Flat Quasiparticle Dispersion in the 2D t-J Model

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A model of weakly interacting hole quasiparticles is proposed to describe the normal state of the high temperature superconductors. The effect of strong correlations is contained in the dispersion relation of the holes, which is obtained accurately using a numerical technique and the t-J model on 8×8, 12×12, and 16×16 clusters. Many-body effects induce anomalous quasiparticle *flat* bands similar to those observed in recent angle-resolved photoemission experiments. We also found that the Hall coefficient is in excellent quantitative agreement with experimental results for $La_{2-x}Sr_xCuO_4$. Several other "anomalous" features of the cuprates can be explained with this model.

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Many normal state properties of the high temperature superconductors are still puzzling. The dc resistivity, ρ_{ab}, of the hole-doped cuprates is linear with temperature (T) when the hole concentration is "optimal" [1]. The Hall coefficient, R_H, at constant temperature changes sign as the hole density is increased away from the insulator parent compound [2,3]. Angle-resolved photoemission experiments (ARPES) suggest the presence of a large Fermi surface in some cuprates [4]. This result is in contradiction with theoretical ideas at $T = 0$ based on electronic models which favor small holelike Fermi surfaces at low hole density [5]. In addition, using ARPES techniques it has been recently reported [6] that an extended region of flat CuO_2-derived bands very near the Fermi energy exists for Bi2212, Bi2201, Y123, and Y124. Such a universal behavior of the cuprates cannot be explained within band structure calculations which use different effective electronic potentials for each compound [6,7].

In this paper we discuss a model of hole carriers in an antiferromagnetic background that explains in a natural way many anomalous properties of the cuprates. The main assumption is that the normal state can be modeled by a noninteracting dilute gas of hole quasiparticles. The influence of antiferromagnetism and strong correlations is contained in the special dispersion relation, $\epsilon(\mathbf{k})$, which is obtained using an unbiased numerical method applied to a one band model description of the CuO_2 planes. Our approach is similar in spirit to that of Trugman [8] where the dispersion relation of holes was calculated variationally using the t-t'-J model. One of the main results of the paper is that the hole dispersion relation contains flat bands at the X and Y points [i.e., $\mathbf{k} = (\pi, 0)$, and $(0, \pi)$], very similar to those described in recent ARPES experiments [6]. The present approach belongs to the family of "narrow band" descriptions of the normal state of the cuprates, but with flat bands caused by strong electronic correlations instead of band structure effects. In agreement with previous approximate calculations [8,9], $\epsilon(\mathbf{k})$ contains a somewhat hidden energy scale, Δ, which is considerably smaller than the total quasiparticle bandwidth of the order of the antiferromagnetic exchange J, and produces an R_H in quantitative agreement with the experimental data [3] for $La_{2-x}Sr_xCuO_4$.

To calculate $\epsilon(\mathbf{k})$, here we used the two dimensional t-J model [10]. However, the intuitive ideas to be discussed below are not dependent on the specific model selected to represent the cuprates, as long as strong antiferromagnetic fluctuations are present in the ground state. The t-J model Hamiltonian is defined as

$$H = -t \sum_{\langle ij \rangle} [(1 - n_{i,-\sigma}) c^{\dagger}_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) + \text{H.c.}] + J \sum_{\langle ij \rangle} [\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j], \quad (1)$$

where the notation is standard. Here $\epsilon(\mathbf{k})$ is calculated using a Green function Monte Carlo (GFMC) method [11] which allows us to obtain results on large clusters of 8×8, 12×12, and 16×16 sites minimizing finite size effects. This technique produces unbiased accurate results for the one hole problem since in this case a good starting variational wave function can be prepared (based on the "string" picture [4]). We checked that other techniques (Lanczos method on clusters from 16 to 26 sites and noncrossing diagrammatic approximations) produce results in good agreement with GFMC [4].

In Fig. 1(a), the numerically evaluated $\epsilon(\mathbf{k})$ is shown for $J/t = 0.4$ along particular directions in the Brillouin zone. Note that finite size effects are negligible. The minimum in the energy is obtained at the $\bar{M}$ point $\mathbf{k} = (\pi/2, \pi/2)$ in agreement with previous approximate calculations [4,8]. The total bandwidth W is severely re-

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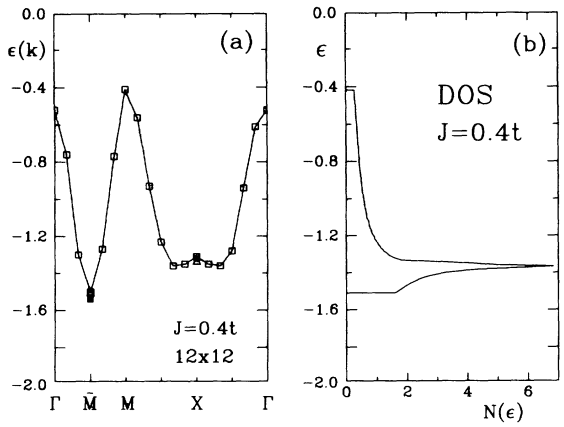

FIG. 1. (a) Energy of a hole in the t-J model, $\epsilon(\mathbf{k})$, vs momentum obtained with the GFMC method on a 12×12 lattice (open squares) and $J/t = 0.4$, (in units of t). Results for an 8×8 cluster (open triangles) and a 16×16 cluster (full squares) are shown for the $\bar{M}$ and X points to illustrate the absence of strong finite size effects in the results. Note the flat region near the X point. The error bars are not shown but typically they are $\approx 0.02t$ at all momenta, with the exception of the Γ and M points where they are $\approx 0.20t$. (b) Density of states obtained from our fit of the numerical data in Fig. 1(a) showing the van Hove singularity between $\bar{M}$ and X. The unit of energy is t.

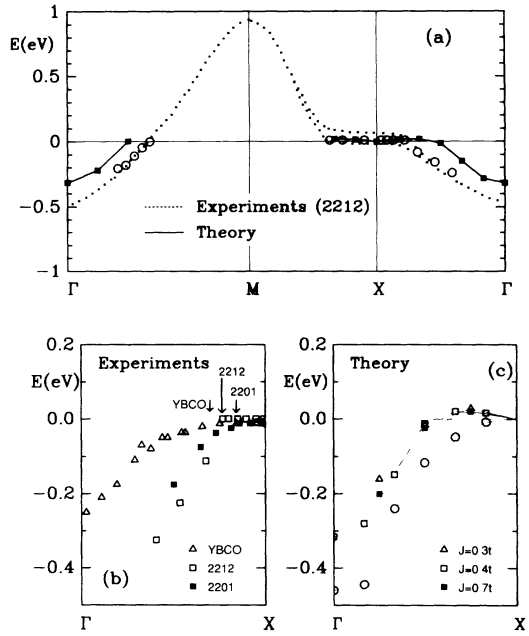

FIG. 2. (a) Energy vs momentum of the experimentally observed quasiparticle band obtained using ARPES techniques (from Ref. [6]; open circles). The dashed line is an extrapolation discussed in [6]. The theoretical predictions of the present paper are shown as full squares joined by a solid line. They correspond to $J/t = 0.4$, on a 12×12 cluster. (b) Experimental ARPES results for three high-T_c compounds. The points show the energy position of the quasiparticle peaks as the momentum interval between Γ and X is scanned. The arrows roughly denote the width of the flat bands in these compounds. (c) Theoretical dispersion of the quasiparticle for several values of J/t as shown in the figure. The circles correspond to $J/t = 0.4$ and a diagonal hopping amplitude $t' = 0.15t$. $t \approx 0.4$ eV is assumed.

duced from that of a gas of noninteracting electrons due to the antiferromagnetic correlations. However, the analysis below suggests that the strong *anisotropy* of $\epsilon(\mathbf{k})$ is more important than the actual bandwidth for calculations carried out near room temperature. The close proximity in energy of momenta $\bar{M}$ and X introduces a small energy scale $\Delta = \epsilon(X) - \epsilon(\bar{M})$ in the problem [8,9]. Actually, all momenta belonging to the noninteracting 2D Fermi surface $\cos k_x + \cos k_y = 0$ are very close in energy in the t-J model. In the range $0.3 \leq J/t \leq 0.7$, we found that Δ is approximately 15% to 20% of the total bandwidth. Since $W \sim J$, then important effects are expected at $T \sim 300$ K. The presence of this small scale can be understood more easily in the context of the Hubbard model. There at $U/t = 0$ and when $U/t \to \infty$, a degeneracy between holes at $\bar{M}$ and X exists (in the latter the whole bandwidth scales like $1/U$ as discussed in Ref. [4]). However, for finite values of U/t there is no *symmetry* causing a degeneracy along the $\cos k_x + \cos k_y = 0$ line, and the $\bar{M}$ and X energies split. Since in two limits the splitting become zero, it is reasonable that Δ remains small for all values of the coupling.

In order to calculate observables, we have fit the numerical results of Fig. 1(a) using a general combination of trigonometric functions. The best fit corresponds to

$$\epsilon(\mathbf{k}) = -1.255 + 0.34 \cos k_x \cos k_y + 0.13(\cos 2k_x + \cos 2k_y).$$

The main *effective* contribution to $\epsilon(\mathbf{k})$ arises from hole hopping between sites belonging to the same sublattice, to avoid distorting the antiferromagnetic background. However, note that $\epsilon(\mathbf{k})$ is not as simple as $\epsilon_{\mathrm{MF}}(\mathbf{k}) \sim J(\cos k_x + \cos k_y)^2$ which is suggested by the standard mean field spin-density-wave (SDW) approximation [5]. In ϵ_{MF} the line $\cos k_x + \cos k_y = 0$ is still degenerate, with important physical implications which are *not* in agreement with experiments.

An important detail of Fig. 1(a) is the near flatness of the energy in the vicinity of $\mathbf{k} = (\pi, 0)$. This feature is in good agreement with ARPES results obtained by Dessau *et al.* [6] for Bi2212 [reproduced in Fig. 2(a)]. These authors remarked that such a flat region near $(0, \pi), (\pi, 0)$ is observed in several high-T_c compounds and seems a universal property of the hole-doped cuprates. To compare the theoretically observed flat region of Fig. 1(a) and the experiments, in Fig. 2(a) the chemical potential of our model was fixed such that $\mathbf{k} = (\pi, 0)$ would approximately be the Fermi momentum p_F, and to set the overall scale we used $t = 0.4$ eV. Only momenta from Γ to the Fermi momentum are plotted since for momenta above p_F the data points of Fig. 1(a) represent poles in the hole spectral function that do not necessarily carry a

large weight, and thus they do not correspond to the large quasiparticle peaks observed in the ARPES experiment [12]. The qualitative agreement between the t-J model prediction and experiments is remarkable showing that the flatness of the $\mathbf{k} = (\pi, 0)$ region in the cuprates may have a many-body origin. Intuitively, it is the presence of saddle points near X and Y (also noticed in Ref. [8]) which is responsible for the abnormal flatness of the hole dispersion. As expected, the density of states presents a van Hove (vH) singularity caused by the saddle points [Fig. 1(b)]. The similarities with the vH scenario widely discussed in the literature are remarkable [13]. In the previous vH ideas the saddle point is generated by band effects, while here *many-body* effects in the CuO_2 planes are crucial, and thus our predictions are universal for all hole-doped cuprates.

Recently, ARPES studies by King *et al.* [7] noticed that the width of the flat band is slightly different for Bi2201, Bi2212, and Y-Ba-Cu-O (Y123 and Y124) [the results are reproduced in Fig. 2(b)]. At first sight, this seems puzzling if the origins of the flat feature are the copper-oxide planes as proposed in this paper. However, in Fig. 2(c) we show our results using the same scale for values of J/t in the narrow interval between 0.3 and 0.7, and also including a small diagonal hopping t' for illustration. Figure 2(c) shows that small changes in the parameters lead to changes in the width of the flat bands of the same order of magnitude as observed experimentally.

The presence of the small scale Δ produces interesting physical consequences. In Fig. 3(a), the hole occupation number in momentum space, n_k, is shown at 10% hole density, and several temperatures ranging from $T = 0$ to ~ 500 K. It is clear that n_k at $\mathbf{k} \approx (\pi/2, \pi/2)$ rapidly decreases as the temperature increases. Reciprocally, the occupation near $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$ increases. Intuitively, this result is understandable since different regions in momentum space will start contributing appreciably to observables once the temperature is comparable to their energy with respect to the $T = 0$ chemical potential. Thus, in our model the near degeneracy between $\bar{M}$ and X implies that a strong temperature dependence in many quantities should be expected. In Figs. 3(b) and 3(c) the Fermi surface is shown as a function of temperature. At $T = 0$ and a realistic hole density $x = 0.10$, the minimum of the hole band located at $\bar{M}$ implies the presence of hole pockets in the Fermi surface [Fig. 3(b)]. However, when the temperature becomes comparable to Δ all levels along the X-Y direction become equally populated and the hole pockets are washed out. To characterize the Fermi surface at a fixed finite temperature, we decided to plot the lines in k space where the Fermi distribution f is appreciably reduced from its maximum value, $f_{\max}$, which is always obtained at $\bar{M}$. To fix ideas, in Fig. 3(c) we plotted the line where the population of a given state has been reduced to only 10% of the maximum $f_{\max}$. At a temperature of the order or larger than Δ no vestige of the hole pockets remains, and the

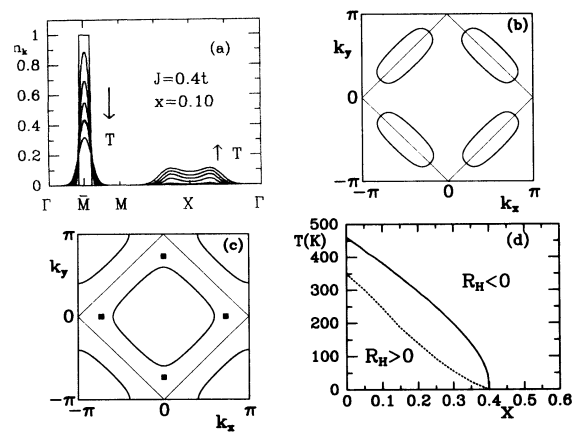

FIG. 3. (a) Occupation number n_k versus momenta at hole concentration $x = 0.10$, $J/t = 0.4$, and several equidistant temperatures ranging from $T = 0$ to $T = 0.10t$. The arrows indicate the direction in which T is growing. The rapid reduction in the hole population near $\bar{M}$ is apparent. (b) Fermi surface as defined in the text corresponding to $J/t = 0.4$, $x = 0.1$, and zero temperature. (c) Same as (b) but at $T \approx 0.08t \approx 400$ K. The full squares denote the position of the saddle points. (d) Sign of the Hall coefficient R_H in the plane temperature-hole density (T, x). The solid line separates holelike ($R_H > 0$) from electronlike ($R_H < 0$) behavior, at $J/t = 0.4$. The dashed line separates the regime where the Fermi surface is small and holelike, from the region where the FS is large and electronlike.

"Fermi surface" is large and electronlike, as observed experimentally [8]. Note also that the Fermi surface shown in Fig. 3(c) has remnants of *nesting* as was also observed experimentally in recent ARPES studies [6,7].

We have also investigated the effect of a small Δ on the weak coupling one band Hubbard model. For example, at $U/t = 4$, diagrammatic approaches suggest that $\Delta \sim 40$ K, i.e., approximately an order of magnitude smaller than for the t-J model at $J/t = 0.4$ [14]. Thus, the disappearance of the hole pockets near half filling will occur at an even lower temperature than for the t-J model. These ideas can actually explain interesting Monte Carlo numerical results reported in the literature. Working on a 16×16 cluster, $T \sim 0.17t$, and electronic density $\langle n \rangle = 0.87$, Moreo *et al.* have observed a large Fermi surface in a numerical simulation of the Hubbard model [15]. However, our analysis shows that only at temperatures as low as $T = 0.009t$ can the near degeneracy between $\bar{M}$ and X be resolved and thus Monte Carlo simulations at currently accessible temperatures treat all the momenta along X-Y as effectively degenerate in energy. Then, the absence of "hole pockets" in the numerical analysis is now understandable. [16]

The value of n_k shown in Fig. 3(a) has important consequences for other experimentally measurable quantities. The change from a pocketlike to a large Fermi surface as the temperature is increased (at low hole density) suggests that R_H may also acquire a strong tem-

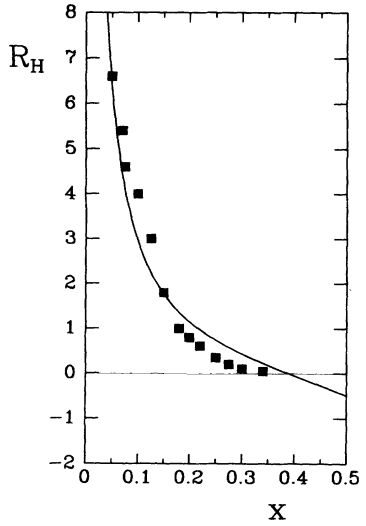

FIG. 4. Hall coefficient (R_H) (in units of 10^{-3} cm^3/C) vs hole density (x). The solid line denotes results for the pure t-J model at $J/t = 0.4$ and $T = 0$. The full squares are experimental results for $La_{2-x}Sr_xCuO_4$ at $T = 50$ K (Ref. [3]).

perature and density dependence in the present model. To check this idea, R_H was calculated in the relaxation-time approximation as [8,17]. To avoid the complexities associated with interplane coupling between adjacent CuO_2 planes, here we compare results exclusively with $La_{2-x}Sr_xCuO_4$ at different Sr concentrations. In this compound, the volume of the unit cell is equal to $3.8 \times 3.8 \times 6.6 \times$Å$^3 \approx 95 \times (10^{-8}$ cm$)^3$. In Fig. 3(d), the sign of the Hall coefficient is shown in the plane T-x. A sign change occurs at low temperature as a function of x at a concentration $x \sim 0.4$, and near half-filling increasing the temperature at $T \sim 400$ K [18]. In Fig. 3(d) the region where the Fermi surface changes from hole to electronlike is shown. Note that there is a novel intermediate regime where R_H is positive while the FS is large, which is reminiscent of the experimentally observed behavior in the cuprates. Figure 4(a) shows the hole density dependence of R_H at low temperature compared with recent experiments by Hwang *et al.* [3]. The agreement between theory and experiment is excellent [19]. Note that on the theoretical side, no other adjustable parameter is used besides J/t.

Summarizing, in this paper we presented a simple model of hole quasiparticles that accounts for several unusual properties of the normal state of the cuprates. The effect of strong correlations is contained in the dispersion relation of holes. A saddle point appears in $\epsilon(\mathbf{k})$, inducing a van Hove singularity in the DOS of many-body origin, and producing a nearly flat hole band near the X point, in agreement with recent ARPES experiments [6,7].

We have recently received a paper by Bulut, Scalapino, and White [20], where similar discussions for the quasiparticle dispersion are given. We thank these authors for sending us an advance copy of their paper. Conversations with S. Trugman, D. J. Scalapino, A. Moreo, Z.-X. Shen, D. M. King, M. Horbach, N. Bonesteel, and R. Laughlin are also acknowledged. E.D. is supported by the Office of Naval Research under Grant No. ONR N00014-93-0495. M. B. is supported by the Office of Naval Research under Grant No. ONR N00014-J-92-1320.

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