Spectral functions of lightly doped antiferromagnets using dressed hole operators

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Literature addressing the existence of ''hole pockets'' in experiments for the high-T_c cuprates and in theoretical analysis of electronic models of correlated electrons is reviewed. It is argued that the issue is not conclusively resolved, both in theory and experiments. The apparently large Fermi surface observed in numerical studies of the doped Hubbard and t-J models suggests the presence of $1-x$ carriers (with x the concentration of holes). However, this is in contradiction with results obtained in similar calculations for the Drude weight which scales with x at low doping. To address such a paradox, *dressed* operators are here used. Their spectral decomposition $A(\mathbf{k},\omega)$ is analyzed specially using the t-J model on ladders, but considering also chains and two-dimensional (2D) clusters. The results are contrasted against those obtained with the standard *bare* operators. It is concluded that substantial changes in the spectral weight can occur by replacing the bare hole creation operator by its dressed version. Apparently large Fermi surfaces can turn into small ones by working with quasiparticle (qp) operators that represent accurately the state of one hole. Thus, large Fermi surfaces in angle-resolved photoemission (ARPES), obtained by the sudden removal of an electron, may not be in contradiction with a visualization of the normal state of lightly doped antiferromagnets as composed of a gas of spin polarons with energies approximately obtained from the rigid band doping of the half-filled dispersion. The coexistence of a large Fermi surface in ARPES with, e.g., a holelike Hall coefficient seems possible in systems with strong correlations. In this paper the expression ''hole pocket'' is used as representing a large accumulation of spectral weight centered at $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ generated by antiferromagnetic correlations in 2D clusters, or in analogous positions for ladders and chains. The subtle issue of whether such hole pockets represent a true small Fermi surface or just large incoherent weight cannot be addressed with finite resolution techniques such as angle-resolved photoemission and numerical studies of electronic models. They only provide information about the location of the dominant weight in $A(\mathbf{k},\omega)$. The ideas discussed here are very general and they can be applied to a variety of problems where quasiparticles are strongly dressed by low energy excitations of the medium in which they are immersed. [S0163-1829(97)03821-6]

I. INTRODUCTION

A. Experiments and theory on hole pockets: Present status

Angle-resolved photoemission (ARPES) experiments continue providing important information for the understanding of the normal and superconducting states of the high critical temperature superconductors.[1] Among the interesting results observed with ARPES in this context is the discovery of flat bands in the neighborhood of $\mathbf{k}=(\pi,0)$, in the two-dimensional (2D) square lattice notation, for a variety of optimally doped compounds.[2–4] These results show the relevance of strong electronic correlations within the planes to properly describe the cuprates. In addition, the dispersion of a hole in an antiferromagnet has been addressed with ARPES through experiments in $Sr_2O_2Cl_2$,[5,6] allowing a comparison with predictions obtained from the t-J and other electronic models for the cuprates at half-filling.[7] Then, both the undoped and optimally doped limits have been studied and the next step is the analysis of the evolution of one result into another as the density of holes is smoothly changed in the underdoped regime. Recently, progress in this direction has been reported in a study of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) by Marshall and collaborators[8] (see also Ref. 9). While along the $\Gamma=(0,0)$ to $M=(\pi,\pi)$ direction the quasiparticle dispersion does not change much with doping, the region near $X=(\pi,0)$ is substantially affected. As the hole doping x grows from zero, the flat quasiparticle band near $(\pi,0)$ moves up in energy towards the Fermi energy which is approximately reached at optimal doping. At very low hole density the flat band at X is 0.2 eV below the chemical potential. These results are supplemented by information along the $X-M$ direction showing that the band crossing of the Fermi level observed at optimal doping actually disappears in the underdoped regime. A possible explanation of the results presented in Ref. 8 involves the presence of ''hole pockets'' induced by antiferromagnetic correlations which are features centered at $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ for x smaller than optimal. It is important to remark that half the pocket (i.e., the region lying at momenta the closest to (π,π) which here is referred to as the ''outside'' part of the pocket) has not been observed experimentally (see Fig. 1). This may be caused by its small intensity. Actually ARPES data for optimally doped Bi2212 obtained by Aebi *et al.* using a technique with high resolution in momentum space have shown features that are compatible with *full* small hole pockets, i.e., with a nonzero signal for both the outside and inside regions of the pocket.[10,11] However, certainly the intensity outside is much smaller than the intensity in the inside pocket wall [the

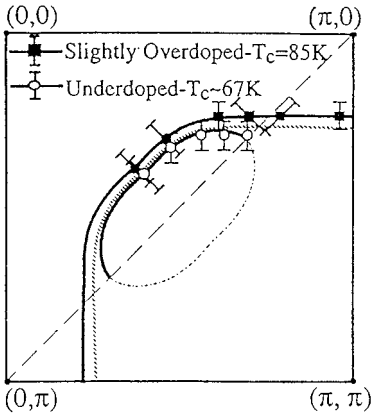

FIG. 1. ARPES results reproduced from Ref. 8. They show the Fermi level crossing of two Bi2212 samples of differing oxygen content (one corresponding to optimal doping and the other to the underdoped regime). The entire BZ can be reconstructed by four-fold rotation about (0,0).

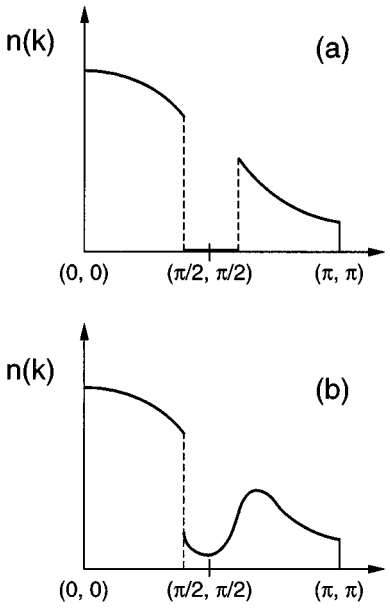

FIG. 2. (a) Schematic representation of $n(\mathbf{k})$ along the diagonal $\Gamma - M$ as predicted by theories with hole pockets (such as those based on the spin-density-wave mean-field approximation), i.e., filling rigidly the quasiparticle dispersion obtained at half-filling. For an actual calculation using a variational state based on the string picture see Fig. 3 of Ref. 22, and using a spin-density-wave mean-field approximation see Ref. 23; (b) Possible behavior of $n(\mathbf{k})$ if an accurate many-body calculation would be implemented for the 2D t-J or Hubbard models. Now the second discontinuity has been replaced by an accumulation of weight.

closest to $(0,0)$] and, in addition, superstructural effects may contaminate the data. Complicating matters further, note that studies of $YBa_2Cu_3O_{6+\delta}$, with $0.2 \leqslant \delta \leqslant 0.9$, by Liu *et al.*[12] do not report appreciable changes in the hole dispersion near X in a wide range of densities contrary to what occurs for Bi2212.[8] More recently, studies by Ding *et al.*[13] found no evidence of small hole pockets in underdoped Bi2212 even in samples with a critical temperature as small as 15 K. Thus, the presence of pocket features in ARPES is still under much discussion.

Regarding the theoretical aspects of the problem, hole pockets have been mentioned since the early studies of holes injected in antiferromagnets.[14–16] These holes are sometimes visualized as spin polarons, i.e., formed by the actual vacancy plus a cloud of spin excitations that reduce the antiferromagnetic order parameter in its vicinity, as in spin-bag approaches.[17] The dispersion of just one hole in the two-dimensional Heisenberg model is accurately known using a variety of techniques.[18,19] The minimum of the hole band, or maximum of the valence band, is at $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ and thus at least naively a small but finite density of holes would populate this region creating the pockets mentioned above. Such rigid filling of hole states has appealing properties as noted by Trugman.[20] Recent effective models for the high-T_c cuprates, such as those used in the ''antiferromagnetic van Hove scenario,''[21] also describe the normal state as made out of weakly interacting quasiparticles with a dispersion calculated from numerical studies at half-filling.[18,19] Flat bands are observed as in experiments. Assuming a rigid filling of this band, reasonable results are obtained for superconductivity once a nearest-neighbor attraction is introduced in the problem to mimic the sharing of spin polarons effects (i.e., real space approach to hole pairing). As the density of holes increase, the pockets start overlapping and eventually the Fermi surface becomes large.[18,20] Thus, in this context a transition from a small to a large Fermi surface is predicted, in apparent agreement with the recent experiments of Marshall *et al.*[8]

However, there are several features of the hole pocket theories that are not satisfactory. First of all it is unclear up to what density it is reasonable to assume that the quasiparticle dispersion has not changed appreciably with respect to the half-filled result. This may occur only very close to the undoped limit. Second, from a rigorous point of view the rigid filling of the half-filled dispersion generates a small Fermi surface with a momentum distribution $n(\mathbf{k})=\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}\rangle$ having *two* discontinuities along the direction from $(0,0)$ to (π,π) [see Fig. 2(a)]. Similar results were obtained in an actual variational calculation based on the string picture by Eder and Becker,[22] and also using the spin-density-wave mean-field approximation by Duffy and Moreo.[23] These two singular points survive even at densities when the four pockets merge into one single structure, i.e., when the Fermi surface could be labeled as ''large.'' It is very unlikely that at large hole density in the real cuprates two such discontinuities along $\Gamma - M$ exist, and thus the pocket scenarios can only be accurate in the underdoped regime at best.

Even though mathematically indeed there are two discontinuities along $\Gamma - M$ in theories with hole pockets, we prefer to interpret these results as follows: if a high resolution calculation for electronic models could be possible it is likely that only one discontinuity in $n(\mathbf{k})$ along $\Gamma - M$ will be present, i.e., the large one close to Γ. However, in addition to this singularity, the presence of robust antiferromagnetic correlations in the system must produce features in the form of a large accumulation of spectral weight at the position where the second discontinuity in $n(\mathbf{k})$ exists in hole pocket approaches [as illustrated in Fig. 2(b)]. This is reasonable since no drastic changes can be expected in the distribution of

weight as the antiferromagnetic correlation length ξ_{AF} varies from ∞ (long range order) to a finite number, as long as it remains robust. Then, hole pocket theories may provide useful guidance for the location of important parts of the spectral weight in ARPES experiments once it is accepted that the second (likely spurious) discontinuity in $n(\mathbf{k})$ along $\Gamma - M$ may be replaced by a sharp crossover in more accurate calculations. Thus, below we will proceed with the analysis of hole pocket ideas and experimental results having this caveat in mind, i.e., in the rest of the paper the expression ''hole pocket'' will be used to refer to a large accumulation of spectral weight generated by short range antiferromagnetic correlations located in momentum space forming a small circle around $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ without any implication on the actual Fermi surface of the problem. This generalization of the term also avoids subtleties related with the Luttinger theorem in the Hubbard and t-J models,[24] and it is suitable for the finite resolution experimental techniques (ARPES) and numerical methods currently available.

Many numerical studies of the spectral weight in the literature have been interpreted as compatible with a large Fermi surface for hole densities $x\sim 0.12$ with only one large peak crossing the Fermi energy along the $\Gamma - M$ line and no vestige of the ''outside'' region of a hole pocket, not even in the form of incoherent weight.[25] However, these calculations have problems. For example, recent studies have shown that Monte Carlo simulations carried out at $U/t=4$ have not reached low enough temperatures to be able to address the presence of hole pockets.[23] In addition, studies at larger couplings supplemented by maximum entropy (ME) techniques to obtain dynamical properties are typically carried out at large temperature due to sign problems. Weight along $\Gamma - M$ above $\mathbf{k}=(\pi/2,\pi/2)$ could be easily missed since the pocket structure can only exist in the presence of strong antiferromagnetic fluctuations that can be washed out at large temperatures. Exact diagonalization methods applied to 2D finite clusters at zero temperature actually show the existence of weight in the region where the pockets are supposed to be located (i.e., ''shadow bands'' vestiges are observed in these studies).[26] However, finite size effects are difficult to control in this approximation. Thus, we believe that the issue of the presence of spectral weight in $A(\mathbf{k},\omega)$ at low temperature in the region where pockets are predicted is still unclear in models of correlated electrons with intermediate range antiferromagnetic fluctuations.

B. Paradox and possible solution

In principle, a large Fermi surface would correspond to $1-x$ conduction electrons. However, all numerical studies of the optical conductivity and the Drude weight D in Hubbard and t-J models have shown that $D\sim x$ in strong coupling and for small doping, i.e., the number of carriers is x rather than $1-x$.[14,27] This occurs up to hole densities as large as $\langle n\rangle = 1-x\sim 0.5$ (''quarter filling''), i.e., clearly in the region where $A(\mathbf{k},\omega)$ data are interpreted as corresponding to a large Fermi surface. These two results are apparently incompatible and such a paradox motivated the study presented in this paper. Not only 2D planes but also the recently much studied ladder systems[28] have a similar behavior[29–31] which seems to be general of models with short range antiferromagnetic fluctuations.

It is important to remark that also in experiments for the cuprates similar results are observed. Uchida *et al.* reported a Drude weight that grows linearly with the hole concentration away from the half-filled case.[32] Other $3d$ transition metals have a similar behavior.[33] In addition, Hall coefficient measurements for the cuprates at low temperature show that R_H changes sign at a very large hole density, implying hole-like behavior in the region where ARPES results indicate a large Fermi surface.[34]

A possible explanation of this paradox relies on the extended character of the hole quasiparticle. As explained before, a hole is not just a pointlike vacancy but also includes a finite region in its vicinity where the spins are distorted from its regular behavior far from the hole. For the purposes of this discussion the issue of whether the distortion decays rapidly with distance away from the empty site (polaron picture) or if it decays slowly as in some calculations, is not important since most of the contribution to the dressing arises from short distance properties, as long as the quasiparticle weight Z remains finite. The size of the distortion is actually a function of the ratio between the exchange J of the $S=1/2$ spins and the hopping amplitude t that regulates the hole kinetic energy, i.e., as J/t is reduced the size of the spin distortion grows and it can easily cover a few dozen sites even for realistic values of J/t.[14] On the other hand, the ARPES experiments are usually interpreted as the sudden creation of a vacancy by the removal of an electron. This abruptly created excitation is not a hole quasiparticle since the spin dressing is missing. Only after some time elapses the spin background can relax around the vacancy and the qp state is reached. The difference between the state created in ARPES and the actual ground state of the hole is reflected on the quasiparticle weight Z of the experimental ARPES peaks. If there is a large difference between a ''one-site'' bare vacancy and the actual dressed hole, then Z is small. Numerical studies of Z for realistic values of J/t in the t-J model have shown that this weight is indeed small namely ~ 0.3, if Z is defined such that $0\leqslant Z\leqslant 1$.[35,36] Then, important potential deviations exist between the actual hole qp and the excitation tested in ARPES experiments. The most important difference lies in the *intensity* of the peaks. In this paper it is conjectured, and numerical evidence supports the claim, that the intensity of the outside part of the hole pockets is negligible or rather small in ARPES and numerical simulations precisely due to the difference between *bare* and *dressed* hole states. In other words, if spin dressed hole states could be created experimentally or in the computational studies, then hole pockets features could be observed as high intensity structures in systems with robust antiferromagnetic correlations. Eder and Ohta arrived recently to similar conclusions.[37]

Note again that this paper does *not* intend to address the important issue of whether the zero-temperature Fermi surface of lightly doped antiferromagnets is small or large. For such a study it would be necessary to calculate $n(\mathbf{k})$ very accurately and search for discontinuities at particular momenta. This is beyond the accuracy of the many-body techniques currently available, both numerical and analytical.

The goal of the paper is more modest. It simply provides numerical information about the regions in energy and momentum where the ARPES and angle-resolved inverse photoemission (ARIPES) signals have the largest weight. In this respect it is here shown that a Fermi surface that apparently is ''large'' according to standard calculations of $A(\mathbf{k},\omega)$ can become ''small'' if the operator used to explore the subspace of N_e-1 electrons is dressed (where N_e is the number of electrons in the ground state).

II. QUASIPARTICLE OPERATORS

How do we proceed to construct the dressed hole operators and test these ideas numerically? The basic procedure was set up several years ago by Dagotto and Schrieffer[35] using string operators. Similar ideas were independently introduced by Eder, Becker and Stephan.[38] More recently Eder and Ohta[37] have implemented the method for two-dimensional (2D) clusters. Ideas from both Refs. 35 and 37 are used below in our discussion of ladders, chains, and planes. For completeness details on the construction of the dressed operators are here provided. It is intuitively clear that spin excitations need to be added to dress the hole vacancy. A variety of techniques have shown that ''strings'' are suitable excitations for this dressing.[14,39] Thus, the hole is injected at a given site **i**, and first allowed to propagate one lattice spacing to site **j** which brings one spin from **j** back to **i**. For a classical Néel state this spin is in the ''wrong'' spin-up-down sublattice, and for a quantum mechanical Néel state it is also in the wrong sublattice most of the time and thus it costs energy. Considering as an example a hole created by annihilating an electron with spin up, this effect can be introduced in the quasiparticle operator by replacing the bare hole operator by

$$\gamma^{\dagger}_{\mathbf{i}\uparrow}=\beta_0\overline{c_{\mathbf{i}\uparrow}}+\beta_1\sum_{\mathbf{j},\sigma}(\overline{c_{\mathbf{j}\sigma}}\,\overline{c^{\dagger}_{\mathbf{i}\sigma}})\overline{c_{\mathbf{i}\uparrow}}, \tag{1}$$

where the sites **j** are the nearest-neighbors (NN) of **i**, $\overline{c^{\dagger}_{\mathbf{i}\sigma}}$ and $\overline{c_{\mathbf{i}\sigma}}$ are creation and annihilation operators of electrons with spin σ. If the t-J model is considered, defining $\overline{c^{\dagger}_{\mathbf{i}\sigma}}=c^{\dagger}_{\mathbf{i}\sigma}(1-n_{\mathbf{i},-\sigma})$ enforces the constraint of no double occupancy. β_0 and β_1 are parameters which give the relative weight between the two components of the dressed operators. These parameters are determined variationally as discussed below. Equation (1) follows the original prescription of Ref. 35 to improve a bare operator. Eder and Ohta[37] used a slightly different approach which amounts to fixing σ to $\downarrow$ in Eq. (1).

Following similar ideas longer strings can be introduced. For example, string excitations of length 2 are included by adding in Eq. (1) the term $\Sigma_{\mathbf{j}',\sigma'}\Sigma_{\mathbf{j},\sigma}(\overline{c_{\mathbf{j}'\sigma'}}\,\overline{c^{\dagger}_{\mathbf{j}\sigma'}})(\overline{c_{\mathbf{j}\sigma}}\,\overline{c^{\dagger}_{\mathbf{i}\sigma}})\overline{c_{\mathbf{i}\uparrow}}$, where **j** are NN sites of **i**, and **j**′ are NN sites of **j**. For each new string excitation another variational parameter must be introduced, and thus this term should be weighted by a parameter β_2.

The general expression for the dressed creation operator of a hole with string of length λ is

$$\gamma^{\dagger}_{\mathbf{i}\uparrow}=\sum_{\mu=0}^{\lambda}\beta_\mu\gamma^{(\mu)\dagger}_{\mathbf{i}\uparrow}, \tag{2}$$

where

$$\gamma^{(\mu)\dagger}_{\mathbf{i}\uparrow}=\sum_{\boldsymbol{l}_\mu,\sigma_\mu}\cdots\sum_{\boldsymbol{l}_1,\sigma_1}(\overline{c_{\boldsymbol{l}_\mu\sigma_\mu}}\,\overline{c^{\dagger}_{\boldsymbol{l}_{\mu-1}\sigma_\mu}})\cdots(\overline{c_{\boldsymbol{l}_1\sigma_1}}\,\overline{c^{\dagger}_{\mathbf{i}\sigma_1}})\overline{c_{\mathbf{i}\uparrow}}, \tag{3}$$

and $\boldsymbol{l}_n$ denote NN sites of $\boldsymbol{l}_{n-1}$ ($\boldsymbol{l}_0\equiv i$ and $\gamma^{(0)\dagger}_{\mathbf{i}\uparrow}\equiv\overline{c_{\mathbf{i}\uparrow}}$).

Actually the hole state should be in a plane wave state due to translational invariance and thus we are finally interested in

$$\gamma^{\dagger}_{\mathbf{k}\uparrow}=\sum_{\mathbf{i}}e^{i\mathbf{k}\cdot\mathbf{i}}\gamma^{\dagger}_{\mathbf{i}\uparrow}=\sum_{\mu=0}^{\lambda}\beta_\mu\gamma^{(\mu)\dagger}_{\mathbf{k}\uparrow}, \tag{4}$$

where $\gamma^{(\mu)\dagger}_{\mathbf{k}\uparrow}$ is the Fourier transformed of Eq. (3). In a similar way, the general expression for the dressed annihilation operator of a hole with string of length λ is

$$\gamma_{\mathbf{k}\uparrow}=\sum_{\mathbf{i}}e^{-i\mathbf{k}\cdot\mathbf{i}}\gamma_{\mathbf{i}\uparrow}, \tag{5}$$

$$\gamma_{\mathbf{i}\uparrow}=\sum_{\mu=0}^{\lambda}\beta'_\mu\gamma^{(\mu)}{}_{\mathbf{i}\uparrow}, \tag{6}$$

where $\gamma^{(\mu)}{}_{\mathbf{i}\uparrow}$ is the Hermitian conjugate of $\gamma^{(\mu)\dagger}_{\mathbf{i}\uparrow}$, given by Eq. (3).

In the results shown below strings of length $\lambda=3$ were considered. Thus, in both the one-dimensional and square lattices, the number of variational parameters β_μ to determine is 4. For ladders, it is necessary to consider different parameters for strings along the longitudinal and the transversal directions. It is easy to verify that the number of variational parameters is 10. Various criteria can be adopted to fix these parameters. One of them is to maximize the weight $Z_{0h\to1h}$ of the first pole found in the spectral decomposition of the dressed hole operator $\gamma^{\dagger}_{\mathbf{k}\uparrow}$ at half-filling defined as

$$Z_{0h\to1h}(\mathbf{k})=\frac{|\langle\Psi^{\mathrm{gs}}_{1h}|\gamma^{\dagger}_{\mathbf{k}\uparrow}|\Psi^{\mathrm{gs}}_{0h}\rangle|}{(\langle\Psi^{\mathrm{gs}}_{0h}|\gamma_{\mathbf{k}\uparrow}\gamma^{\dagger}_{\mathbf{k}\uparrow}|\Psi^{\mathrm{gs}}_{0h}\rangle)^{1/2}}, \tag{7}$$

where $|\Psi^{\mathrm{gs}}_{nh}\rangle$ is the normalized ground state in the subspace of nh holes. Alternatively, the β's could be chosen by minimizing the energy of the state with one dressed hole, $|\Psi_{1h}(\mathbf{k})\rangle=\gamma^{\dagger}_{\mathbf{k}\uparrow}|\Psi^{\mathrm{gs}}_{0h}\rangle$. In practice it was observed that both criteria lead to similar results. From these procedures it becomes quite apparent that the relative weights among the different length string contributions turn out to be momentum dependent. In our calculations we did not observe a systematic behavior worth discussing here regarding the actual optimal values of the parameters β's as the couplings, densities and cluster geometries were changed. Nevertheless we observed that there is no need to fine-tune these parameters to their best values to obtain accurate numbers. In other words, the β dependence of the results is in general mild.

In order to determine the parameters β'_μ, similar procedures were followed. That is, they could be selected by maximizing the weight:

$$Z_{1h\to0h}(\mathbf{k})=\frac{|\langle\Psi^{\mathrm{gs}}_{0h}|\Psi_{0h}(\mathbf{k})\rangle|}{(\langle\Psi_{0h}(\mathbf{k})|\Psi_{0h}(\mathbf{k})\rangle)^{1/2}}, \tag{8}$$

where $|\Psi_{0h}(\mathbf{k})\rangle=\gamma_{\mathbf{k}\uparrow}|\Psi^{\mathrm{gs}}_{1h}\rangle$, or by minimizing the energy

$$E_{0h}(\mathbf{k})=\frac{\langle\Psi_{0h}(\mathbf{k})|H|\Psi_{0h}(\mathbf{k})\rangle}{\langle\Psi_{0h}(\mathbf{k})|\Psi_{0h}(\mathbf{k})\rangle}, \tag{9}$$

where H is the Hamiltonian of the model (e.g., the t-J model defined below). These criteria adopted to determine the parameters β'_μ by relating the states of 0 and 1 holes are the closest to the idea of considering the operator $\gamma_{\mathbf{k}\uparrow}$ as the Hermitian conjugate of $\gamma^\dagger_{\mathbf{k}\uparrow}$. A different criterion has been adopted in Ref. 37. The set of parameters β_μ and β'_μ are completely determined, using either the overlap or the energy criteria, except for an overall constant that is fixed by normalizing the wave functions $\gamma^\dagger_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$ and $\gamma_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$, respectively. Another possibility is to adopt those parameters relative to β_0,β'_0.

The PES and IPES spectra for dressed operators are defined, respectively, as

$$A^{(-)}_{nh}(\mathbf{k},\omega)=\sum_\nu |\langle\Psi^\nu_{nh+1}|\gamma^\dagger_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle|^2\delta[\omega-(E^\nu_{nh+1}-E^{\rm gs}_{nh})], \tag{10}$$

$$A^{(+)}_{nh}(\mathbf{k},\omega)=\sum_\nu |\langle\Psi^\nu_{nh-1}|\gamma_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle|^2 \times\delta[\omega-(E^\nu_{nh-1}-E^{\rm gs}_{nh})],$$

where $\Psi^\nu_{nh\pm1}$ and $E^\nu_{nh\pm1}$ are the νth eigenstate and eigenenergy in the subspace with $(nh\pm1)$ holes. These spectral functions are completely determined once the parameters β,β' of the dressed operators have been calculated as explained before. Normalizing the states $\gamma^\dagger_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$ and $\gamma_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$ to 1, it is easy to see that $\int_{-\infty}^{\infty}A^{(\pm)}_{nh}(\mathbf{k},\omega)d\omega=1$.

It is important to notice that the standard sum rules for the density of states $N^{(\pm)}_{nh}(\omega)=(1/N)\Sigma_{\mathbf{k}}A^{(\pm)}_{nh}(\mathbf{k},\omega)$ (N = number of sites) using bare operators in the t-J model are usually stated as

$$\int_{-\infty}^{\infty}N^{(+)}_{nh,\rm bare}(\omega)d\omega=x,\quad \int_{-\infty}^{\infty}N^{(-)}_{nh,\rm bare}(\omega)d\omega=\frac{1-x}{2}, \tag{11}$$

where x is the doping fraction. These sum rules are no longer valid for dressed operators, even in the case where β_μ and β'_μ are defined relative to β_0 and β'_0, i.e., when the states $\gamma^\dagger_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$ and $\gamma_{\mathbf{k}\uparrow}|\Psi^{\rm gs}_{nh}\rangle$ are not normalized to 1. This is due to the fact that the anticonmutation relations for dressed operators differ from the anticonmutation relations for the bare operators $\overline{c_{\mathbf{i}\sigma}},\overline{c^\dagger_{\mathbf{i}\sigma}}$ for a string length greater than zero. This is reasonable since now the quasiparticle operators have a finite ''size'' and they behave as normal fermionic operators only when the excitations created by them are well separated from each other. The standard sum rules for individual moments using bare operators, namely

$$\int_{-\infty}^{\infty}[A^{(+)}_{nh,\rm bare}(\mathbf{k},\omega)+A^{(-)}_{nh,\rm bare}(\mathbf{k},\omega)]d\omega=\frac{1+x}{2}, \tag{12}$$

are also no longer satisfied for dressed operators with the normalizations discussed above.

Note that one could take advantage of the arbitrariness of the overall normalization of the parameters β_μ and β'_μ in such a way that $A^{(+)}_{nh}(\mathbf{k},\omega)$ and $A^{(-)}_{nh}(\mathbf{k},\omega)$ for dressed operators indeed satisfy the sum rules (11) and (12). Such a procedure would be appropriate if a detailed comparison with experimental results is intended, especially for the quantities $N^{(+)}_{nh}(\omega)$ and $N^{(-)}_{nh}(\omega)$. However, in the present work we have *not* carried out such a normalization of spectral functions since our main goal is to study the redistribution of weight, for each momentum, produced by the dressing of quasiparticles. Thus, in the results below the integral over ω of the PES and IPES spectra is 1 for each case, regardless of the density of holes and for *both* the bare and dressed operators.

III. MODEL AND TECHNIQUE

In this paper the t-J model is used for the calculations, which is defined as

$$H=J\sum_{\langle\mathbf{ij}\rangle}\left(\mathbf{S_i}\cdot\mathbf{S_j}-\frac{1}{4}n_in_j\right)-t\sum_{\langle\mathbf{ij}\rangle,\sigma}(\overline{c^\dagger_{\mathbf{i}\sigma}}\,\overline{c_{\mathbf{j}\sigma}}+\text{H.c.}), \tag{13}$$

in the standard notation. Note, however, that the main idea discussed here, namely that a possible transition from apparently large to apparently small Fermi surfaces can be achieved by changing bare to dressed hole operators, should be valid for a wide variety of models where spin or other type of fluctuations appreciably dress the bare vacancies. As geometrical setup for the present study 2D clusters, ladders and chains will be used. Of special importance will be the results in ladders since in this case sufficiently long clusters in the leg direction can be studied numerically. Certainly it would also be very important to carry calculations on doped 2D systems.[37] However, the linear size of these clusters may not be large enough to clearly disentangle real physics from size effects. In addition, a large body of literature[28] has shown that doped ladders and doped planes have very similar features and thus a study of ladders can shed light on the physics of planes as well.

The numerical technique used in this paper is exact diagonalization (ED) which allows for the study of dynamical properties of models of correlated electrons on finite clusters.[14] The calculation of the spectral functions, Eq. (10), is performed using the formalism of continued fraction expansion.[14] Although in principle the quasiparticle operators could be implemented in quantum Monte Carlo simulations, in practice the evaluation of static correlations in this context would involve expectation values in the ground state of a product of several fermionic creation and destruction operators. This observable will likely be very noisy (i.e., carrying large error bars) specially if there are ''sign'' problems in the simulations. In addition, the study of dynamical properties with maximum entropy techniques is still being developed and noisy signals dramatically decrease the reliability of the results. Thus, here our analysis is limited to the ED method.

IV. 2D CLUSTERS

Let us begin our study by considering two-dimensional clusters. In this case Eder and Ohta[37] have already performed calculations of the PES and IPES spectra for dressed operators following the quasiparticle ideas of Dagotto and

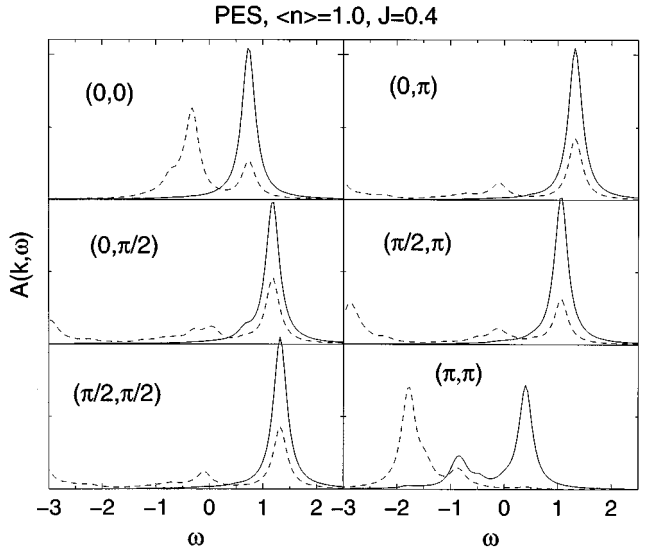

FIG. 3. PES spectral weight for the 2D t-J model at half-filling and $J=0.4$ ($t=1$) using a 4×4 cluster. The solid (dashed) lines correspond to dressed (bare) operators.

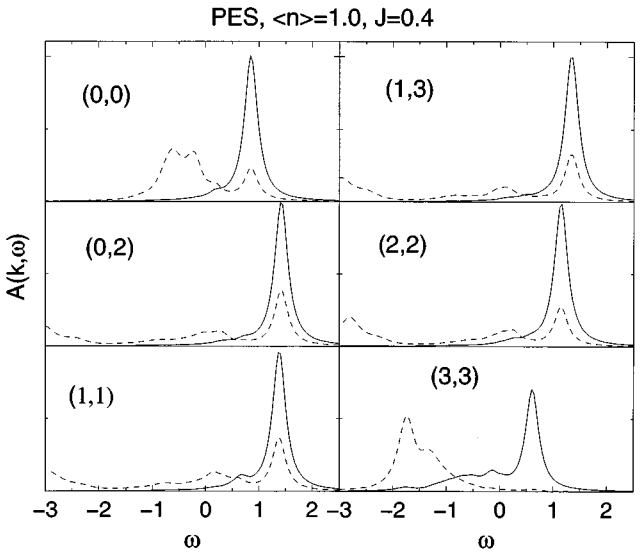

FIG. 4. Same as Fig. 3 but for a $\sqrt{18}\times\sqrt{18}$ cluster. The label of momenta is in units of $\pi/3$.

Schrieffer[35] discussed before. Since the dressed operators used here are not identically the same as theirs (although they are very similar) it is worth comparing our results with their predictions, at least for some special cases. In Fig. 3, the PES signal at half-filling obtained with the bare operators and the dressed operators Eqs. (1)–(3) is shown for a 4×4 cluster at $J/t=0.4$. In agreement with Ref. 37, and the intuitive expectations discussed in the Introduction, a substantial change in the weight distribution is observed here changing from bare to dressed operators. For momenta near the naive Fermi momentum, such as $(\pi/2,\pi/2)$ and $(0,\pi)$, the dominant peaks have grown substantially in weight indicating that the operatorial form of the dressed operator Eqs. (1)–(3) is suitable for this calculation (a ''bad'' operator would not have been able to increase the quasiparticle weight Z even with several free parameters in its definition).

Note specially the dramatic change in the distribution of weight near (π,π) in Fig. 3 (see also Ref. 37). The bare $A(\mathbf{k},\omega)$ corresponding to this momentum carries a negligible weight in its first pole. However, after dressing the hole by string excitations, this same pole becomes the dominant structure in the spectrum through a huge change in the quasiparticle weight. A similar situation occurs for momentum $(0,0)$. After the introduction of the dressed operators now the six momenta of Fig. 3 have peaks with similar intensities, quite different from the result found with the bare operators. In Fig. 4, similar results are shown using a tilted square cluster of 18 sites that allow us to test other momenta in the Brillouin zone. The effects are qualitatively the same as observed for the 16-site cluster. The dramatic change at (π,π) and $(0,0)$ remain. It was observed that increasing J/t, the peaks obtained with the bare operators increase their intensity, since the reduction in hole mobility makes the hole state resemble more a plain near-static vacancy. Nevertheless the use of qp operators still helps in increasing even further their intensity. At $J/t=1$ (not shown), it was observed that the changes are still quite substantial specially at momentum (π,π). Then, the study of half-filled 2D clusters presented here is in excellent agreement with the expectations discussed in the Introduction and also with previous literature.[37]

V. LADDERS

A. Undoped ladders

In Fig. 5, results corresponding to an undoped ladder at $J/t=0.3$ are shown. For the case of bare operators the PES spectral function previously presented in Ref. 31 is recovered. The first pole in the spectrum carries only a small fraction of the total weight. Especially for the antibonding band and $k=\pi$, and also for the bonding band and $k=0$, the bare weight at low energy is very small. This result qualitatively resembles those obtained at half-filling for the 2D cluster

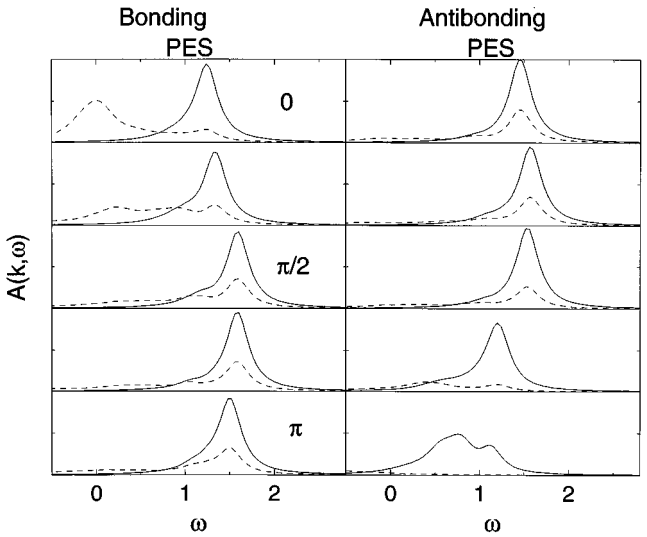

FIG. 5. PES spectral weight for the t-J model on a 2×8 ladder. $t=1$ is the unit of energy. The density is $\langle n\rangle=1$ and the Heisenberg coupling $J=0.3$. Bonding (antibonding) denotes results for momentum along the rung equal to 0 (π). The solid (dashed) lines are obtained with dressed (bare) operators.

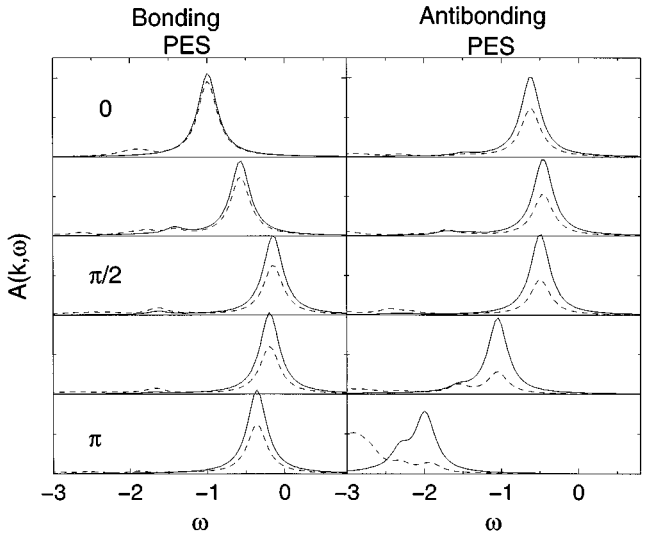

FIG. 6. Same as Fig. 5 but for $J=1.0$.

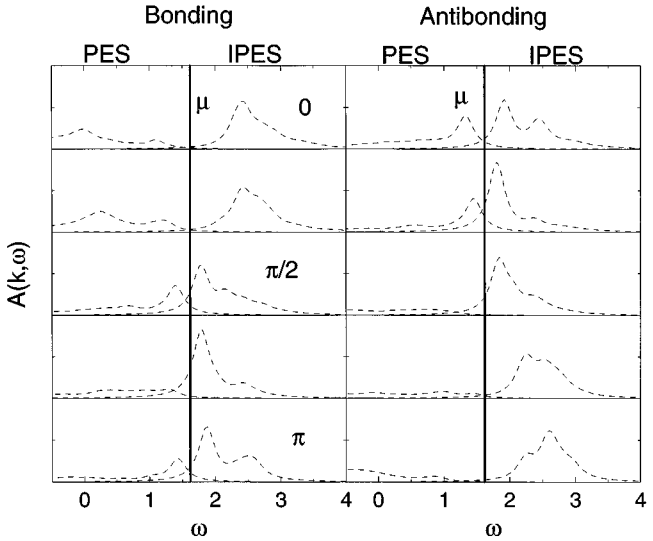

FIG. 7. PES and IPES spectral weight for the t-J model on a 2×8 ladder using *bare* operators. $t=1$ is the unit of energy. The density is $\langle n\rangle=0.875=2/16$ and the coupling $J=0.3$.

(Figs. 3 and 4). However, when the dressed operators are used a substantial rearrangement of the spectral weight occurs. The incoherent part of $A(\mathbf{k},\omega)$ is drastically reduced and most of the weight moves to the first pole in the spectrum. This occurs for all momenta, and specially dramatic is the improvement for the antibonding $k=\pi$ case where the region with negligible weight is replaced by a broad two-peak structure carrying most of the weight of the spectral function. For both bands there is now virtually no distinction between the different momenta.

Similar conclusions are reached for other values of the coupling J/t. In Fig. 6, results for $J/t=1$ are presented. At this large coupling most of the momenta already have a large peak dominating the spectral weight even when bare operators are employed, and the use of dressed operators simply increase that weight even further. An exception is once again the antibonding $k=\pi$ case where even at such large coupling, the bare operator fails to produce a robust peak at low energy. However, the dressed operator is here as effective as it was at $J/t=0.3$, and it produces for this band and momentum a peak as intense as for other momenta, similarly as it occurs in 2D clusters. Then, it is concluded that even though ladders do not have long range antiferromagnetic order, the short distance antiferromagnetic correlations are strong enough to influence on the propagation of holes. The success of the hole operator Eqs. (1)–(3) both for planes and ladders indirectly proves this statement.

B. Doped ladders

The most important results of this paper have been obtained for lightly doped ladder systems. It is here where the use of bare and dressed operators produces drastically different results regarding the large vs small character of the Fermi surface. In Figs. 7 and 8, the spectral functions obtained on a 2×8 cluster with two holes (i.e., $\langle n\rangle=0.875$), $t=1$ and $J=0.3$ are presented. Let us first consider the data corresponding to PES bare operators (Fig. 7):[29,31] here a large peak is observed near the chemical potential only at $k=\pi/2$ (bonding) and $k\leqslant\pi/4$ (antibonding). In the rest the weight is scattered in a large window of energy. For the IPES case, well-defined peaks appear near μ for several momenta in both the bonding and antibonding bands. Actually weight at energies $\sim1t$ above μ can be found in all cases. Especially notable is the antibonding $k=\pi$ spectrum where the PES part has a rather small weight at low energies, while on the contrary the IPES sector presents a large signal at $\omega\sim1t$ above μ. Taken at face value, these results suggest that in the antibonding case a quasiparticle band has crossed the chemical potential somewhere in the interval $\pi/4<k<\pi/2$. For the bonding band the situation is similar but with the crossing located in the vicinity of $k\sim\pi/2$. It is clear that inspecting by eye the numerical results obtained with bare operators would lead to the conclusion that the doped ladder has a large Fermi surface, i.e., the quasiparticle band crosses μ just once in both bands and it disperses into the IPES region.[29]

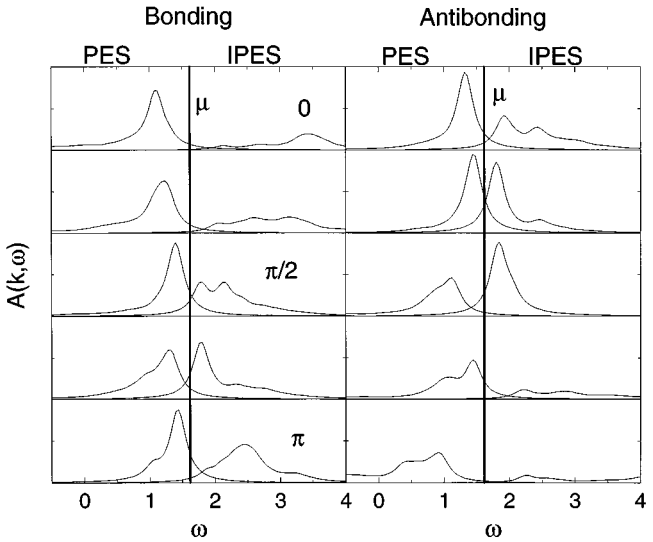

FIG. 8. Same as Fig. 7 but now for *dressed* operators.

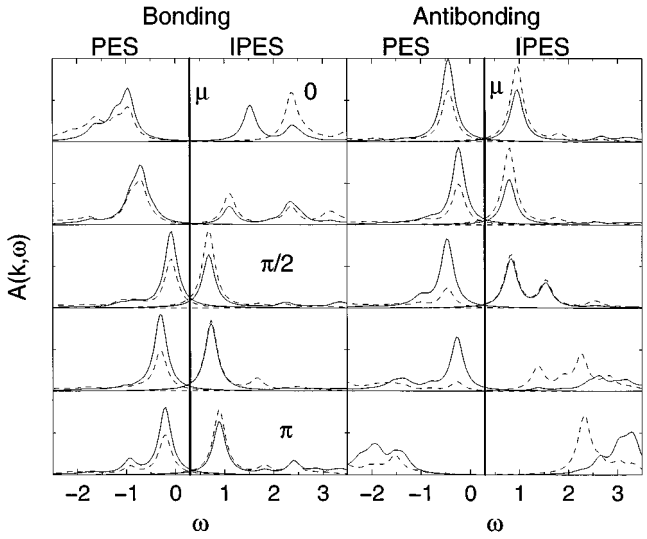

FIG. 9. PES and IPES spectral weight for the t-J model on a 2×8 ladder. $t=1$ is the unit of energy. The density is $\langle n\rangle = 0.875 = 2/16$ and the coupling $J=1.0$. The solid (dashed) lines denote results using dressed (bare) operators.

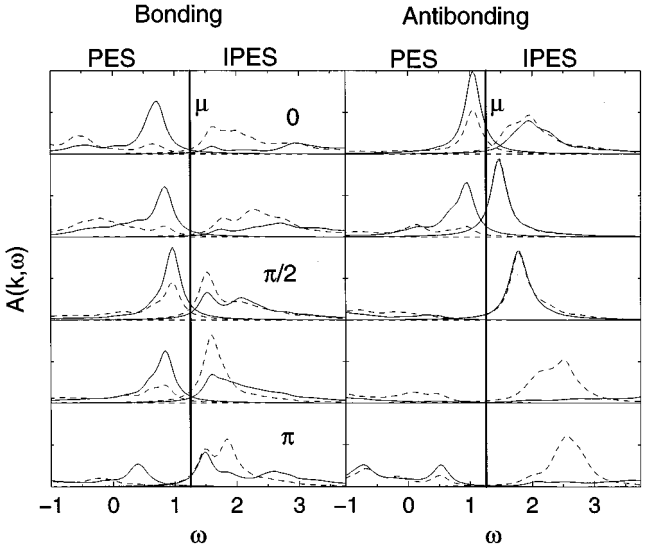

FIG. 10. Same as Fig. 9 but for $\langle n\rangle = 0.75$ and $J=0.3$.

Let us now consider the case when dressed operators are used (Fig. 8). The situation is dramatically different for the antibonding band. The IPES weight appearing at $\omega-\mu\sim t$ for $k\geqslant 3\pi/4$ is now shifted to high energies beyond the range shown in Fig. 8. Conversely, weight in the PES sector moves closer to the Fermi energy. In the range of energies shown the net effect amounts to a transfer of weight from IPES to PES at large momenta $k\sim\pi$ in the antibonding sector. The quasiparticle peak described by the dressed operators resembles the quasiparticle dressed peak found at half-filling (Fig. 5) but now with the chemical potential located slightly below the energy of the first pole at $k=\pi/2$. In other words, the hole momentum distribution corresponding to dressed operators will now have a minimum in the vicinity of $\pi/2$, as if there were hole pockets at this momenta. For the bonding band, important changes are also observed. The dominant features are now in the PES region and the band appears as fully populated.

The J/t dependence of the results is illustrated by the data at $J=1.0$ obtained for $\langle n\rangle = 0.875$ (Fig. 9). In the bonding band below μ, the dressed operators still improve on the bare operators but by a smaller factor than at $J=0.3$, as in 2D clusters. The interpretation of Fig. 9 for the bonding band as a large vs small Fermi surface is complicated by the fact that the two holes actually form a tight *bound* state at this coupling. The splitting between the two dominant peaks at $k\sim\pi/2$ is likely related to the binding energy Δ which for $J/t=1.0$ is $\sim 1t$. For the antibonding band the situation at this large coupling is similar as for $J=0.3$. The most substantial changes occur at large momenta, notably $k=3\pi/4$, where again a shift of weight from IPES to PES transforms an apparent large Fermi surface into a small one. It is interesting to remark that in Ref. 29 an ''intriguing'' duality between metalliclike features and lightly hole doped insulating features was reported. The results present here contribute to the solution to this apparent paradox.

Data at $\langle n\rangle = 0.75$ and $J/t=0.3$ are shown in Fig. 10. The results in the bonding sector are very similar to those obtained at $\langle n\rangle = 0.875$. Only at $k=\pi$ the PES weight has decreased substantially compared with Figs. 7 and 8. The antibonding band is more affected by the reduction of the electronic density, as expected. Now, the PES region for $k\geqslant\pi/2$ has been drastically depleted compared with the results for $\langle n\rangle = 0.875$ suggesting a ''large'' Fermi surface for this band and density even using dressed operators. Results at $\langle n\rangle = 0.50$ (Fig. 11) show that this trend continues as the hole density grows. At this or smaller densities the Drude weight no longer grows as the number of holes,[14] and thus there is no paradox as described in the Introduction. At $\langle n\rangle = 0.50$ the antibonding band is empty regardless of whether bare or dressed operators are used, while the bonding band is approximately half-filled. Increasing J/t to 1, effects similar to those shown in Figs. 10 and 11 have been observed. It is quite reasonable to find no qualitative changes between the dressed and bare operators at large hole density since the antiferromagnetic correlations are negligible and

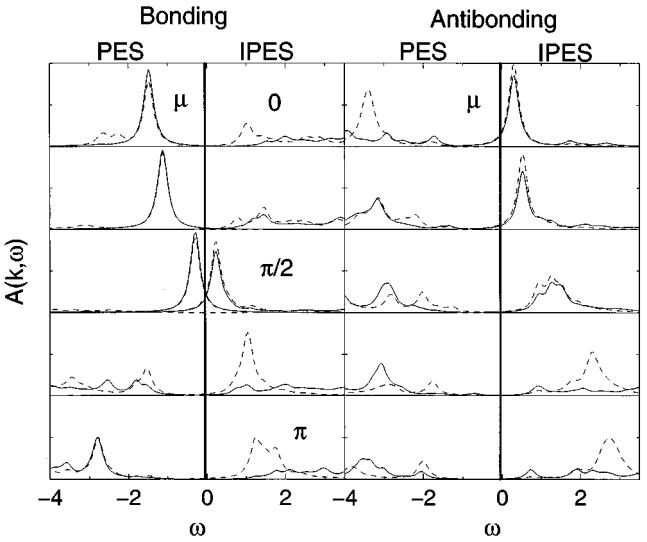

FIG. 11. Same as Fig. 9 but for $\langle n\rangle = 0.50$ and $J=0.3$.

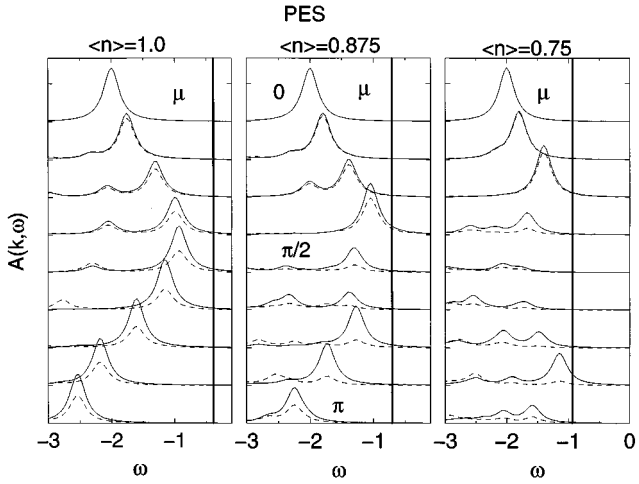

FIG. 12. PES spectral weight for the 1D t-J model on a chain of 16 sites at $J=2.0$ ($t=1$) and several densities. The dressed (bare) operator results are shown with solid (dashed) lines.

thus the form of the dressed operator Eqs. (1)–(3) is no longer operative. Certainly the largest differences between bare and quasiparticle operators have appeared in this study close to half-filling where ξ_{AF} is not negligible.

VI. CHAINS

The study of the PES spectra discussed for ladders and planes can be easily extended to one dimensional systems. However, here the special properties of electronic 1D models complicates the interpretation of the data. Actually, it is known *a priori* that there is no quasiparticle peak in the spectral function of the 1D t-J model, but instead two divergences appear in the spectra due to spin-charge separation.[40] Numerical studies on finite chains produce a collection of discrete δ functions that only in the thermodynamic limit become the continuum between the two divergences. In spite of this complication note that the purpose of this paper is to discuss the general notion that there is a potential redistribution of spectral weight when operators different from bare fermionic ones are used in creating the charge excitations. Thus, independent on whether the peaks found in $A(k,\omega)$ for 1D systems correspond to true quasiparticles or are part of a continuum, repeating for chains the calculation performed for ladders and planes can illustrate the generality of the ideas discussed in this paper. Both numerical simulations and PES experiments have a coarse resolution and it is difficult for them to decide whether a given peak is a quasiparticle peak or a sharp cusp in the spectrum. However, using these techniques at least it is possible to state with confidence the position of the dominant weight in the data. This position may be altered by replacing bare operators by dressed ones in any dimension including 1D.

Results for the t-J model on a chain of 16 sites, $J/t=2.0$ and several densities are shown in Fig. 12. For the half-filled case the spectra are qualitatively similar to those discussed for ladders and planes. Working with the bare operator the largest peak is at $k=0$, and it slightly decreases in intensity as k grows. Above $k=\pi/2$, a reflected signal caused by strong antiferromagnetic fluctuations is observed. This is the 1D equivalent of the ''shadow bands'' recently extensively discussed in the literature.[17,41–43] To construct the dressed operators in 1D the same procedure as in higher dimensions was followed since the Heisenberg model on a chain has strong short distance antiferromagnetic correlations in spite of its long distance power-law decaying behavior. For their motion the holes react mainly to their local spin environment and thus the dominant short distance hole dressing is common to chains, ladders, and planes. The results at half-filling working with the dressed operator indeed show a substantial increase in the intensity of the dominant peak which becomes approximately uniform for all momenta.

Away from half-filling the effects observed in chains are still similar to those found in ladders and planes. Consider, for example, $\langle n\rangle=0.875=2/16$ (we will concentrate our attention on PES results only for simplicity). Above $k\sim\pi/2$, the bare operator peak has reduced drastically its intensity. However, using dressed operators a large weight is found not only at small momenta but also for $k\geqslant 3\pi/4$. Actually the shape of the spectral function for the quasiparticle operator resembles what would be obtained if the region near $k=\pi/2$ of the half-filled result would have been removed by hole doping, i.e., as if hole pockets would have been created in the system. Certainly the momentum distribution of the dressed operators will have a sharp minimum at $\pi/2$. The results at $\langle n\rangle=0.75$ show similar features. The bare operators have a large signal only at small k, while the dressed operators in addition still have some nonnegligible weight at large k. Thus, once again, even in models without sharp quasiparticle peaks in the thermodynamic limit, a large redistribution of weight can occur when bare operators are replaced by dressed operators resembling a transformation from a large Fermi surface to a small Fermi surface.

VII. CONCLUSIONS

In this paper it has been argued that apparently ''large'' Fermi surfaces obtained with techniques that have a finite resolution in momentum and energy such as those found with ARPES and in numerical studies of correlated electrons, can be changed into ''small'' Fermi surfaces by using dressed quasiparticle hole operators rather than bare operators. Examples have been provided for ladders, planes, and chains described by the t-J model. This result is especially clear for ladders at density $\langle n\rangle=0.875$. As the density grows further the antiferromagnetic correlations become negligible and no important differences are found between bare and dressed holes (if the dressing is attributed to antiferromagnetic correlations). Note that the subtle issue of whether the ''hole pockets'' define a small Fermi surface at zero temperature has not been addressed here. The techniques employed only allows for a study of the location of the main spectral weight in the spectrum, but not of singularities in $n(\mathbf{k})$.

Intuitively, the sensitivity of (i) momentum (π,π) in 2D clusters and (ii) the antibonding band with $k=\pi$ in ladders to the change of operators from bare to dressed can be understood by noticing that near half-filling holes reduce their energy by having those momenta.[16] This is clear from typical distributions $n(\mathbf{k})$ such as those illustrated in Fig. 2 (see also Refs. 22 and 23). Evolving in time (Fig. 13), a hole vacancy

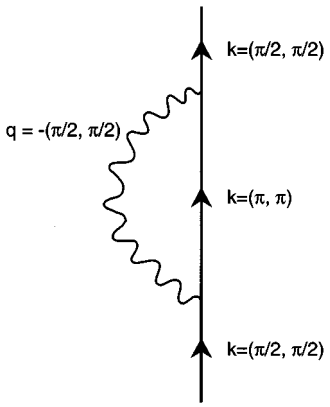

FIG. 13. Schematic representation of the time evolution of a hole quasiparticle near half-filling. The hole may spend a considerable part of the time in a state of momentum close to (π,π) (see Ref. 16).

that forms part of a quasiparticle (made out of a vacancy plus its dressing) may reside with high probability into a state with momentum in the vicinity of (π,π) to improve its kinetic energy. This is especially true in the small J/t regime where having spin excitations that are not energetically optimal [i.e., with $\mathbf{k}=-(\pi/2,\pi/2)$ rather than (π,π)] is compensated by the gain in the hole kinetic energy. In such a regime the bare IPES signal will be large close to (π,π), as observed, while for dressed operators the movement of the whole quasiparticle is considered and such effects do no longer affect the results.

The main experimental implication of our study is that materials can exist for which ARPES would signal a large Fermi surface while other measurements, such as optical conductivity and Hall coefficient, could suggest that holes are the carriers and that the Fermi surface is small. In other words, *ARPES is associated with bare holes while transport measurements react to dressed holes*. Our results also have consequences for theories that construct the doped regime starting with results for the quasiparticle behavior obtained at half-filling.[21] The fact that dressed operators may transform a large Fermi surface into a small one provides support for these theories.

The ideas discussed here are very general and they can be applied to models for heavy fermions, quasi-one-dimensional systems, and manganites. If the dressing of hole excitations in a given compound or theoretical model is large, then calculations using dressed operators are needed to study the accuracy of theories that treat doped regimes as composed of hole excitations obtained in the undoped limit. Apparent experimental paradoxes where large Fermi surfaces are obtained in ARPES while holelike behavior is found in the Drude weight of the optical conductivity $\sigma(\omega)$ should not be surprising when the quasiparticles are strongly dressed.

ACKNOWLEDGMENTS

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