Quasiparticle dispersion of the t-J and Hubbard models

A. Moreo, S. Haas, A. Sandvik, and E. Dagotto

Department of Physics and National High Magnetic Field Lab, Florida State University, Tallahassee, FL 32306, USA
(August 14, 2018)

The spectral weight $A(p,\omega)$ of the two dimensional $t-J$ and Hubbard models has been calculated using exact diagonalization and quantum Monte Carlo techniques, at several densities $1.0 \leq \langle n \rangle \leq 0.5$. 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 (AF) correlations are robust. The results give support to theories of the copper oxide materials based on the behavior of holes in antiferromagnets, and it also provides theoretical guidance for the interpretation of experimental photoemission data for the cuprates.

PACS numbers: 74.20.-z, 74.20.Mn, 74.25.Dw

Angle resolved photoemission (ARPES) techniques applied to the high temperature superconductors have produced interesting data that introduces important constraints on theories for the copper oxide planes. Recently, it has been shown [1] that the hole-doped compounds $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$, $\text{Bi}_2\text{Sr}_2\text{CuO}_8$, $\text{YBa}_2\text{Cu}_3\text{O}_7$, and $\text{YBa}_2\text{Cu}_4\text{O}_8$ exhibit universal properties likely induced by the behavior of carriers in their common $\text{Cu}_2\text{O}_2$ 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 ($\sim 0.15\text{eV}$). 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. [3,4] 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 $\xi_{AF}$ remains large. Theories based on this assumption have been proposed. [5,6] In particular, in Refs. [6,8] 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. [7] The rigid band hypothesis has also been studied by other authors. [8] On the experimental side, recent ARPES results by Aebi et al. [9] 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 $A(p,\omega)$ 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 $2D$ $t-J$ 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. $A(p,\omega)$ 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, [10] and finite hole density. [11] We found that the disagreement with our present results is avoided once the influence of finite temperature effects is considered, and a more sophisticated ME method is used.

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.1a, $A(p,\omega)$ 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 mo-
mentum 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. 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 \((\pi, \pi)\), 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.1b, the position of the low-energy peak is shown with full dots, with the convention that the area of the dot is proportional to the intensity of the peak. The bandwidth of this sharp quasiparticle-like peak is \(\sim 0.8t = 2J\), in excellent agreement with our previous discussion.

From their position it can be shown that the bandwidth of the hole carriers is of order \(J\), the particular details of the dispersion may differ from common features of similar intensity and bandwidth. The clear similarity between the experimental bandwidth of the Bi2212 PES data, and recent results for the \(\text{insulating} \) \(\text{Sr}_2\text{CuO}_2\text{Cl}_2\) compound, 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 \(\text{Sr}_2\text{CuO}_2\text{Cl}_2\), the addition of a small \(t'\)-term to the 2D \(t – J\) model is necessary. Thus, care must be taken when the fine details of different compounds at different dopings are compared.

Now consider the inverse photoemission (IPES) \((\omega > 0)\) intensity in Fig.3a,b. The observed spectral weight in the vicinity of \((\pi, \pi)\) somewhat resembles the distribution for a non-interacting 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 have shown that if proper \textit{quasiparticle} operators 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.

Fig.4a,b shows ED results for \(A(p, \omega)\) 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 \(\xi_{AF}\) 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 \(A(p, \omega)\) resembles the behavior of a non-interacting \(\cos px + \cos py\) band.

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

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, \(A(p, \omega < 0)\) has a sharp quasiparticle-like 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 \(\xi_{AF}\) is robust. When the AF fluctuations become negligible then 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 crossover 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, \[\text{[23]}\] and provides 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 preprint by Preuss, Hanke and von der Linden \[\text{[22]}\] where conclusions similar to ours were reached. E.D., A.M. and A.S. are supported by the Office of Naval Research under grant ONR N00014-93-0495. E. D. is also supported by the donors of the Petroleum Research Fund administered by the American Chemical Society. S. H. is supported by SCRI, at FSU. We thank the NHMFL and MARTECH at FSU for its partial support.
[1] D.S. Dessau et al., Phys. Rev. Lett. 71, 2781 (1993); A. A. Abrikosov, J. C. Campuzano, and K. Gofron, Physica C 214, 73 (1993); D. M. King et al., Phys. Rev. Lett. 73, 3298 (1994); K. Gofron et al., Phys. Rev. Lett. 73, 3302 (1994).

[2] For a comprehensive review, see E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

[3] E. Dagotto, A. Nazarenko and M. Boninsegni, Phys. Rev. Lett. 73, 728 (1994).

[4] Z. Liu and E. Manousakis, Phys. Rev. B 45, 2425 (1992).

[5] N. Bulut, D. J. Scalapino and S. R. White, Phys. Rev. B 50, 7215 (1994).

[6] R. Putz, R. Preuss, A. Muramatsu, and W. Hanke, preprint.

[7] A. Kampf and J. R. Schrieffer, Phys. Rev. B 41, 6399 (1990).

[8] E. Dagotto, A. Nazarenko and A. Moreo, Phys. Rev. Lett. 73, 00 (1994).

[9] S. Haas, A. Moreo and E. Dagotto, Oct. 1994, preprint.

[10] S. Trugman, Phys. Rev. Lett. 65, 500 (1990); R. Eder, Y. Ohta, and T. Shimozato, Phys. Rev. B 50, 3350 (1994).

[11] P. Aebi et al., Phys. Rev. Lett. 72, 2757 (1994).

[12] N. Bulut, D. J. Scalapino and S. R. White, Phys. Rev. Lett. 73, 748 (1994).

[13] E. Dagotto and J. R. Schrieffer, Phys. Rev. B 43, 8705 (1991).

[14] The third structure immediately after the quasiparticle peak has been extensively analyzed under the name of “string-states”. These features should be more sensitive to doping than the dominant quasiparticle state, and thus they are not discussed in detail here.

[15] M. Jarrell and J. E. Gubernatis, unpublished; R. N. Silver, D. S. Sivia, and J. E. Gubernatis, Phys. Rev. B 41, 2380 (1990).

[16] E. Dagotto, F. Ortolani and D. Scalapino, Phys. Rev. B 46, 3183 (1992).

[17] The simulations of Ref. [12] did not observe such structure mainly due to finite temperature effects and also the use of a different ME technique with less resolution.

[18] B.O. Wells, et al., Phys. Rev. Lett. xx, yy (1994).

[19] A. Nazarenko, K. Vos, S. Haas, E. Dagotto, and R. Gooding, preprint (1994).

[20] R. Eder and Y. Ohta, Phys. Rev. B 50, 10043 (1994), and references therein.

[21] This result is to be contrasted with \( \langle n \rangle \approx 0.75 \) i.e. 4 holes on the 16 and 18 sites clusters: (b) Same as Fig.3a but for density \( \langle n \rangle \approx 0.50 \) i.e. 8 holes on the 16 and 18 sites clusters.

Figure Captions

1. (a) Spectral weight \( A(p, \omega) \) 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 \( \delta \)-functions have been given a width \( \epsilon = 0.25t \) in the plots; (b) position of the two dominant peaks in \( A(p, \omega) \) 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 Fig.1a (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.

2. Spectral weight \( A(p, \omega) \) of the 2D Hubbard model obtained with the QMC method supplemented by Maximum-Entropy, on an \( 8 \times 8 \) cluster, \( U/t = 10 \), and \( T = t/4 \).

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.

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