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Quasiparticle dispersion in the cuprate superconductors and the two-dimensional Hubbard model

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The momentum dispersion of the peak structure of the single-particle spectral weight $A(\mathbf{p},\omega)$ of the two-dimensional Hubbard model is discussed. Using results obtained from Monte Carlo simulations on lattices up to 12×12 in size, we determine the low-lying quasiparticle dispersion relation. This dispersion relation is anomalously flat near the $(\pi,0)$ and $(0,\pi)$ points of the Brillouin zone, similar to the results of recent angular resolved photoemission measurements of the hole-doped cuprates. We argue that the generic nature of the quasiparticle dispersion relation observed in these materials arises from the strong Coulomb interaction and reflects the hole-spin correlations rather than the one-electron interactions which customarily determine the band structure.

Recent angular resolved photoemission experiments on $Bi_2Sr_2CaCu_2O_{10}$ (Bi 2212), $Bi_2Sr_2CuO_8$ (Bi 2201),[1] $YBa_2Cu_4O_8$ (YBCO 124),[2] and $YBa_2Cu_3O_7$ (YBCO 123) (Refs. 3 and 2) suggest a "generic" quasiparticle dispersion $E(\mathbf{p})$ for these hole-doped copper oxide materials.[4] These studies find that the Fermi surface is a rounded square centered around (π,π) with an extended region of flat bands near the Fermi energy located around the $X(Y)$ points $(\pi,0)$ $[(0,\pi)]$.[5] The saddle-point behavior near the $X(Y)$ points is much more extended than the usual van Hove band-structure form. While some of the general features of the initial angular resolved photoemission spectroscopy (ARPES) results appeared consistent with band-structure calculations, more recent measurements have shown that the band-structure results for $E(\mathbf{p})$ exhibit a much larger dispersion near the X and Y points.[1–4] In addition, the generic behavior is difficult to understand within a band-structure picture which involves different one-electron potentials for each of these materials. An alternative possibility, which we explore here, is that the generic features arise from the presence of a strong Coulomb interaction and reflect the structure of the many-body correlations rather than the one-electron interactions. Recent Monte Carlo calculations[6] of the single-particle density of states for the two-dimensional Hubbard model doped away from half-filling show that when the Coulomb interaction U is of order the bandwidth $8t$, a peak develops at the top of the lower Hubbard band near the Fermi level. This resonant peak is associated with low-lying quasiparticle excitations near the Fermi energy. Here we use Monte Carlo simulations to study how the peaks in the single-particle spectral weight for a two-dimensional Hubbard model disperse with $\mathbf{p}$. Focusing on the behavior of the peak near the Fermi surface, we find that it exhibits a remarkably flat dispersion near the $(\pi,0)$ $X(Y)$ points, while cutting through the $(\pi/2,\pi/2)$ point in a similar manner to the ARPES data. Thus we conclude that the striking similarity of the quasiparticle dispersion $E(\mathbf{p})$ of the hole-doped cuprates listed above can arise as a consequence of the strong Coulomb repulsion and the resulting hole-spin correlations in these materials. In addition, we discuss the nature of the Fermi surface. We find that the Fermi surface is centered around (π,π), if the Fermi level lies above the flat region in $E(\mathbf{p})$, but when the doping increases sufficiently to put the Fermi level below the flat region, the Fermi surface is closed around (0,0).

The two-dimensional Hubbard model that we study has a Hamiltonian given by

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+c^{\dagger}_{j\sigma}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where t is the near-neighbor hopping amplitude and U is the on-site Coulomb repulsion. The operator $c^{\dagger}_{i\sigma}$ creates an electron of spin σ on site i and $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. A chemical potential μ is used to set the filling $\langle n\rangle=\langle n_{i\uparrow}+n_{i\downarrow}\rangle$. Using quantum Monte Carlo techniques,[7,8] we have calculated the single-particle finite-temperature Green's function

$$G_{ij}(\tau)=-\langle T_{\tau}c_{j\sigma}(\tau)c^{\dagger}_{i\sigma}(0)\rangle, \tag{2}$$

where τ is the imaginary time variable. The corresponding spectral weight is defined as

$$A(\mathbf{p},\omega)=-\frac{1}{\pi}\,\mathrm{Im}\,G(\mathbf{p},\omega). \tag{3}$$

In order to obtain $A(\mathbf{p},\omega)$ from $G(\mathbf{p},\tau)$, an analytic continuation is necessary. The maximum entropy procedure[9,10] provides an effective way to perform the analytic continuation provided one has Monte Carlo data with good statistics. The results reported here typically consisted of averages over

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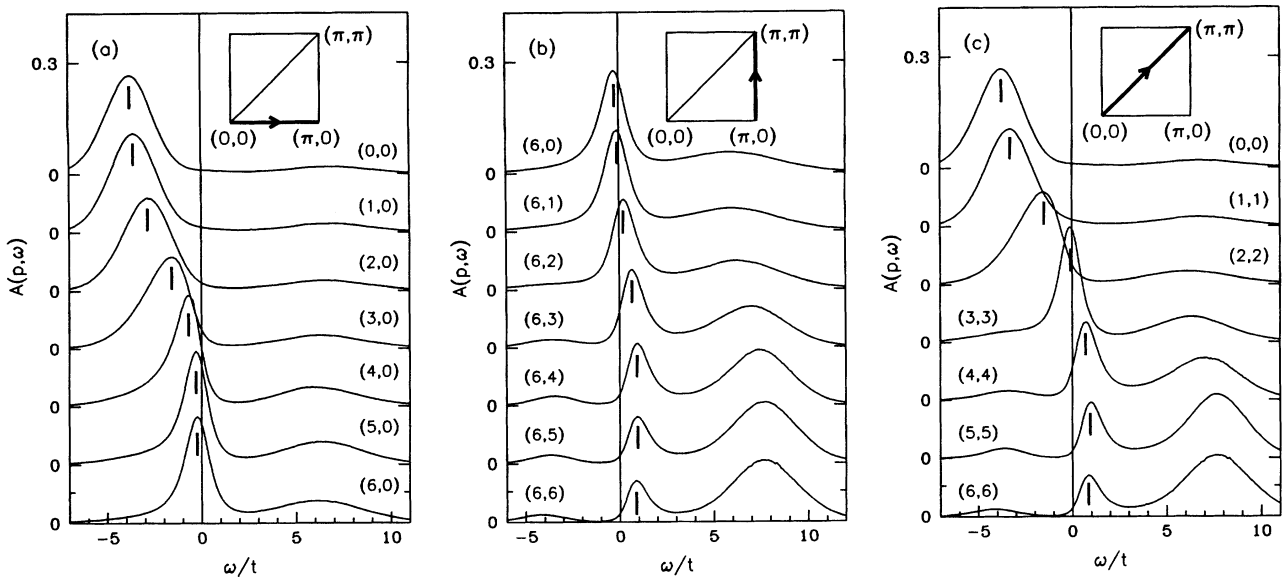

FIG. 1. Single-particle spectral weight $A(\mathbf{p},\omega)$ versus ω for various values of $\mathbf{p}$. These results are for $U=8t$ and $\langle n\rangle=0.87$ on a 12×12 lattice at a temperature $T=0.5t$. The inset in each panel shows the location of the momentum cuts through the Brillouin zone. Here the momentum $\mathbf{p}$ is given in units of $\pi/6$.

10^5 updates of all the Hubbard-Stratonovich variables and $G(\mathbf{p},\tau)$ had statistical error of less than 0.5%. The reliability of the analytic continuation has been tested in a number of ways, including comparisons with 4×4 exact diagonalization results.[11]

The results which we will discuss were obtained on lattices up to 12×12 in size with $U=8t$ for various fillings and temperatures. We begin by examining the single-particle spectral weight $A(\mathbf{p},\omega)$ for a filling of $\langle n\rangle=0.87$. In Figures 1(a)–1(c), we plot $A(\mathbf{p},\omega)$ versus ω for $\mathbf{p}$ moving along the momentum cuts shown in the Brillouin zone insets. Here we see that the peak in $A(\mathbf{p},\omega)$ disperses very slowly around $(\pi,0)$ relative to its behavior near $(\pi/2,\pi/2)$.

As previously noted,[6] the spectral weight of the doped system shows remnants of the upper and lower Hubbard bands present in the insulating state along with a quasiparticle peak which remains much closer to the Fermi level at the top of the lower Hubbard band. It is this peak that we are particularly interested in following. When $\mathbf{p}$ is on the Fermi surface, it should be centered at $\omega=0$. As $\mathbf{p}$ moves outside the Fermi surface, as shown for example in Fig. 1(b), we can clearly resolve both the quasiparticle peak near the Fermi energy and the upper Hubbard band peak. However, when $\mathbf{p}$ moves below the Fermi surface our resolution is such that we lose the quasiparticle peak, if it exists, in the lower Hubbard band. With this limitation in mind, we have plotted the peaks in $A(\mathbf{p},\omega)$ as $E(\mathbf{p})$ versus $\mathbf{p}$ (for various sized lattices to obtain different values of $\mathbf{p}$) in Fig. 2(a). The dotted curve in Fig. 2(a) represents the band-structure result for the Hubbard model $\varepsilon(\mathbf{p})=-2t(\cos p_x+\cos p_y)-\mu$.

We note the flat dispersion of the Monte Carlo results near $(\pi,0)$ and the small rise at (π,π) compared to the band-structure result. The existence of the flat dispersion can also be seen in the behavior of $A(\mathbf{p},\omega)$ for $\mathbf{p}$ near $(\pi,0)$, shown in Fig. 1. For this filling and temperature, the Fermi level lies slightly above the flat region in $E(\mathbf{p})$. By comparing results for $E(\mathbf{p})$ obtained at different temperatures, we find that $E(\mathbf{p})$ near $(\pi,0)$ gets flatter as T is lowered. This is also observed as U is increased from $8t$ to $12t$. In addition, the single-particle density of states for this system exhibits a sharp resonant peak near the Fermi energy. While this is reminiscent of a van Hove peak, it is stronger and much more robust. The usual band-structure peak is washed out by the lifetime broadening for the interacting problem. Here we have a structure characteristic of the strong spin correlations which form around the hole. These results for $N(\omega)$ are similar to those found by Jarrell for the infinite-dimensional Hubbard model, where the problem can be exactly mapped to a single-impurity Anderson model.[12]

As discussed, in the region below the Fermi surface the quasiparticle peak can be obscured, within our present resolution, by the lower Hubbard band. We believe that there is in fact a quasiparticle band near the Fermi surface, for which the energy scale is set by $J\sim4t^2/U$. This is what has been found for one-hole doped in an antiferromagnetic t-J model.[13] Furthermore, a narrow quasiparticle band was observed for finite dopings in the exact diagonalization calculations of the t-J (Ref. 14) and the one-band Hubbard[11] models, as well as in the Monte Carlo simulations of the three-band Hubbard model.[15] The peaks associated with the upper and lower Hubbard bands are also seen in Fig. 2(a). We believe that the low-lying quasiparticle peak nearest the Fermi energy represents a hole strongly correlated with the local spin background and that its dispersion is basically set by J rather than the one-electron band structure.

For $\langle n\rangle=0.87$, we see in Fig. 2(a) that the Fermi level lies slightly above the flat band at $(\pi,0)$. This would lead to a

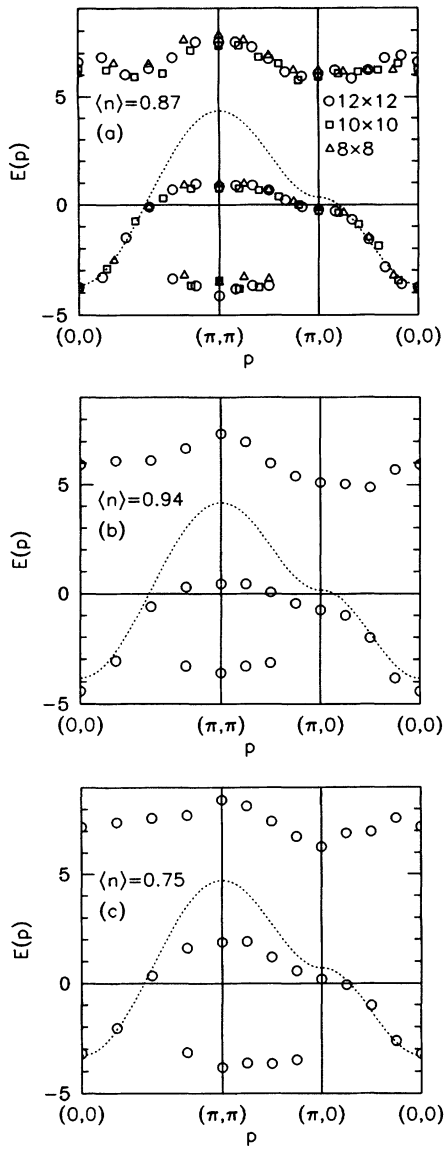

FIG. 2. Dispersion $E(\mathbf{p})$ of the peaks in the spectral weight versus $\mathbf{p}$ for fillings (a) $\langle n\rangle=0.87$, (b) $\langle n\rangle=0.94$, and (c) $\langle n\rangle=0.75$ obtained using $U=8t$ and $T=0.5t$. The dotted lines are the dispersion of the noninteracting system $\varepsilon(\mathbf{p})=-2t[\cos(p_x)+\cos(p_y)]-\mu$. The results for $\langle n\rangle=0.87$ are given for 8×8, 10×10, and 12×12 lattices, and the results for $\langle n\rangle=0.94$ and $\langle n\rangle=0.75$ are given for the 8×8 lattice.

Fermi surface that is closed around (π,π). When the doping is varied, the flat band region near $(\pi,0)$ moves with respect to the Fermi energy, lying below it for $\langle n\rangle=0.94$ and slightly above it for $\langle n\rangle=0.75$ as seen in Figs. 2(b) and 2(c). Thus for $\langle n\rangle=0.75$, when the Fermi level lies just below the flat band region of $E(\mathbf{p})$, the Fermi surface will be closed around (0,0). In agreement with these results, we find that the density of states, $N(0)$, is a maximum when the filling is such that the Fermi level lies at the flat portion of $E(\mathbf{p})$. At $T=0.5t$, this maximum in $N(0)$ occurs for $\langle n\rangle\sim0.84$. Thus, in the case where there is only a near-neighbor hopping, the change in the Fermi surface topology[16] occurs for a site filling $\langle n\rangle\sim0.84$.

In order to make more direct comparisons with the superconducting cuprates, we have included a next-nearest-neighbor hopping t' in the simulations. For $t'=-0.15t$, we find that a similar flat band exists near the $X(Y)$ point, and the change in the topology of the Fermi surface occurs at $\langle n\rangle\sim0.7$. If one assumes that the curvature of the Fermi surface determines the sign of the Hall coefficient, R_H, then these results would be in agreement with the observed doping dependence of R_H in $La_{2-x}Sr_xCuO_4$.[17]

From these results, we conclude that the dispersion of the spectral weight near the Fermi energy of the doped Hubbard model has a generic behavior similar to the hole-doped cuprates. In particular, there is a flat band of states near the Fermi energy around the $(\pi,0)$ and $(0,\pi)$ points. This is clearly seen in the variation of the peak position shown in Fig. 1 and gives rise to the resonant peak in the single-particle density of states $N(\omega)$.[6] We believe that this is part of a band of quasiparticles characterized by an energy scale set by J which has an anomalously flat band region near X and Y. The dispersion relation of these excitations is determined by the strong Coulomb interactions which give rise to local hole-spin correlations and is not simply determined by the one-electron band structure. In addition, depending on whether the Fermi level lies above or below the flat region in $E(\mathbf{p})$, the Fermi surface is closed around the (π,π) or (0,0) point, respectively. We find that, when only a near-neighbor hopping t is included, this change in the topology of the Fermi surface occurs at $\langle n\rangle\sim0.84$. Monte Carlo results in which a next-near-neighbor hopping $t'=-0.15t$ is introduced show a similar flat band near $X(Y)$ with a change in the topology of the Fermi surface at $\langle n\rangle\sim0.7$. It has been suggested[1,2] that the generic many-body flattening of the bands near the Fermi energy may play a role in enhancing T_c. As we have seen here, this is not a van Hove band structure effect but rather a many-body effect.

We have recently received a paper by Dagotto *et al.*,[18] where a similar discussion regarding the quasiparticle dispersion of a hole in the t-J model is given.

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[16] An alternative way of getting information on the Fermi surface topology is to use the criterion $\langle n_{\mathbf{p}} \rangle = 0.5$. Since these calculations are done at relatively high temperatures, this criterion is crude and the resulting Fermi surface is more similar to that of the $U=0$ system.

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