Validity of the rigid-band picture for the t-J model

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We present an exact diagonalization study of the doping dependence of the single-particle Green's function in 16-, 18-, and 20-site clusters of the t-J model. We find evidence for the validity of the rigid-band picture starting from the half-filled case: upon doping, the topmost states of the quasiparticle band observed in the photoemission spectrum at half-filling cross the chemical potential and reappear as the lowermost states of the inverse photoemission spectrum. Features in the inverse photoemission spectra, which are inconsistent with the rigid-band picture, are shown to originate from the nontrivial point-group symmetry of the ground state with two holes, which enforces different selection rules than at half-filling. Deviations from rigid-band behavior which lead to the formation of a large Fermi surface in the momentum distribution are found to occur at energies far from the chemical potential. A Luttinger Fermi surface and a nearest-neighbor hopping band do not exist.

A well-known problem in the description of high-temperature superconductors is the volume of the Fermi surface. Since these systems are close to a metal-to-insulator transition, there arises the following question: Should one model them by a system of quasiparticles which correspond to the doped holes and populate the dispersion relation calculated for a single hole (rigid-band approximation) or should one assume that the ground state can still be obtained by adiabatic continuation from the noninteracting one, so that the Fermi surface corresponds to a slightly less than half-filled band of noninteracting electrons? Based on numerical studies of the momentum distribution and single-particle spectral function for the frequently used t-J model, it has been argued[1] that the single hole represents a "problem of only marginal relevance" for the doped case: Already for two holes in clusters with 16–20 lattice sites (corresponding to a nominal hole concentration of $\sim$10%) a kind of phase transition has occurred so that both the Fermi surface and the quasiparticle band structure in its neighborhood resemble that for noninteracting particles. In this paper we present evidence against this widely accepted picture: As far as the photoemission spectrum is concerned the rigid-band approximation (RBA) is in fact an excellent one; to fully understand the inverse photoemission spectrum one has to take into account the nontrivial symmetry of the two-hole ground state, which enforces transitions into a second, symmetry-different band of many-body states.

The t-J model reads

$$H = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}\right).$$

The $\mathbf{S}_i$ are the electronic spin operators and the sum over $\langle i,j\rangle$ stands for a summation over all pairs of nearest neighbors. The operators $\hat{c}_{i,\sigma}$ are expressed in terms of ordinary fermion operators as $c_{i,\sigma}(1 - n_{i,-\sigma})$. We study the single-particle spectral function $A_n(\mathbf{k},\omega) = A_{n,-}(\mathbf{k},-\omega) + A_{n,+}(\mathbf{k},\omega)$, where the photoemission (PES) spectrum $A_{n,-}(\mathbf{k},\omega)$ and inverse photoemission (IPES) spectrum $A_{n,+}(\mathbf{k},\omega)$ are defined as

$$\begin{aligned} A_{n,-}(\mathbf{k},\omega) &= \sum_{\nu} |\langle \Psi_{\nu,n+1}|\hat{c}_{\mathbf{k},\sigma}|\Psi_{0,n}\rangle|^2 \\ &\quad \times \delta(\omega - (E_{\nu,n+1} - E_{\text{ref}})), \\ A_{n,+}(\mathbf{k},\omega) &= \sum_{\nu} |\langle \Psi_{\nu,n-1}|\hat{c}^{\dagger}_{\mathbf{k},\sigma}|\Psi_{0,n}\rangle|^2 \\ &\quad \times \delta(\omega - (E_{\nu,n-1} - E_{\text{ref}})). \end{aligned} \tag{1}$$

Here $|\Psi_{\nu,n}\rangle$ ($E_{\nu,n}$) is the νth eigenstate (eigenenergy) with n holes (in particular $\nu = 0$ implies the ground state) and the reference energy E_{ref} is chosen as $E_{0,n}$ (although other values will be advantageous later on). All spectra were evaluated exactly by the Lanczos method.

Let us first recall a few constraints due to sum rules. The momentum distribution $n(\mathbf{k}) = \langle \Psi_{0,n}|\hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma}|\Psi_{0,n}\rangle$ in the n-hole ground state is the zeroth moment of $A_{n,-}(\mathbf{k},\omega)$; the zeroth moment of $A_{n,+}(\mathbf{k},\omega)$ is given by $1 - N/2L - n(\mathbf{k})$, where N is the number of electrons and L the number of sites (for an even number of electrons and total z spin 0). Introducing $\mathbf{Q} = (\pi,\pi)$ and $\delta n(\mathbf{k}) = n(\mathbf{k}) - n(\mathbf{k}+\mathbf{Q})$, the expectation value of the kinetic energy can be written as

$$\langle H_t \rangle = \sum_{\mathbf{k}\in \text{AFBZ}} \epsilon(\mathbf{k}) \delta n(\mathbf{k}), \tag{2}$$

where $\epsilon(\mathbf{k})$ is the free-particle energy, and the summation over $\mathbf{k}$ is restricted to the interior of the antiferromagnetic Brillouin zone (AFBZ). Since $\epsilon(\mathbf{k}) < 0$ in the range of summation, in order to have $\langle H_t \rangle < 0$ the average of $\delta n(\mathbf{k})$ in the AFBZ must be positive; i.e., $n(\mathbf{k})$ must be larger inside the AFBZ than outside, so that there is always a tendency towards the formation of a "large Fermi surface" in $n(\mathbf{k})$. To exemplify this, Table I compares $n(\mathbf{k})$ for the two-hole ground state of the fully isotropic t-J model and of the t-J_z model (where the transverse part of the Heisenberg exchange is discarded) with an added staggered field. The latter model has explicitly

TABLE I. Momentum distribution in the ground state of the t-J_z model ($t/J_z = 2$) in a staggered magnetic field ($0.1J_z$) and the t-J model (t/J=2) in a 4×4 cluster. To stabilize a ground state with the same point-group symmetry (B_1) as for the t-J model, a second nearest neighbor hopping term of strength $-J_z/10$ has been added to the t-J_z model.

$\mathbf{k}$	$(0,0)$	$(\frac{\pi}{2},0)$	$(\pi,0)$	$(\frac{\pi}{2},\frac{\pi}{2})$	$(\frac{\pi}{2},\pi)$	(π,π)
$n(\mathbf{k})(t\text{-}J_z)$	0.5481	0.5374	0.3491	0.4993	0.3387	0.2522
$n(\mathbf{k})(t\text{-}J)$	0.5565	0.5421	0.3378	0.4974	0.3225	0.3197

broken symmetry (the ground state expectation value of the staggered magnetization is 61.3% of the value for the Néel state) which rigorously excludes a large Fermi surface. In spite of this, $n(\mathbf{k})$ is almost indistinguishable for the two models and in particular always would suggest a large Fermi surface. This shows that use of $n(\mathbf{k})$ to assign a Fermi surface may be quite problematic. The key problem is that for strongly correlated systems the "quasiparticle peak" near the chemical potential carries only a small fraction of the total PES weight; if we decompose $n(\mathbf{k})$ into a component from the coherent peak, $n_{\mathrm{QP}}(\mathbf{k})$, and from the integration over the incoherent continua, $n_{\mathrm{inc}}(\mathbf{k})$, we usually have $n_{\mathrm{inc}}(\mathbf{k}) > n_{\mathrm{QP}}(\boldsymbol{k})$. Then, when only $n(\mathbf{k})$ is considered, for example, a change in $n_{\mathrm{inc}}(\mathbf{k})$ (which is unrelated to low-energy physics) may mimic a Fermi surface. As will be seen below, this is precisely what happens when the t-J model is doped with holes. Next, the sum rules for the spectral function enforce that in the doped case PES weight (IPES weight) is concentrated inside (outside) of the AFBZ, so that not only $n(\mathbf{k})$ but also the distribution of spectral weight in $\mathbf{k}$ space is reminiscent of free electrons.

Let us next discuss what can be reasonably expected if the RBA were to hold: A variety of diagonalization studies[2–4] have shown that two holes in the t-J model form a bound state with a binding energy ($E_B \sim 0.8J-J$) that is a sizable fraction of the single-hole bandwidth ($W \sim 2J$). The two-hole ground state thus should be modeled by a state of the type $|\Phi_0\rangle = \sum_{\mathbf{k}} \Delta(\mathbf{k}) a^{\dagger}_{\mathbf{k},\uparrow} a^{\dagger}_{\mathbf{k},\downarrow}|0\rangle$, where $a^{\dagger}_{\mathbf{k},\sigma}$ is the creation operator for a holelike "quasiparticle" in the band observed in $A_{0,-}(\mathbf{k})$. The wave function $\Delta(\mathbf{k})$ may differ appreciably from zero for all quasiparticle states within $\sim E_B$ above the ground state so that a "Fermi surface" does not exist. In IPES we annihilate a hole (with momentum $\mathbf{k}$), and so the remaining hole should be in a state belonging to the single-hole band with momentum $-\mathbf{k}$; the intensity should be proportional to the quasiparticle occupation $\tilde{n}(\mathbf{k})$. Conversely, in photoemission we add a third hole and, neglecting all interactions except for the Pauli principle, should observe the same spectrum as for a single hole with the intensity of the peaks near the Fermi energy E_F being reduced by a factor $1-\tilde{n}(\mathbf{k})$. Adding up the weights of the peaks in $A_{2,+}(\mathbf{k},\omega)$ and $A_{2,-}(\mathbf{k},\omega)$ closest to E_F we should therefore ideally obtain the weight of the "unsplit" peak in $A_{0,-}(\mathbf{k},\omega)$, a sensitive quantitative test for the RBA. Moreover, the $d_{x^2-y^2}$ symmetry of the two-hole ground state[3] implies that in the 16- and 18-site cluster $\Delta(\mathbf{k})$ must have a node along the $(1,1)$ direction and hence $\tilde{n}(\mathbf{k}) = 0$ for these momenta.

Let us now check how much these expectations are borne out by the exact spectra. Figure 1 compares $A(\mathbf{k},\omega)$ in the half-filled and two-hole ground state for all allowed momenta in the 4×4 and 18-site cluster [(0,0) and (π,π) are from the 18-site cluster]; Fig. 2 displays the same information for the 20-site cluster. No adjustment of any kind has been performed. In agreement with the above discussion Fig. 1 shows that for momenta along the (1,1) direction (left panel) there is a striking similarity between the PES spectra for the doped and undoped case, $A_{2,-}(\mathbf{k},\omega)$ and $A_{0,-}(\mathbf{k},\omega)$, particularly near the Fermi energy $E_F \sim +1.7t$. A band of peaks with practically identical dispersion and weight can be clearly identified in both groups of spectra [a possible exception is $(\frac{2\pi}{3},\frac{2\pi}{3})$; this momentum might play a special role since the single-hole ground states at this momentum and (π,π) have total spin $S = 3/2$, whereas all other single-hole ground states are dubletts[3]]. Away from (1,1) (right panel of Fig. 1) doping leads to a shift of weight from the PES band to IPES peaks immediately above E_F: This suggests the "split peak" situation $\tilde{n}(\mathbf{k}) \neq 0$. The situation is the same for the 20-site cluster; Fig. 2 shows the same similarity between the low-energy parts of the PES spectra for the doped and undoped cases. Again the dominant low-energy PES peaks near the Fermi energy (right panel) remain either unaffected by doping or

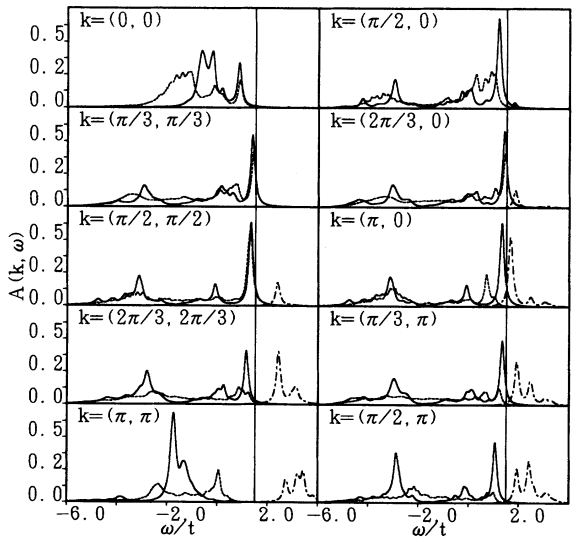

FIG. 1. Comparison of the photoemission spectra at half-filling and in the ground state with two holes: $A_{0,-}(\mathbf{k},-\omega)$ (solid line) $A_{2,-}(\mathbf{k},-\omega)$ (dotted line), and $A_{2,+}(\mathbf{k},\omega)$ (dash-dotted line) for the 16- and 18-site cluster. The Fermi energy is marked by the vertical line; δ functions have been replaced by Lorentzians of width $0.1t$.

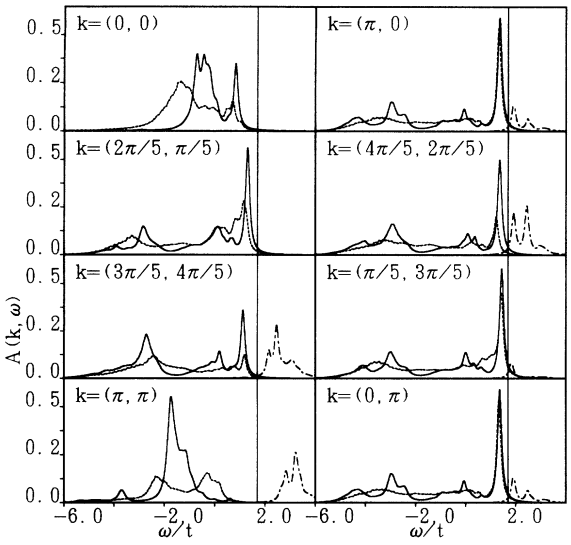

FIG. 2. Same as Fig. 1 but for the 20-site cluster.

seem to (partially) cross the chemical potential to reappear as low-energy IPES peaks. Point-group symmetry poses no significant constraint on the hypothetical pair wave function $\Delta(\mathbf{k})$ in this cluster [all momenta except (0,0) and (π,π) have low symmetry] and consequently we observe low-energy IPES weight for all momenta where low-energy PES peaks were present at half-filling.

It is only at energies remote from E_F that major changes in the PES spectra occur upon doping: For momenta around (0,0) and (π,π) there is a pronounced addition or depletion of incoherent spectral weight at energies $\sim 3t$ below E_F. The increase or decrease of the integrated spectral weight near $(0,0)/(\pi,\pi)$ and the corresponding formation of a "large Fermi surface" in $n(\mathbf{k})$ upon doping therefore is clearly not the consequence of the phase-transition-like emerging of a nearest neighbor hopping band[1] in the range $2J \ll 3t$ around E_F [note that the spectral weight near E_F at $(0,0)/(\pi,\pi)$ even diminishes or increases upon doping]. Rather it is accomplished by the reshuffling of incoherent spectral weight deep below E_F, and thus is certainly unrelated to any low-energy physics. As a matter of fact, the actual form of $A(\mathbf{k},\omega)$ for the doped 20-site cluster rules out the Luttinger Fermi surface postulated[1] for this cluster on the basis of the momentum distribution. Despite the fact that $(\pi,0)$ and $(\pi/5,3\pi/5)$ are on opposite sides of the Luttinger Fermi surface, the low-energy peak structure in $A(\mathbf{k},\omega)$ is practically identical for these momenta: Both photoemission spectra show a pronounced low-energy peak, indicating that these momenta are "occupied." The criterion $n(\mathbf{k}) < 1/2$ [$n(\mathbf{k}) > 1/2$], employed in Ref. 1 to decide whether a $\mathbf{k}$ point is inside [outside] the Fermi surface obviously has no significance for predicting the low-energy behavior of the spectral function.

Next, we proceed to a quantitative check of the rigid-band approximation: We set $E_{\mathrm{ref}} = E_{0,2}$ in the photoemission spectral function at half-filling, $A_{0,-}(\mathbf{k},\omega)$, and do not invert the sign of ω, so that we can directly compare the positions of peaks in this function and in the inverse photoemission spectrum for the doped ground state, $A_{2,+}(\mathbf{k},\omega)$ (both spectra involve the single-hole subspace in their final states, so that direct comparison of states is possible). Then, Fig. 3 confirms that in the 16- and 18-site cluster the final states for the lowest IPES peaks at all momenta off the (1,1) direction (right panel) indeed belong to the single-hole band observed in PES at half-filling (the energies of the respective lowest peaks agree to $10^{-10}t$, essentially the limit of the Lanczos procedure). Figure 4 shows that the same holds true in the 20-site cluster for all momenta except $(0,0)$ and (π,π). In complete agreement with the RBA, the lowermost peaks of the IPES spectrum for the doped case are thus identified as the uppermost states in the PES spectrum for the undoped case. It is only at higher energies ($\sim J$ above the quasiparticle states) that there are states with appreciable weight in the IPES spectra which have vanishing or small weight in the PES spectrum at half-filling. The low-energy physics thus should be completely consistent with rigid-band behavior.

It should be noted that the above result is in contradiction to the "large Fermi surface" scenario.[1] This would necessitate the assumption that the uppermost states of the completely filled, next nearest neighbor hopping band observed in PES at half-filling simultaneously belong to a half-filled, nearest neighbor hopping (i.e., topologically different) band "observed" for the two-hole ground state. It would moreover require the assumption that upon doping a full-scale transition to a topologically different band structure can occur, while simultaneously the states next to the chemical potential remain unaffected and merely cross the Fermi level.

Let us now turn to a discussion of the IPES final states in the 16- and 18-site cluster along the (1,1) direction (left panel of Fig. 3). Obviously, these states are not observed in $A_{0,-}(\mathbf{k},\omega)$ so that we seem to have found "new states," which were "generated by dop-

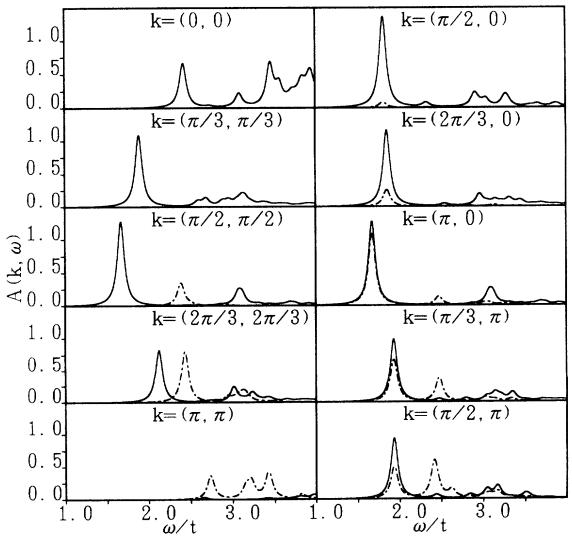

FIG. 3. PES spectrum $A_{0,-}(\mathbf{k},\omega)$ (solid line) and IPES spectrum $A_{2,+}(\mathbf{k},\omega)$ (dash-dotted line) for the 16- and 18-site cluster. The reference energies are identical so that direct comparison of the peaks is possible; δ functions have been replaced by Lorentzians of width $0.05t$.

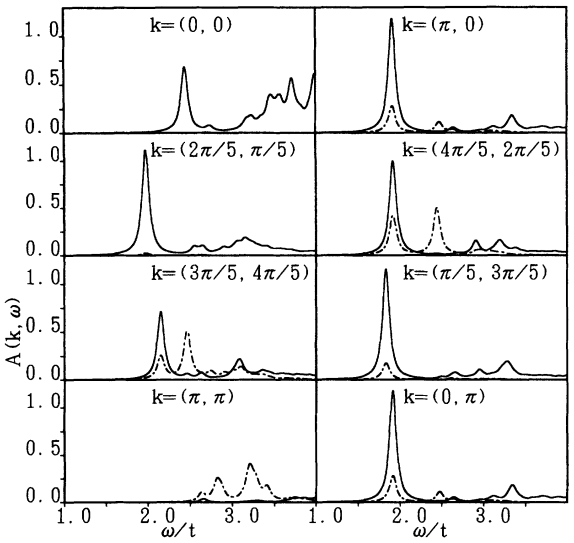

FIG. 4. Same as Fig. 3 but for the 20-site cluster.

ing." The true explanation, however, is much simpler: For each momentum along (1,1) the little group comprises the reflection by a plane along the (1,1) direction (which we denote by T_m). The ground state at half-filling is totally symmetric, and consequently even under T_m, whereas the two-hole ground state has $d_{x^2-y^2}$ symmetry and hence is odd under T_m. Consequently, for any single-hole state $|\Psi_{\nu,1}(\mathbf{k})\rangle$ the matrix element $\langle\Psi_{\nu,1}(\mathbf{k})|\hat{c}_{\mathbf{k},\sigma}|\Psi_{0,0}\rangle$ $[\langle\Psi_{\nu,1}(\mathbf{k})|\hat{c}^{\dagger}_{\mathbf{k},-\sigma}|\Psi_{0,2}\rangle]$ is different from zero only if $|\Psi_{\nu,1}(\mathbf{k})\rangle$ is even [odd] under T_m. The appearance of the "new states" thus is simply the consequence of a group theoretical selection rule.[5]

We thus have to explain single-hole states with an odd parity under T_m [for the highly symmetric $\mathbf{k}$ points $(0,0)$ and (π,π) they must have the full $d_{x^2-y^2}$ symmetry]. The totally symmetric single-hole states observed in PES at half-filling can be understood in terms of the string picture,[6-9,14] where the hole is assumed to be dressed by a cloud of spin defects. We thus adopt the hypothesis[5] that the odd-parity states in question are similar in nature, but that the cloud of spin defects surrounding the hole has a nontrivial symmetry. Hence we define

$$d_{j,\uparrow} = S^-_j \hat{c}_{j+\hat{x},\downarrow} + S^-_j \hat{c}_{j-\hat{x},\downarrow} - S^-_j \hat{c}_{j+\hat{y},\downarrow} - S^-_j \hat{c}_{j-\hat{y},\downarrow},$$

where $j+\hat{x}$ denotes the nearest neighbor of j in the positive x direction, etc. When acting on the Néel state, $d_{j,\uparrow}$ generates the four strings of length 1 beginning at site j. Their relative signs makes sure that the resulting state has $d_{x^2-y^2}$ symmetry under rotations around j. A coherent superposition of such operators with momentum along (1,1) consequently creates a state with the desired transformation properties and we assume that the states in question can be described by such a wave function. Then, for momenta along (1,1), in $A_{0,-}(\mathbf{k},\omega)$ we replace $\hat{c}_{\mathbf{k},\sigma}$ by the Fourier transform of $d_{j,\sigma}$. We denote the resulting function by $\tilde{A}_{0,-}(\mathbf{k},\omega)$ and it is shown in Fig. 5. Again we choose $E_{\mathrm{ref}} = E_{0,2}$ to facilitate comparison with the IPES spectra for the two-hole ground state. $\tilde{A}_{0,-}(\mathbf{k},\omega)$ is similar in character to $A_{0,-}(\mathbf{k},\omega)$ in that

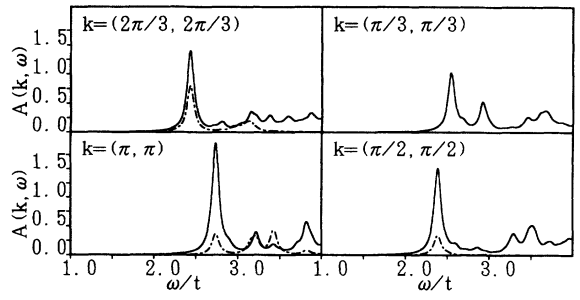

FIG. 5. PES spectrum $\tilde{A}_{0,-}(\mathbf{k},\omega)$ (solid line) and IPES spectrum $A_{2,+}(\mathbf{k},\omega)$ (dash-dotted line) for momenta along (1,1) in the 16- and 18-site cluster. The reference energies are identical so that direct comparison of the peaks is possible; δ functions have been replaced by Lorentzians of width $0.05t$.

there is a "quasiparticle peak" at the bottom of an incoherent continuum. We conclude that there indeed exists a band of many-body states, where a hole surrounded by a spin defect cloud with intrinsic $d_{x^2-y^2}$ symmetry propagates coherently. Next, the dominant peaks in the IPES spectra along (1,1) fall precisely into this band (the energies of the respective lowest peaks agree to an accuracy of 10^{-10}), so that we have clarified their nature.

As a more quantitative check of the RBA we next consider the weight of the peaks near E_f: Figure 6 compares the weight of the peak at $(\pi/2,\pi/2)$ in $A_{0,-}(\mathbf{k},\omega)$ [where it equals the weight at $(\pi,0)$] and $A_{2,-}(\mathbf{k},\omega)$ as well as the sum of the weights of the lowest peak in $A_{2,+}(\mathbf{k},\omega)$ and highest peak in $A_{2,-}(\mathbf{k},-\omega)$ at $(\pi,0)$. The RBA predicts all three quantities to be equal and Fig. 6 shows that they indeed agree remarkably well over a wide range of t/J.

Finally, let us discuss the "band structure" near E_f, summarized in Fig. 7 for the 16- and 18-site cluster. In $A_{2,-}(\mathbf{k},\omega)$ we observe very much the same band as in $A_{0,-}(\mathbf{k},\omega)$, the dispersion of the peaks close to E_f being practically identical to that for the half-filled band. For the doped case, there is moreover an obvious correlation between the peak intensity and the distance from E_F as one would expect for a Fermi liquid: Comparison of Figs.

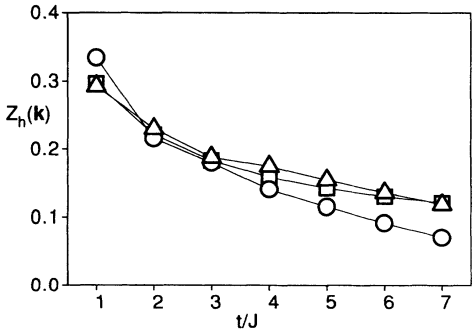

FIG. 6. Comparison of the t/J dependence of the PES pole strength at $(\pi/2,\pi/2)$ at half-filling (squares) and in the two-hole ground state (triangles) and the added weights of the lowest IPES peak and highest PES peak at $(\pi,0)$ in the two-hole ground state (circles)

1 and 7 shows that sharp peaks exist for those momenta which are closest to the Fermi energy in their respective clusters; weak or diffuse peaks are seen for momenta which are more distant from E_F [for momenta outside the AFBZ there is in addition a depletion of intensity over the whole width of the spectra, as necessitated by the kinetic-energy sum rule (2)]. The same overall trend can also be seen in the 20-site cluster (Fig. 2). In IPES for the 16- and 18-site cluster, the situation is more complicated due to the novel selection rule for momenta along the $(1,1)$ direction. Away from this line we observe in $A_{2,+}(\mathbf{k},\omega)$ a portion of the band seen in $A_{0,-}(\mathbf{k},\omega)$ (as is the case for all momenta in the 20-site cluster, where no selection rule exists). In the sense of the RBA these states have partially crossed the Fermi energy; due to the interaction between the holes, however, there is no Fermi surface but rather a zone of partially occupied momenta (indicated by the box in Fig. 7) where the quasiparticle peaks are split between PES and IPES. For IPES along the (1,1) direction in the 16- and 18-site cluster the selection rule prohibits transitions back into the single-hole band and a different band of many-body states with odd parity under reflection by the $(1,1)$ axis is seen. We have identified them as a hole dressed by a cloud of spin defects with intrinsic $d_{x^2-y^2}$ symmetry. This band has almost no dispersion and for all momenta accessible to our diagonalization study remains $\sim 2J$ above E_f, and thus is unrelated to any low-energy physics.

While there is no well-defined Fermi surface in the bound states we have studied, the obvious validity of the rigid-band approximation suggests that if a Fermi surface exists at all, it takes the form of small hole pockets. The precise location of these pockets in an infinite system is impossible to predict on the basis of exact diagonalization results; due to the near degeneracy of the states near the surface of the magnetic Brillouin zone, the interaction between the holes is decisive. Whereas the 16- and 18-site cluster both suggest $(\pi,0)$ as the locus of the pockets, this momentum seems to be largely unoccupied by holes in the 20-site cluster, where the largest shift from PES to IPES occurs at $(2\pi/5,4\pi/5)$. The best one can say is that there seems to be a trend for hole occupation at or near $(\pi,0)$. Since it is the interaction between the holes which favors these $\mathbf{k}$ points, the apparent contradiction with the well-known fact that the single-hole ground state has momentum $(\pi/2,\pi/2)$ is not surprising.

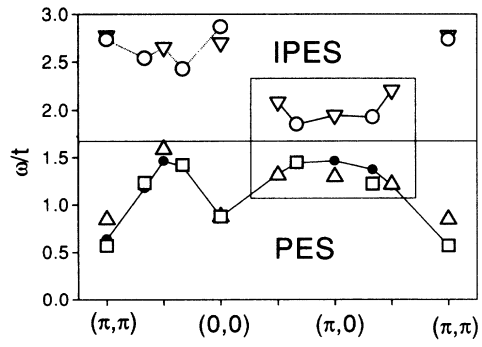

FIG. 7. Schematic quasiparticle band structure in the neighborhood of E_f for the 16- and 18-site cluster. Up triangles (squares) give the position of the highest peak in $A_{2,-}(\mathbf{k},-\omega)$, down triangles (circles) the position of the lowest peak in $A_{2,+}(\mathbf{k},\omega)$ for the 4×4 (18-site) cluster. The positions of the highest peaks in $A_{0,-}(\mathbf{k},-\omega)$ (dots) are also given. The various groups of spectra have been shifted so that the energies of the respective PES peak at $(0,0)$ coincide (shift between doped 16- and 18-site cluster: $0.275t$).

Rigid-band behavior and hole pockets in the $t-J$ model are consistently suggested by a number of previous exact diagonalization works. Poilblanc and Dagotto[10] studied the $A(\mathbf{k},\omega)$ for single-hole states and concluded that the two-hole ground state in the 4×4 cluster shows hole pockets at $(\pi,0)$, in agreement with the present result. Stephan and Horsch[1] studied $n(\mathbf{k})$ and $A(\mathbf{k},\omega)$ for the two-hole ground state and concluded on the contrary that there is neither rigid-band behavior nor hole pockets. It should be noted, however, that whereas Poilblanc and Dagotto employed a quantitative criterion (presence or absence of a quasiparticle peak at the position of the two-hole ground state energy), Stephan and Horsch based their conclusions solely on the qualitative inspection of a rather limited data set; as discussed above (see Table I) $n(\mathbf{k})$ is not reliable for assigning the Fermi surface and our results for the spectral function in the 20-site cluster show for example that the Luttinger Fermi surface assigned there by Stephan and Horsch does not exist. Next, Castillo and Balseiro[11] computed the Hall constant and found its sign near half-filling to be consistent with a holelike Fermi surface. Gooding *et al.*[12] studied the doping dependence of the spin correlation function in clusters with special geometry and also found indications of rigid-band behavior. Finally, a study of $n(\mathbf{k})$ in the range $J > t$ (where the incoherent continua are negligible) with an added density repulsion to preclude hole clustering[13] shows unambiguous hole pockets. It seems fair to say that the available numerical results for the t-J model when interpreted with care are all consistent with rigid-band behavior and/or hole pockets.

In summary, we have performed a detailed study of the doping dependence of the single-particle spectral function up to the largest clusters that are numerically tractable. The results show unambiguously that rigid-band behavior is realized in small clusters of t-J model: Near the chemical potential, the main effect of the doping consists in moving the Fermi energy into the "band" of peaks observed at half-filling. Thereby the parts of the quasiparticle band which remain on the photoemission side are essentially unaffected; the uppermost states of this band simply cross the Fermi level and reappear as the lowermost states of the inverse photoemission spectrum. This behavior is always realized, unless it is prohibited by a trivial reason, namely, a symmetry-related selection rule. In the latter case, there is no low-energy IPES weight at all. On the PES side, modifications of the spectral function which deviate from the rigid-band picture occur predominantly at energies far from E_f, and hence should be unrelated to any Fermi surface physics. In particular, the gains and losses of PES weight which lead to the formation of a "large Fermi surface" in the momentum distribution upon doping originate from addition and de-

pletion of incoherent weight deep below the Fermi energy. On the IPES side, there is no indication of the emerging of "new states" at low energies in the course of doping. Such new states in the IPES spectrum are seen only at high energies, and hence also should be unrelated to any low-energy physics. Available exact diagonalization data are all in all consistent with this interpretation.

Then, we are left with the problem to reconcile the emerging picture for the t-J model with experiments on high-temperature superconductors. While some transport properties are quite consistent with a rigid-band/hole pocket scenario,[14] the main problem is with angular-resolved photoemission experiments.[15] These show peaks which disperse towards the Fermi energy and vanish there, as one would expect for a band crossing. Thereby the locus of the "crossing points" is remarkably consistent with the predictions of band theory, which in turn is inconsistent with hole pockets. In a Fermi liquid, the contradicting quantities actually fall into two distinct classes: Photoemission spectra depend on the wave function renormalization constant Z_h; transport properties do not. Hence, if one wants to resolve the discrepancy concerning the volume of the Fermi surface entirely within a Fermi-liquid-like picture, the simplest way would be to assume a "small" Fermi surface (to model the transport properties) and explain the photoemission results by a systematic variation of Z_h along the band which forms the Fermi surface, i.e., similar to the "shadow band" picture.[16] A trivial argument for such a strong variation in Z_h would be that irrespective of the actual band structure, a distribution of PES weight in the Brillouin zone that resembles the noninteracting (band theory) Fermi surface always optimizes the expectation value of the kinetic energy. Also, it should be noted that the spectral weight in the shadow band should even decrease when the charge fluctuations in the original Hubbard model are taken into account: When going back to the Hubbard model, the (negative) exchange energy in the t-J model then is split into a (positive) contribution from the Hubbard repulsion and a (negative) gain in kinetic energy, so that the total expectation value of the kinetic energy certainly becomes more negative than for the t-J model. Via the kinetic-energy sum rule (2), one can infer that this necessarily leads to an even more free-electron-like distribution of spectral weight. All in all adopting the rigid-band behavior found above, the available diagonalization data for the t-J model[1,10–12] as a whole are reasonably consistent with the above scenario.

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