hole doping. We predict that the strength of the signal above $\mathbf{p}_F$ should increase as the system moves away from the optimal doping level towards half filling. Possible candidates for such a study are YBCO ($T_c = 60$ K) or $Bi_2Sr_2Ca_{1-x}Lu_xCu_2O_{8+\delta}$ and $Bi_2Sr_{2-x}La_xCaCu_2O_{8+\delta}$ which are underdoped [15].

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[1] T. Imai et al., Phys. Rev. B **47**, 9158 (1993).
[2] P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994); J. Osterwalder *et al.* (to be published).
[3] A. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990); **42**, 7967 (1990).
[4] E. Dagotto, A. Nazarenko, and M. Boninsegni, Phys. Rev. Lett. **73**, 728 (1994); E. Dagotto, A. Nazarenko, and A. Moreo, Phys. Rev. Lett. **74**, 310 (1995).
[5] B. O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995).
[6] R. N. Silver *et al.*, Phys. Rev. B **41**, 2380 (1990); S. R. White, *ibid.* **44**, 4670 (1991).
[7] D. Duffy and A. Moreo, Phys. Rev. B **51**, 11 882 (1995); R. Eder and Y. Ohta (to be published); S. Trugman, Phys. Rev. Lett. **65**, 500 (1990).
[8] For similar QMC ME results, see N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **50**, 7215 (1994).
[9] E. Dagotto, F. Ortolani, and D. Scalapino, Phys. Rev. B **46**, 3183 (1992); N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **73**, 748 (1994).
[10] Note also that naively the position of the peaks in states (1,1) and (3,3) of Fig. 2 at $\langle n\rangle = 1$ seem different in disagreement with our expectations. This is caused by the low accuracy of the ME method.
[11] Here, we *assume* that the PES spectral weight induced by antiferromagnetism is mainly a function of ξ_{AF} i.e., we compare numerical and experimental results at different temperatures, but having the same spin correlation.
[12] Let us define when a theoretically calculated PES signal can be predicted to be "observable" in an experiment [with the help of B. O. Wells (private communication)]. PES spectra have large backgrounds, superimposed on the actual relevant signal. This background depends on the momentum, and changes from sample to sample with fluctuations as large as 50%. Since the background is convex, the natural requirement for a PES theoretically calculated signal to be observable is that the combination background-signal produces a local maximum (i.e., a peak in the measured intensity). From the data shown in Fig. 1(b), and the intensity of the signal at the last point where the dispersion is observed, i.e., $\mathbf{p} = (0.7\pi, 0.7\pi)$, it is concluded that a peak with an intensity of roughly 10% of the largest signal [located at $\mathbf{p} = (0.5\pi, 0.5\pi)$] would be at the verge of being detected. This is the criterion followed in this paper to label a result as observable.
[13] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[14] E. Dagotto *et al.*, Phys. Rev. B **41**, 9049 (1990).
[15] Y. Koike *et al.*, Physica (Amsterdam) **159C**, 105 (1989).