Exact Diagonalization Study of Strongly Correlated Electron Models: Hole pockets and shadow bands in the doped $t$-$J$ model

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Abstract. A detailed exact-diagonalization study is made for the doping dependence of the single-particle spectral function $A(k, \omega)$ and momentum distribution function $n(k)$ of the two-dimensional $t$-$J$ model as a representative model for doped Mott insulators.

The results for $A(k, \omega)$ show unambiguously that the rigid-band behavior is realized in the small-cluster $t$-$J$ model: upon doping, the uppermost states of the quasiparticle band observed at half filling simply cross the Fermi level and reappear as the lowermost states of the inverse photoemission spectrum, while the photoemission side of the band remains essentially unaffected. We discuss problems in directly determining the Fermi surface from $n(k)$ and make a situation where they are largely avoided; we then find clear signatures of a Fermi surface which takes the form of small hole pockets. The identical scaling with $t/J$ of the quasiparticle weight $Z_h$ and difference in $n(k)$ between neighboring $k$-points suggests the existence of such a Fermi surface in the physical regime of parameters. We construct spin-bag operators which describe the holes dressed by the antiferromagnetic spin fluctuations and find that elementary electronic excitations of the system can be described well in terms of weakly-interacting spin-1/2 Fermionic quasi-particles corresponding to the doped holes. We make a comparison with other numerical calculations and recent angle-resolved photoemission experiment and argue that, adopting this rather conventional Fermi-liquid scenario with non-Luttinger Fermi surface, one would explain many quasiparticle-relating properties of doped cuprates in a very simple and natural way. We also show that the dynamical spin and charge excitations deviate from the particle-hole excitations of this Fermi liquid: e.g., the dominant low-energy spin excitation at momentum transfer $(\pi, \pi)$ reflects excitations of the incoherent spin background and is identified as a collective mode comparable to spin waves in the Heisenberg antiferromagnet.

1. Introduction

Physics of correlated electrons near a Mott-Hubbard metal-to-insulator transition has been of great interest in recent years after the discovery of high-temperature superconductors. Here a well-known particularly intriguing problem is the volume of the Fermi surface (FS) for the slightly less than half-filled band. Should one model the doped insulator by a dilute gas of quasiparticles corresponding to the doped holes [this would imply that the volume of the FS is proportional to the hole concentration] or can the ground state still be obtained by adiabatic continuation from the noninteracting one with all electrons taking part in the formation of the FS so that its volume is identical to that of free electrons? Based on numerical studies of the two-dimensional (2D) $t$-$J$ model, we present evidence that the first picture is a correct one [1–3]: the calculated photoemission spectrum can be interpreted very well in the rigid-band approximation (RBA), the low-energy electronic excitations can be described as holes dressed by antiferromagnetic spin fluctuations as expected in the string or spin bag picture, and the FS with the form of small hole pockets can be seen clearly in the momentum distribution function if obvious problems are circumvented.

This non-Luttinger ‘small’ FS picture, shown [4,5] to be consistent with majority of transport properties in the normal state of high-temperature superconductors, was
discarded some time ago because of the apparent contradiction to the angle-resolved photoemission (ARPES) experiment where the existence of a ‘large FS’ consistent with the LDA band-structure calculations was claimed. Most recently, however, this picture has been put under reconsideration; results of newly reported ARPES (and other) experiment [6,7] can be interpreted as indications of the small FS picture, as we will discuss in §6. Some doubts have also been casted to numerical studies of the $t$–$J$ and Hubbard models [8–11]: e.g., a recent quantum Monte Carlo calculation suggests the existence of such a hole-pocket–like FS in the 2D Hubbard model [11]. Here we report results of our exact-diagonalization studies of the $t$–$J$ model.

The $t$–$J$ model is defined by the Hamiltonian

$$H = -t \sum_{<ij>\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) + J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

(1)

where the operators $\hat{c}_{i\sigma}$ are expressed in terms of ordinary Fermion operators as $c_{i\sigma}(1 - n_{i\bar{\sigma}})$, $n_i = n_{i\uparrow} + n_{i\downarrow}$ are the electron number operators, and $\mathbf{S}_i$ are the electronic spin operators. The summation is taken over all the nearest-neighbor pairs $<ij>$ on the 2D square lattice. The photoemission (PES) and inverse photoemission (IPES) spectra are defined respectively as

$$A_n^-(\mathbf{k}, \omega) = \sum_\nu |\langle \Psi^{(n+1)}_\nu | c_{k\sigma} | \Psi^{(n)}_0 \rangle|^2 \delta(\omega - (E^{(n+1)}_\nu - E^{(n)}_0))$$

$$A_n^+(\mathbf{k}, \omega) = \sum_\nu |\langle \Psi^{(n-1)}_\nu | c_{k\sigma}^\dagger | \Psi^{(n)}_0 \rangle|^2 \delta(\omega - (E^{(n-1)}_\nu - E^{(n)}_0))$$

(2)

with the single-particle spectral function $A(\mathbf{k}, \omega) = A_n^-(\mathbf{k}, -\omega) + A_n^+(\mathbf{k}, \omega)$. Here $|\Psi^{(n)}_\nu\rangle$ ($E^{(n)}_\nu$) is the $\nu$-th eigenstate (eigenenergy) with $n$ holes ($\nu = 0$ implies the ground state).

2. Problems in Identifying the Fermi Surface

Various authors have computed the momentum distribution function $n(\mathbf{k}) = \langle \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} \rangle$ and single-particle spectral function $A(\mathbf{k}, \omega)$ for the two-hole ground state of small clusters of this model (corresponding to a nominal doping of ~10%), and found that $n(\mathbf{k})$ is maximum at $\mathbf{k} = (0,0)$ and minimum at $\mathbf{k} = (\pi, \pi)$ and roughly consistent with a free-electron picture and a quasiparticle-like band structure can be assigned in $A(\mathbf{k}, \omega)$ in the neighborhood of the Fermi energy which resembles that for noninteracting particles. It has become customary [12] to cite this as evidence that already at such fairly low doping levels the $t$–$J$ model has a free-electron–like ‘large’ FS. However, it is straightforward to see that this shape of $n(\mathbf{k})$ is simply the consequence of elementary sum rules and has no significance for the actual topology of the FS [10]: The expectation value of the kinetic-energy term of Eq. (1) may be expressed as

$$\langle H_t \rangle = \sum_{\mathbf{k} \in \text{AFBZ}} \varepsilon(\mathbf{k}) \delta n(\mathbf{k})$$

(3)

with $\delta n(\mathbf{k}) = n(\mathbf{k}) - n(\mathbf{k} + \mathbf{Q})$, where $\varepsilon(\mathbf{k})$ is the free-particle energy, $\mathbf{Q} = (\pi, \pi)$, and the summation is restricted to inside of the antiferromagnetic Brillouin zone (AFBZ). Since $\varepsilon(\mathbf{k}) < 0$ inside the AFBZ, the average of $\delta n(\mathbf{k})$ must be positive there to ensure $\langle H_t \rangle < 0$. Also, denoting by $M_0^-$ ($M_0^+$) the 0th moment of the PES (IPES) spectrum, we have $M_0^- = n(\mathbf{k})$ and $M_0^+ = \text{const} - n(\mathbf{k})$. The mere requirement $\langle H_t \rangle < 0$ thus enforces that (i) $n(\mathbf{k})$ be larger inside the AFBZ than outside and (ii) IPES weight predominantly appear
outside the AFBZ and PES weight be concentrated within the AFBZ. Thus, such ‘nearestneighbor hopping’ band and ‘free-electron–like’ FS mainly reflect generic properties of any Hamiltonian where the kinetic energy is a nearest-neighbor hopping term. It is also easy to construct a counterexample of a system, where the dispersion of lowest-energy sharp peaks can fit to the nearest-neighbor hopping band, while it is guaranteed that a free-electron–like FS is rigorously excluded due to a build-in broken symmetry [10].

We must therefore consider how the more subtle questions, such as the existence and shape of the FS and the band structure near the Fermi energy, can be answered in our numerical method. Besides the above elementary sum rules, the key problems which we have to bear in mind are as follows:

A: For strongly correlated systems, the ‘quasiparticle peak’ near the chemical potential carries only a small fraction \( Z_h \) of the total weight of the single-particle spectral function; in other words, the small ‘Fermi-edge discontinuity’ in \( n(k) \), which has to be equal to \( Z_h \), is superimposed over a substantial background stemming from the integration of the incoherent continua. Then, when only \( n(k) \) is considered, a systematic change in the weight of the background, which is unrelated to low-energy physics, may mimic an FS.

B: A variety of diagonalization studies have shown that two holes in the \( t-J \) model form a bound state with a binding energy \( (E_B \approx 0.8J - J) \) that is a sizeable fraction of the single-hole bandwidth \( (W \approx 2J) \). The ground state with two ‘holelike quasiparticles’ should thus be modeled by a state of the type

\[
|\Psi_0\rangle = \sum_k \Delta(k) a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger |\text{vac}\rangle
\]

where \( a_{k\sigma}^\dagger \) is the quasiparticle creation operator in the undoped vacuum state \( |\text{vac}\rangle \). The wave function \( \Delta(k) \) may differ appreciably from zero for all quasiparticle states within \( \sim E_B \) above the ground state: no signatures of the FS can be seen unless \( \Delta(k) \) is well localized in \( k \)-space, i.e., \( \Delta(k) \sim \delta_{k,k_0} \). In this situation, the quasiparticle peak at any momentum splits into two peaks, one in the IPES spectrum with intensity proportional to the quasiparticle occupation \( \tilde{n}(k) \) and the other in the PES spectrum with the intensity proportional to \( 1-\tilde{n}(k) \). Adding up these weight, one should then ideally obtain the weight of the ‘unsplit’ quasiparticle peak. Moreover, the \( d_{x^2-y^2} \) symmetry of the two-hole ground state (in, e.g., 16 site- and 18-site clusters) implies that \( \Delta(k) \) must have a node along \( (1,1) \) direction and hence \( \tilde{n}(k)=0 \) for these momenta; the peak splitting should thus occur predominantly near \( (\pi,0) \).

C: There is a (near) degeneracy of the quasiparticle dispersion along the surface of the AFBZ, which is unfavorable in identifying the location of the quasiparticles in \( k \)-space: a ‘dilution’ occurs because few holes are distributed over many \( k \)-points with almost the same energy. A marginal next-nearest-neighbor hopping term \( t' \) may be included in the Hamiltonian to lift this degeneracy (see §5): The negative sign of \( t' \), in particular, favors hole occupancy of \( k=(\pi,0) \) which has a low multiplicity favorable for avoiding the additional dilution. Moreover, in the 16-site cluster, this term breaks the spurious symmetry due to the mapping of a \( 2^4 \) hypercube and selects a unique two-hole ground state with momentum \( (0,0) \).

3. Rigid-Band Picture

The RBA states that, upon doping, the chemical potential shifts across the quasiparticle band at half filling, while no change occurs in the quasiparticle band structure; the lowermost peaks of the IPES spectrum for the doped case are identical as the uppermost states in the PES spectrum for the undoped case. Let us see whether this is realized in the spectra obtained by the exact diagonalization.
Figure 1 compares $A(k, \omega)$ in the half-filled and two-hole ground states for all allowed momenta in the 16- and 18-site clusters. We find that along the $(1, 1)$ direction, where the pair wave function $\Delta(k)$ vanishes, there is a striking similarity between the PES spectra near the Fermi energy $E_F$ for the doped and undoped cases: a band of peaks with practically identical dispersion and weight can be clearly identified in both groups of spectra [a possible exception is $(2\pi/3, 2\pi/3)$: the single-hole ground states of this momenta and $(\pi, \pi)$ have total spin $S=3/2$]. Away from $(1, 1)$, doping leads to a shift of weight from the PES band to IPES peaks immediately above $E_F$; as expected from the symmetry of $\Delta(k)$, this shift is most pronounced near $(\pi, 0)$ (see B of §2). The results for the 20-site cluster also indicate the same similarity between the low-energy parts of the PES spectra for the doped and undoped cases: the dominant low-energy PES peaks near $E_F$ remain either unaffected or (partially) cross the chemical potential to reappear as lowest-energy IPES peaks. At energies remote from $E_F$ (and thus unrelated to any low-energy physics), there is a reshuffling of incoherent spectral weight [pronounced addition at $(0, 0)$ and depletion at $(\pi, \pi)$], which causes the formation of a ‘large FS’-like $n(k)$.

Fig. 1. Comparison of the photoemission spectra at half filling and in the ground state with two holes: $A_0^-(k, -\omega)$ (solid line), $A_{-2}^-(k, -\omega)$ (dotted line), and $A_{-2}^+(k, \omega)$ (dot-dashed line) for the 16- and 18-site clusters with $J/t=0.4$ are shown. The Fermi energy is marked by the vertical line, and $\delta$ functions have been replaced by Lorentzian of width $0.1t$.

A quantitative check of the validity of RBA is to see whether the lowest-energy IPES peaks in the two-hole ground state exactly observe the single-hole quasiparticle band observed in PES at half filling. We choose $E_0^{(2)}$ as the ‘ground-state’ energy in the PES spectrum at half-filling and do not invert the sign of $\omega$: we can thus make a direct comparison of the positions of peaks in this spectrum and in the IPES spectrum for the two-hole ground state because both spectra involve the single-hole subspace in their final states. The calculated results in the 16-, 18-, and 20-site clusters confirm that the final states for the lowest IPES peaks at all momenta off the $(1, 1)$ direction indeed belong
to the single-hole band observed in PES spectrum at half filling within an accuracy of $10^{-10}t$ [there is no low-energy IPES peak along the $(1,1)$ direction because $\delta(k)=0$ (see B in §2)]. It is only at higher energies ($\sim J$ above the quasiparticle states) that there is a significant difference in the spectra. Note that this result is in clear contradiction to the ‘large FS’ scenario: this would necessitate the assumption that the uppermost states of the next-nearest-neighbor hopping band at half filling simultaneously belong to a topologically different nearest-neighbor hopping band obtained under a ‘full-scale transition’ upon doping of two holes.

Another quantitative check of the RBA is to compare the spectral weight of the peaks near $E_F$. Figure 2 (a) compares the weight of the peak at $(\pi/2, \pi/2)$ in $A_0^-(k,\omega)$ [which has the same weight at $(\pi,0)$] and $A_2^-(k,\omega)$ as well as the sum of the weights of the lowest peak in $A_2^+(k,\omega)$ and highest peak in $A_2^-(k,-\omega)$ at $(\pi,0)$ [which are in the ‘split-peak’ situation]. The RBA predicts all three quantities to be equal, and as seen in Fig. 2 (a), they are indeed agree remarkably well over a wide range of $t/J$.

The quasiparticle band structure near $E_F$ is summarized in Fig. 2 (b): The dispersion in the two-hole states agree very well with that of the half-filled band, as the RBA predicts. Also, comparing Fig. 1 with 2 (b), we note an obvious correlation between the quasiparticle peak intensity and the distance from $E_F$, as one would expect for a Fermi liquid. Due to the interaction between the holes, there is no FS but rather a zone of partially occupied momenta where the quasiparticle peaks are split between PES and IPES. However, the obvious validity of the RBA suggests that, if the FS exists at all, it takes the form of small hole pockets, although, due to the near degeneracy of the states on the surface of the AFBZ, the precise location of the pockets are decided by the interaction between holes. Along the $(1,1)$ direction, another band of many-body states with intrinsic $d_{x^2-y^2}$ symmetry is also identified (see Ref. [1] for details): this band has almost no dispersion and remains $\sim 2J$ above $E_F$, and thus is unrelated to any low-energy physics.
We construct a ‘spin-bag’ operator to describe the low-energy states thus found near $E_F$, in terms of elementary excitations, i.e., weakly or moderately interacting quasi-particles, whereby the spectral function becomes an almost free-particle form with the incoherent continua being removed and the peaks near $E_F$ being enhanced. Because a ‘single-hole problem’ can be described well by the string picture where the hole is dressed by antiferromagnetic spin fluctuation, we make the ansatz for the operator:

$$\tilde{\psi}_{k\sigma} = \sum_{\lambda=0}^{\lambda_{\text{max}}} \alpha_{\lambda}(k) A_{\lambda}(k)$$

where $A_{\lambda}(k)$ is the Fourier transform of $A_{\lambda}(R_j)$ which creates all strings of length $\lambda$ around site $j$ when acting on the Néel state (see Ref. [2] for details). From the spectral functions for $\tilde{\psi}_{k\sigma}$ with coefficients $\alpha_{\lambda}$ determined variationally, we find the following: (i) The spin-bag operator optimized at half filling works well even for the two-hole case: this suggests the continuity in the development of low-energy states upon doping to the single-hole problem in an antiferromagnet. (ii) The Pauli principle works for the spin-bag operator: in the spectrum of adding a bag with up-spin from the one-hole ground state [containing 8 up-spin and 7 down-spin electrons in the 16-site cluster] at momentum $(\pi/2, \pi/2)$, there is a large elimination of the incoherent continua and enhancement of the peaks at $E_F$, whereas in the spectrum of adding a bag with down-spin, the hole pocket is clearly seen at $(\pi/2, \pi/2)$. (iii) The degree of broadening of the spin-bag peaks is reminiscent of a Fermi liquid: there are sharp peaks close to $E_F$ and diffuse peaks at lower energies. (iv) We find an approximate adjoint (or spin-bag annihilation) operator which works well to simplify the IPES spectrum. Thus, all in all the doped cluster behaves very much like a system of weakly interacting ‘effective Fermions’ corresponding to the doped holes.

4. Hole Pockets

We now present evidence that the FS as deduced from the momentum distribution function takes the form of small hole pockets. We first note that the magnitude of the Fermi-edge discontinuity in $n(k)$ has to be equal to the weight $Z_h$ of the quasiparticle peak in $A(k, \omega)$. Then, to identify the FS, we can take advantage of the fact that $Z_h$ has a pronounced (and characteristic) dependence on $t/J$ [13]: i.e., a potential FS discontinuity must have the same characteristic dependence on $t/J$.

Figure 3 (a) shows $n(k)$ calculated for the single-hole ground state with momentum $k_0=\langle \pi/2, \pi/2 \rangle$. We find the $k$-dependence roughly consistent with free electrons, i.e., larger near $(0,0)$ and smaller near $(\pi, \pi)$, which ensures the negative kinetic energy (see §2), and also we note a dip at $k_0$ for the minority-spin $n(k)$. The question arises which of these features should be associated with the FS: do we have a ‘large FS’ already for a single hole or is there a ‘hole pocket’ at $k_0$? Figure 3 (b) shows a comparison between the ‘depth’ of the dip at $k_0$ ($\Delta_{\text{dip}}$) [estimated by forming the difference in $n(k)$ with a symmetry equivalent $k$ point] and the weight of the quasiparticle peak [obtained from the single-particle spectral function for momentum transfer $k_0$ at half filling] for various values of $t/J$. Obviously, $\Delta_{\text{dip}}=Z_h$ over the entire range of $t/J$, so that the dip clearly originates from the Fermi level crossing of the quasiparticle band, i.e., we have a hole pocket at $k_0$. On the other hand, differences $\Delta n(k)$ across the ‘large FS’ always show the opposite behavior under a variation of $t/J$ as $Z_h$, indicating that these drops in $n(k)$ are unrelated to any FS crossing; it seems reasonable to associate this structure in $n(k)$ with the well-known backflow for interacting Fermi systems [14].

Let us proceed to the two-hole case. A free-electron–like variation of $n(k)$ is clearly seen in, e.g., the 20-site cluster and thus one would be tempted to assign this to the existence of a ‘Luttinger FS’ by adopting a criterion like $n(k)>1/2$ [12]. However, such a
Fig. 3. (a) Momentum distribution for the single-hole ground state with \( S_z = 1/2 \) (i.e., with a ‘down’ hole) for the 16-site cluster with \( t/J = 4 \) (upper panel) and \( t/J = 1 \) (lower panel). The upper (lower) values in the lists refer to the majority (minority) spin, and the ground-state momentum \( k_0 \) is marked by a black box and \( k_0 + (\pi, \pi) \) by a dotted box. (b) Comparison of the \( t/J \) dependence of \( Z_h \) at half filling (dark squares) and various differences \( \Delta n(k) \) in the single-hole ground states with \( S_z = 1/2 \). Shown is the ‘depth’ of the pockets (light circles) and differences across the ‘large FS’ (up and down triangles).

Luttinger FS is ruled out by the same arguments as for a single hole: Fig. 4 (b) compares between the \( t/J \) dependence of \( \Delta n(k) \) across the respective Luttinger FS and that of the quasiparticle weight \( Z_h \) in the spectral function for the two-hole ground state. \( Z_h \) decreases sharply, while \( \Delta n(k) \) increase monotonically with \( t/J \). Thus, the drop in \( n(k) \) upon crossing the ‘large FS’ is obviously unrelated to any true Fermi-level crossing. We note [3] that, if we assume that the backflow contribution for the two holes is simply additive of that for the single hole, the magnitude and \( t/J \) scaling of \( \Delta n(k) \) can be explained very well.

Thus, we expect that the hole pocket is superimposed over the smooth backflow contribution as in the single-hole case, only with the additional complication that the pockets are now ‘washed out’ due to the interaction between holes. Hence, \( n(k) \) may be written as

\[
n(k) = n_{\text{back}}(k) - Z_h \cdot |\Delta(k)|^2
\]

with the pair wave function \( \Delta(k) \) introduced in Eq. (4). Because the calculated results suggests that to a good approximation the backflow contribution \( n_{\text{back}}(k) \) is a function of \( |k_x| + |k_y| \) only (see, e.g., Fig. 3 (a)), this contribution can be eliminated by forming the difference of two momenta with (almost) equal \( |k_x| + |k_y| \). Next, if we choose one of these momenta along (or near) the \((1, 1)\) direction [where \( \Delta(k) \) vanishes (or is small)] and the other at (or near) \((\pi, 0)\), we should obtain \( \Delta n(k) = Z_h \cdot |\Delta(\pi, 0)|^2 \), so that, in contrast to the ‘large FS’ differences indicated in Fig. 4 (b), this difference should scale with \( Z_h \). To check this prediction, the \( t/J \) dependence of various such differences is shown in Fig. 4 (c): obviously, to an excellent approximation, they are proportional to \( Z_h \) over a wide range of \( t/J \). The scaling of \( n(k) \) with \( t/J \) is thus completely consistent with the assumptions that (i) there are washed-out hole pockets at \((\pi, 0)\) and (ii) these are
superimposed over the smooth backflow contribution which is the sum of the backflows for the two individual holes.

Now the last question would be whether one can really make the true FS visible in the structure of \( n(k) \). The answer is simply to circumvent the problems listed in A, B, and C of §2: For A, since diagonalization studies have shown that \( Z_h \approx 1 \) for the parameter region \( J > \sim t \), we choose \( J/t = 1 \) and 2. For B, we introduce a density repulsion term \( H_V = V \sum_{\langle ij \rangle} n_i n_j \) and adjust \( V \)-value so as to cancel the intrinsic attractive interaction between holes and obtain homogeneous distribution of holes. And for C, we introduce a next-nearest-neighbor hopping term with a fixed strength \( t' = -0.1t \) to lift the (near) degeneracy of the momenta along the surface of the AFBZ. Thus, we have the ‘ideal’ situation for observing the FS: large Fermi-edge discontinuity, weak interaction, and a unique single-hole ground state. The results are shown in Fig. 5: In the spectral function, \( E_F \) is located near the top but within a group of pronounced peaks which are well separated from another such group in the IPES spectrum. There are pronounced peaks both immediately above and below \( E_F \) which comprise the bulk of spectral weight for each momentum, indicating well-defined quasiparticle peaks. Correspondingly, \( n(k) \) exhibits a sharp variation: i.e., there are hole pockets at \( (\pi, 0) \) and \( (0, \pi) \). They are superimposed over the familiar backflow contribution, which again has the generic free-electron–like form to ensure negative kinetic energy. Figure 5 also gives the values of the quasiparticle weight at the ‘Fermi momenta’: we note that the depth of the pockets approximately equals \( Z_h \) and both quantities consistently decrease with decreasing \( J/t \). The location of the pockets at \( (\pi, 0) \) rather than at \( (\pi/2, \pi/2) \) might be somehow surprising. This can be traced back to the point-group symmetry of the two-hole ground state: when the symmetry of the ground state at half filling is \( A_1 \) (or \( s \)), that of the two-hole ground state is \( B_1 \) (or \( d_{x^2-y^2} \) and vice versa. Thus, addition of two holes is equivalent to adding an object with \( d_{x^2-y^2} \) symmetry. This implies that the pair wave function \( \Delta(k) \) in Eq. (4) should have this symmetry as well, and in turn implies that \( \Delta(k)=0 \) for all \( k \)-s along the
Fig. 5. (a) Single-particle spectral function for the $t-t'-J-V$ model with two holes: $J/t=2$ and $V/t=2.5$ (2.4) are used for the 20-site (16-site) cluster. The upper four rows refer to the 20-site cluster, and the lower three rows to the 16-site cluster. The frequency region $\omega<0$ ($\omega>0$) corresponds to the PES (IPES) spectrum. Delta functions have been replaced by Lorentzian of width $0.05t$. (b) Momentum distribution in the two-hole ground state of the $t-t'-J-V$ model. In the upper panel, $J/t=2$ and $V/t=2.5$ (2.4) are used for the 20-site (16-site) cluster, and in the lower panel, $J/t=1$ and $V/t=3.0$ (2.0) are used for the 20-site (16-site) cluster. For the ‘Fermi momenta’, the quasiparticle weight $Z_h$ is given in brackets.

(1,1) direction, so that the hole occupation of $(\pi,0)$ is favored.

A possible explanation for the hole-pocket FS could be spin-density-wave–type broken symmetry: although the ground states under consideration are spin singlets, this might be realized if the fluctuations of the staggered magnetization $M_s$ were slow as compared to the hole motion, so that the holes move under the influence of an ‘adiabatically varying’ staggered field. A possible criterion for this situation would be $\tau_{tr} \cdot \omega_{AF} \ll 2\pi$, where $\tau_{tr}$ is the time it takes for a hole to transverse the cluster and $\omega_{AF}$ is the frequency of fluctuations of $M_s$. We estimate (for $J/t=2$) the group velocity of the holes from the dispersion of the ‘quasiparticle peak’ in the PES spectrum [i.e., from the energies indicated by arrows in Fig. 5 (a) for the 20-site cluster and the peaks at $(\pi/2,0)$ and $(\pi/2,\pi/2)$ for the 16-site cluster] and find $\tau_{tr} \simeq 2\pi/0.5t$ (or $\simeq 2\pi/0.2t$) for the 20-site (or 16-site) cluster. Typical frequencies for fluctuations of $M_s$ can be obtained from its correlation function, which, up to a constant, equals the dynamical spin susceptibility for momentum transfer $(\pi,\pi)$; a rigorous lower bound on $\omega_{AF}$ thus can be obtained by subtracting the ground state energy from the energy of the lowest state with total momentum $(\pi,\pi)$ with the same point-group symmetry as the ground state. This gives $\omega_{AF} > 0.9t$ (or $1.2t$) for the 20-site (or 16-site) cluster, i.e., $\tau_{tr} \cdot \omega_{AF} > 2\pi$. ‘Almost static’ Néel order can thus be ruled out as origin of the small FS, even for this fairly large value of $J/t$.

As an additional check, we have introduced exchange terms $J'$ between second- and third-nearest neighbors to reduce the spin correlations and again optimized the density repulsion term to enable ‘free’ hole motion. For this (highly artificial) model, we calculate the momentum distribution, density correlation function $g(R)$ for holes,
and spin correlation function $S(R)$. We find [3] that the density correlation function is homogeneous (i.e., no charge ordering), the spin correlations decay rapidly (i.e., no long-range AF or spiral ordering), but still there are unambiguous hole pockets in $n(k)$. The only possible conclusion is that it is solely the large $Z_h$ that makes the pockets visible in the large $J/t$ region, and not the onset of any kind of ordering.

While the hole pockets can be made clearly visible for large $J$, the situation is more involved for $t>J$. In this parameter region, the small overlap between 'quasiparticle' and 'bare hole' (as manifested by the small $Z_h$) makes the $V$-term (which couples only to the bare hole) increasingly inefficient in enforcing a noninteracting state: the two holes remain bound on second-nearest neighbors up to fairly large values of $V$. However, because the scaling of $\Delta n(k)$ with $t/J$ works very well over a wide range of $t/J$ as we have shown above and also because the overlap of the ground-state wave function with that at $J/t=1$ indicates no significant drop over $J/t=2−0.2$, it seems reasonable to accept the continuity of the presence of hole pockets to the physically realistic (smaller $J/t$-parameter) regime.

5. Comparison with Other Numerical Studies and Experiment

While we have shown the validity of RBA, the presence of hole-pocket FS, and the spin-bag description for the quasiparticles, their evidence is based solely on small-cluster studies. A comparison with other numerical calculations and experiments on cuprate (and other) materials is therefore necessary. As far as numerical studies on small clusters are concerned, hole pockets and/or rigid-band behavior upon doping have been continually suggested: Poilblanc and Dagotto [15] studied the PES spectrum for single-hole states in the $t-J$ model and concluded that the two-hole ground state in the 16-site cluster shows hole pockets at $(\pi,0)$, in agreement with the present results. Castillo and Balseiro [16] computed the Hall constant and found its sign near half filling to be consistent with a hole-like FS, i.e., with hole pockets. Gooding et al. [17] studied the doping dependence of the spin correlation function in clusters with special geometry and also found indications of rigid-band behavior. The situation is quite similar for the Hubbard model: While the generic free-electron–like shape of $n(k)$ found in earlier Monte Carlo studies was initially considered as evidence against hole pockets, more careful and systematic analysis [11] showed that hole pockets are in fact remarkably consistent with the numerical data, their nonobservation in the earlier studies being simply the consequence of thermal smearing. It seems fair to say that the available numerical results for small clusters of both Hubbard and $t-J$ models, when interpreted with care, are all consistent with the RBA and/or hole-pocket FS.

Let us next discuss experimental results on high-temperature superconductors assuming that the hole pockets found in the cluster studies persist in the real materials. The volume of the FS associated with bands for the CuO$_2$ plane presents a well-known puzzle: Early ARPES experiments show bands which disperse towards the Fermi energy and vanish at points in k-space which are roughly located on the free-electron FS corresponding to electron density $1−\delta$, where $\delta$ is the hole concentration. Transport properties, on the other hand, can be modeled well [4,5] by assuming an FS with a volume $\sim \delta$. In a Fermi liquid, these apparently contradicting quantities actually fall into distinct classes: PES spectra depend on $Z_h$, transport properties do not. Hence, if one wants to resolve the discrepancy entirely within a Fermi-liquid–like picture, the simplest way would be to assume a ‘small FS’ and explain the PES results by a systematic variation of $Z_h$ along the band which forms the FS, similar to the ‘shadow band’ picture [18]. A trivial argument for such strong k-dependence of the quasiparticle weight is that a distribution of PES weight in the Brillouin zone (and hence $n(k)$) that resembles the noninteracting FS always optimizes the expectation value of the kinetic energy, and therefore it is favorable if those parts of the band structure, which lie inside the free-electron FS, have large spectral weight, and the parts outside have small weight. Then, it is noticed that, in a
recent ARPES study by Aebi et al. [6], spectral structures which are very consistent with such a shadow-band scenario have indeed been observed. Moreover, another key feature of the dispersion relation for a single hole, namely the extended flat region near \((\pi, 0)\) (see Fig. 2 (b)), has also been found as a universal feature of high-temperature superconductors [19–21]. Thus, adopting a rigid band/hole pocket scenario would explain many experiments in a very simple and natural way, which is moreover remarkably consistent with the existing numerical data as a whole. A recent finding of noncooper quasi-2D materials exhibiting similar anomalies to cuprates [22] seems to suggest that features discussed above should be generic and common to a class of doped Mott insulators.

6. Conclusions

We have performed a detailed study of the doping dependence of the single-particle spectral function and momentum distribution function up to the largest clusters that are numerically tractable. The results show unambiguously that the rigid-band behavior is realized in small clusters of the \(t-J\) 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. We have discussed the problems in directly determining the Fermi surface from the momentum distribution function and made a situation where they are largely avoided; then we found clear signatures of a Fermi surface which takes the form of small hole pockets. Both the high degree of continuity of the ground-state wave function with decreasing \(J/t\) and the identical scaling with \(t/J\) of the quasiparticle weight \(Z_h\) and difference in \(\alpha(k)\) between neighboring \(k\)-points suggest the existence of such a Fermi surface also in the physical regime of parameters. We have also found the spin-bag operators which describe the holes dressed by the antiferromagnetic spin fluctuations, whereby elementary excitations of the system can be described in terms of weakly-interacting spin-1/2 Fermionic quasiparticles, corresponding to the doped holes. We have discussed that adopting this rather conventional Fermi-liquid scenario would explain many experimental results for high-temperature superconductors in a very simple and natural way.

If one adopts the above Fermi-liquid picture, it seems natural to distinguish between two types of spin excitations: the first is the particle-hole excitation of the ‘hole liquid’, which should resemble that of a Fermi liquid with a Fermi-surface volume corresponding to the number of doped holes. In addition, there are the excitations of the ‘spin background’, which may, with some modifications, resemble the spin-wave collective mode of the Heisenberg antiferromagnet. The former part of the excitations can quantitatively explain the Pauli susceptibility at low temperatures and the latter can explain the dynamical spin correlations at momentum transfer \((\pi, \pi)\) observed in neutron scattering experiments. The charge excitation spectrum, on the other hand, resolves the internal structure of the spin bags and observes the bare-hole excitation within the bags, leading also to relevant physics in cuprate materials. In the doping region over \(\sim 30\%\), the spin and charge excitation spectra as well as the single-particle excitation spectrum become consistent with those of noninteracting systems with a large electronic Fermi surface. Details have been discussed in Refs. [23,24].

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