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Quasiparticle dispersion of the t-J and Hubbard models

A. Moreo, S. Haas, A. W. Sandvik,* and E. Dagotto
Department of Physics and National High Magnetic Field Lab, Florida State University, Tallahassee, Florida 32306
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The spectral weight $A(\mathbf{p},\omega)$ of the two-dimensional t-J and Hubbard models has been calculated using exact diagonalization and quantum Monte Carlo techniques, at several densities $0.5 \leq \langle n \rangle \leq 1.0$. The photoemission ($\omega<0$) region contains two dominant distinct features, namely a low-energy quasiparticle peak with bandwidth of order J, and a broad valence band peak at energies of order t. This behavior *persists* away from half-filling, as long as the antiferromagnetic correlations are robust. The results give support to theories of the copper oxide materials based on the behavior of holes in antiferromagnets, and they also provide theoretical guidance for the interpretation of experimental photoemission data for the cuprates.

Angle-resolved photoemission spectroscopy (ARPES) techniques applied to the high-temperature superconductors have produced interesting data that introduce important constraints on theories for the copper oxide planes. Recently, it has been shown[1] that the hole-doped compounds $Bi_2Sr_2CaCu_2O_8$, $Bi_2Sr_2CuO_8$, $YBa_2Cu_3O_7$, and $YBa_2Cu_4O_8$ exhibit universal properties likely induced by the behavior of carriers in their common CuO_2 planes. In particular, it has been reported that the quasiparticle dispersion has a small bandwidth governed by an energy scale of the order of the exchange J of the Heisenberg model (~ 0.125 eV). In addition, in the vicinity of momenta $Y=(0,\pi)$ and $X=(\pi,0)$, the dispersion is anomalously flat. These results give support to theoretical ideas based on strongly correlated electrons, since (i) it is well established[2] that at half-filling the spectral function of a hole in an antiferromagnet contains a sharp quasiparticle peak at the top of the valence band spectra with a bandwidth of order J and (ii) careful studies of the fine details of the hole dispersion in one-band models have revealed the presence of flat regions near the X and Y points in momentum space.[3–6] The existence of these two features is a direct consequence of the presence of strong correlations and antiferromagnetism in the cuprates.

It is reasonable to assume that the behavior of holes in systems with long-range antiferromagnetic order will not change qualitatively as the density of holes is increased away from half-filling, as long as the antiferromagnetic correlation length ξ_{AF} remains large. Theories based on this assumption have been proposed.[7,8] In particular, in Refs. 3 and 8 it was shown that it is possible to reproduce many of the anomalous properties of the cuprates, including the presence of a d-wave superconducting state and the existence of an optimal doping, with the economical assumption that the sharp quasiparticle peak observed at half-filling at the top of the valence band remains robust as the electronic density decreases to phenomenologically realistic values. This assumption (i.e., approximate rigidity of the quasiparticle dispersion with doping) received support from recent calculations addressing the presence of "shadow bands" in the cuprates.[9] The rigid band hypothesis has also been studied by other authors.[10] On the experimental side, recent ARPES results by Aebi *et al.*[11] have shown that features induced by the AF correlations at half-filling are also present at optimal doping. Since the closest structure to the Fermi level in $A(\mathbf{p},\omega)$ is likely to dominate the low-temperature properties of the model, then it is important to establish theoretically whether the quasiparticle peaks observed at half-filling survive in the presence of a finite density of holes.

The purpose of this paper is to report results of an extensive analysis of the spectral weight for both the two-dimensional (2D) t-J and Hubbard models using exact diagonalization (ED) and quantum Monte Carlo (QMC) methods, supplemented by maximum entropy (ME) techniques, and carried out at several densities. $A(\mathbf{p},\omega)$ is shown to contain a two-peak structure, with dispersing features near the top of the valence band dominated by the scale of antiferromagnetism J, while a secondary broad structure appears at energies of order t. We discuss the range in parameter space where this behavior is to be expected, and its influence on the physics of carriers in the cuprates. However, note that recent QMC results have reported the presence of only *one* PES peak for the Hubbard model at both half-filling[12] and finite hole density.[5] We found that the disagreement with our present results is avoided once the influence of finite-temperature effects is considered and QMC data of higher accuracy are used for the ME method.

The technical details of the present computational study, as well as the Hamiltonians of the Hubbard and t-J models, are the standard ones, unless otherwise stated. In Fig. 1(a), $A(\mathbf{p},\omega)$ is shown for the t-J model at half-filling and $J/t=0.4$ using the ED technique applied to 2D clusters with 16 and 18 sites. The combination of these clusters allows enough resolution in momentum space to quantitatively analyze the dispersion of the main features in the spectral weight. The present results have been obtained using approximately 100 iterations in the standard continued fraction expansion (CFE) method to obtain dynamical properties using the Lanczos technique.[2] However, the figure shows that only a small number of poles are dominant. It is clear that near the Fermi energy ($\omega=0$) there is a robust peak that weakly disperses in the scale of the figure. Remnants of this low-energy peak exist at momenta (0,0) and (π,π), in the latter barely visible to the eye (but its intensity and position can be easily studied with the CFE approach mentioned above). In Fig. 1(b), the position of the low-energy peak is shown with full dots, with the convention that the area of the

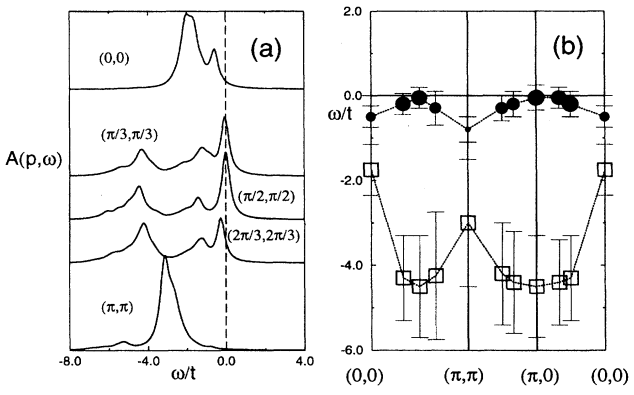

FIG. 1. (a) Spectral weight $A(\mathbf{p},\omega)$ of the 2D t-J model at $J/t=0.4$ using clusters of 16 and 18 sites along the diagonal in momentum space. The δ functions have been given a width $\epsilon=0.25t$ in the plots. (b) Position of the two dominant peaks in $A(\mathbf{p},\omega)$ as a function of momentum. The area of the circles is proportional to the intensity of the quasiparticle peak they represent. The error bars denote the width of the peak as observed in (a) (sometimes to a given broad peak several poles contribute appreciably). The full squares at $\omega\sim-4t$ represent the center of the broad valence-band weight, and the area of the squares is not proportional to their intensity.

dot is proportional to the intensity of the peak. The bandwidth of this sharp quasiparticlelike peak is $\sim 0.8t=2J$, in excellent agreement with our expectations based on previous calculations.[2–4] The flat region near $(\pi,0)$ is also visible in the figure. From Fig. 1(a) it is clear that additional PES spectral weight in $A(\mathbf{p},\omega)$ is located at higher energies $|\omega|$. As discussed before in the literature, the strong correlation effects force the hole quasiparticle to carry only a fraction of the integrated weight,[13] and thus the presence of considerable incoherent intensity deep in energy is reasonable. A rough estimation of their position is shown in Fig. 1(b) (open squares).[14] This feature is not relevant for the low-temperature behavior of the model which is dominated by the quasiparticle peak at the top of the valence band.

Before describing the density dependence of our results, let us clarify the importance of finite-size effects in Figs. 1(a) and 1(b), as well as the differences between our results and those of previous QMC simulations.[5,12] To address both issues simultaneously, we have carried out an extensive QMC simulation of the 2D Hubbard model. The results reported here correspond to $U/t=10$ (i.e., the strong-coupling regime where the model should behave similarly to the t-J model), temperature $T=t/4$, and using $\sim 10^5$ sweeps over the entire lattice to reduce the statistical errors. Here we use the "classic" ME technique.[15] The analytically continued $A(\mathbf{p},\omega)$ obtained at half-filling on an 8×8 cluster is shown in Fig. 2 at several momenta. The results are both qualitatively and quantitatively similar to those obtained for the t-J model in Figs. 1(a) and 1(b), and also in good agreement with ED studies for the Hubbard model.[16] Two peaks in the PES region are clearly identified for all momenta. From their position it can be shown that the bandwidth of the peak at the top of the valence band is of order J, in excellent agreement with our previous discussion. The second broader feature observed in the ED study of the t-J model is also present in the QMC simulation results. Studies at larger U/t couplings in the Hubbard model and in the region $0.2\leq J/t\leq 0.8$ of the t-J model show basically the same features. Then, here it is concluded that the qualitative physics of both models is very similar in the strong-coupling region, where an $A(\mathbf{p},\omega<0)$ with a double-peak structure is observed, as properly assumed in previous analytical studies.[7,3,17]

Let us now discuss our results away from half-filling. In the relevant regime of density for the high-T_c superconductors, namely in the vicinity of "optimal doping" $\langle n\rangle\approx 0.85$, the QMC+ME method at large U/t produces stable results only at temperature $T=t/2$ which is too high to resolve the two-peak structure *even* at half-filling. Thus, in this density regime only the ED results are reliable. In Figs. 3(a) and 3(b), ED data at density $\langle n\rangle\approx 0.88$ are shown (two holes in the 16 and 18 sites clusters). In this case ξ_{AF} is approximately two lattice spacings.[9] The PES results along the diagonal in momentum space present structure very similar to that discussed at half-filling. The low-energy peak is well

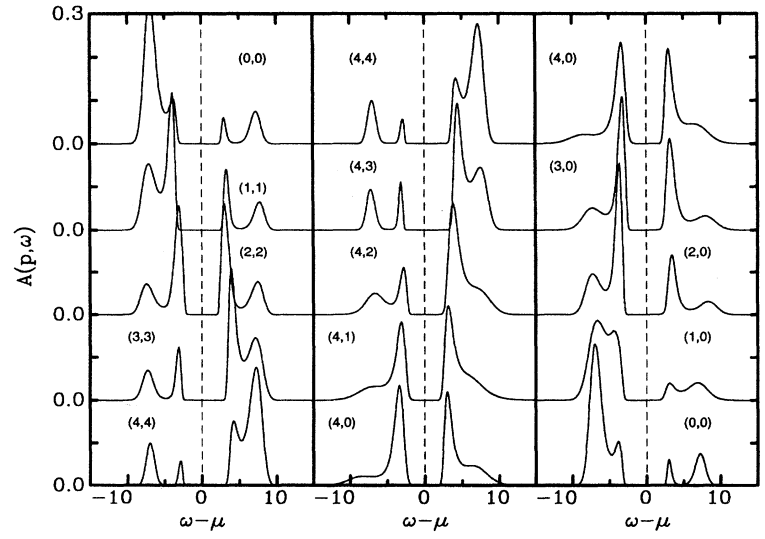

FIG. 2. Spectral weight $A(\mathbf{p},\omega)$ of the 2D Hubbard model obtained with the QMC method supplemented by maximum entropy, on an 8×8 cluster, $U/t=10$, and $T=t/4$.

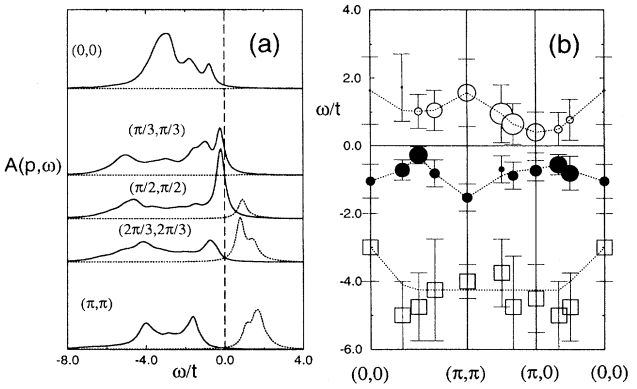

FIG. 3. Same as Fig. 1 but for density $\langle n\rangle \approx 0.88$ (i.e., two holes on the 16 and 18 sites clusters). In (a) the PES intensity is shown with a solid line, while the IPES intensity is given by a dotted line. The chemical potential is located at $\omega=0$. In (b) the full and open circles represent the PES and IPES intensities, respectively, of the peaks the closest to the Fermi energy. Their area is proportional to the intensity. The full squares have a meaning similar to Fig. 1(b).

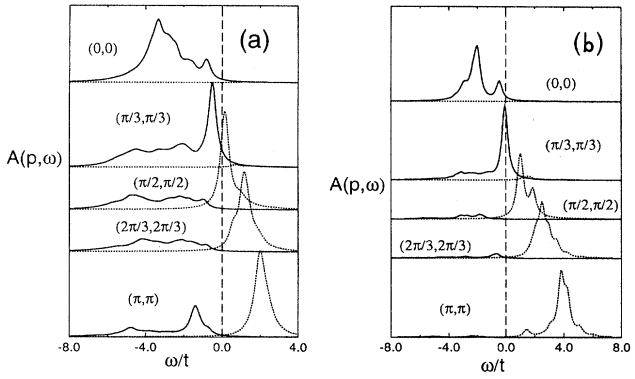

FIG. 4. (a) Same as Fig. 3(a) but for density $\langle n\rangle \approx 0.75$, i.e., 4 holes on the 16 and 18 sites clusters. (b) Same as Fig. 3(a) but for density $\langle n\rangle \approx 0.50$, i.e., 8 holes on the 16 and 18 sites clusters.

defined at all momenta, even those above the naive noninteracting Fermi momentum located near $(\pi/2,\pi/2)$, and still it disperses with a bandwidth of order J. The large accumulation of weight at higher energies $|\omega|$ remains localized at $\omega\sim 4t$. Then, to the extent that the one-band models reproduce the physics of the high-T_c cuprates, it is reasonable to expect that PES experiments carried out at half-filling and near the optimal doping should produce dispersive features of similar intensity and bandwidth. The clear similarity between the experimental bandwidth of the Bi2212 PES data, and recent results for the insulating $Sr_2CuO_2Cl_2$ compound,[18] provides more evidence for the validity of strongly correlated one-band models for the cuprates. However, it is important to remark that while the concrete prediction of our calculations is that the bandwidth of the hole carriers is of order J, the particular details of the dispersion may differ from compound to compound. For example, it has been recently remarked that to reproduce the data for $Sr_2CuO_2Cl_2$, the addition of a small t' term to the 2D t-J model is necessary.[19] Thus, care must be taken when the fine details of different compounds at different dopings are compared.

Now consider the inverse photoemission spectroscopy (IPES) ($\omega>0$) intensity in Figs. 3(a) and 3(b). The observed spectral weight in the vicinity of (π,π) somewhat resembles the distribution for a noninteracting Fermi system. In principle, this effect does not seem reproduced by a rigid band filling of the states at half-filling. However, recently Eder and Ohta[20] have shown that if proper quasiparticle operators[13] are used in the calculation of the spectral weight (i.e., operators dressed by spin fluctuations, instead of bare electronic operators), then the intensity of the IPES region is much reduced and the quality of the rigid-band description of the t-J model appears more clearly. This is an important point not much emphasized in the literature, namely that the robustness of the rigid-band picture in a given model cannot be tested by analyzing the removal of "bare" electrons (sudden approximation) as produced by a PES experiment, but instead "dressed" carriers must be used. Thus, PES and transport experiments may differ in their predictions if holes are heavily renormalized as in the cuprates.

Figures 4(a) and 4(b) show ED results for $A(\mathbf{p},\omega)$ using the same clusters and coupling as at half-filling, but now reducing further the density to $\langle n\rangle \approx 0.75$ and 0.50 (i.e., 4 and 8 holes in the 16 and 18 sites clusters). In this case, through the spin correlations we observed that ξ_{AF} is less than one lattice spacing and thus the influence of AF fluctuations should be small at these densities. Indeed the two-peak structure discussed before at higher densities is now difficult to identify. While the broad valence-band feature at $\omega\sim 4t$ remains, only remnants of the AF-induced intensity above the naive Fermi momentum can be observed. The IPES signal increased its intensity and now $A(\mathbf{p},\omega)$ resembles the behavior of a noninteracting "$\cos p_x+\cos p_y$" band, especially at $\langle n\rangle=0.5$.

An interesting detail of Figs. 1(a), 3(a), 4(a), and 4(b) is that the intensity of PES weight at $\mathbf{p}=(\pi,\pi)$ changes appreciably as the density is varied. This is to be expected since $\mathbf{p}=(\pi,\pi)$ is the momentum the most sensitive to the presence of AF correlations. In particular, when $\xi_{AF}\to 0$, we expect that the PES weight at $\mathbf{p}=(\pi,\pi)$ will be mostly transferred to the IPES regime. The presence of PES weight at (π,π) and $\langle n\rangle=1$ is a direct consequence of the AF correlations, while for a paramagnetic background $A[(\pi,\pi),\omega<0]$ should be negligible.[21]

Summarizing, in this paper the quasiparticle dispersion of the 2D t-J and Hubbard models was analyzed as a function of the electronic density. At half-filling, $A(\mathbf{p},\omega<0)$ has a sharp quasiparticlelike peak at the top of the valence band with a bandwidth of order J. This structure is the relevant one for the low-temperature behavior of the models. A second broad feature deeper in energy was also identified. As the electronic density decreases, the two-peak structure remains clearly visible as long as the antiferromagnetic correlation length ξ_{AF} is robust. When the AF fluctuations become negligible a crossover exists into a dispersion for the quasiparticles which resembles a weakly interacting system. For realistic values of the coupling, namely $U/t=10$, this cross-

over from an antiferromagnetic metal to a paramagnetic ground state occurs between $\langle n \rangle = 0.88$ and 0.75. Then, in the interesting regime for the copper oxide materials the AF correlations govern the behavior of the spectral weight. The present results give strong support to theories of the cuprates based on the behavior of carriers in an antiferromagnet[7,8] and provide information about the crossover from a half-filled to a doped system that can guide the analysis of ARPES data.

After completing this work we received a copy of unpublished work by Preuss, Hanke, and von der Linden[22] where conclusions similar to ours were reached. E.D., A.M., and A.S. were supported by the Office of Naval Research under Grant No. ONR N00014-93-0495. E.D. was also supported by the donors of the Petroleum Research Fund administered by the American Chemical Society. S.H. was supported by SCRI at FSU. We thank the NHMFL and MARTECH at FSU for its partial support.

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*On leave from Department of Physics, Åbo Akademi University, Finland.

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