Photoemission Spectra in t-J Ladders with Two Legs

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Abstract

Photoemission spectra for the isotropic two-leg t-J ladder are calculated at various hole-doping levels using Exact Diagonalization techniques. Low-energy sharp features caused by short-range antiferromagnetic correlations are observed at finite doping levels close to half-filling, above the naive Fermi momentum. These features should be observable in angle-resolved photoemission experiments. In addition, the formation of a d-wave pairing condensate as the ratio J/t is increased leads to dynamically generated spectral weight for momenta close to k_F where the d_{x^2-y^2}-order parameter is large.
The recent discovery of two-leg spin-1/2 ladders such as vanadyl phosphorate \((\text{VO})_2\text{P}_2\text{O}_7\) and \(\text{SrCu}_2\text{O}_3\) has received considerable attention. On one hand they represent a physical realization of RVB spin-liquids, with a ground state dominated by spin singlets, mostly along the rungs. On the other hand, they are a lower-dimensional analogue of the much-studied two-dimensional high-\(T_c\) cuprates and thus a test-ground for generic ideas underlying the physics of strongly correlated electrons. Furthermore, recently progress has been made in doping \(\text{SrCu}_2\text{O}_3\) with holes by substituting some of the Sr-sites by La. Then it is of much interest to test predictions for the Fermi surface of correlated electrons in this novel geometry and contrast them with results in two dimensions.

In this paper we study the isotropic t-J model on a two-leg ladder defined by the Hamiltonian:

\[
H = -t \sum_{j, \sigma} \left[ \sum_{a=1}^{2} \tilde{c}_{a \sigma}^{\dagger}(j)\tilde{c}_{a \sigma}(j+1) + \tilde{c}_{1 \sigma}^{\dagger}(j)\tilde{c}_{2 \sigma}(j) + \text{h.c.} \right] \\
+ J \sum_{j, a} [\mathbf{S}_a(j) \cdot \mathbf{S}_a(j+1) - \frac{1}{4} n_a(j)n_a(j+1)] \\
+ J \sum_{j} [\mathbf{S}_1(j) \cdot \mathbf{S}_2(j) - \frac{1}{4} n_1(j)n_2(j)],
\]

where \(j\) is the rung index, and \(\sigma(=\uparrow, \downarrow)\) and \((=1,2)\) are spin and leg indices. A powerful way to study the Fermi surface of this system is by Angle Resolved Photoemission Spectroscopy (ARPES) which measures the imaginary part of the one-hole Green’s function \(A_h(p, \omega)\), and corresponds to the sudden removal of an electron from the material (likewise the \(A_e(p, \omega)\) corresponds to the process of creating an additional electron).

As shown in previous reports, two-leg ladders close to half-filling belong to the universality class of Luther-Emery Liquids. Then, it is reasonable to consider the non-interacting picture of two coupled chains to understand the topology of the Fermi surface for this special geometry. In Fig. 1 the available single-particle states in two coupled 8-site chains with periodic boundary conditions in the chain-directions are shown for different filling levels. While at finite hole doping a splitting between a bonding and an antibonding band (of order \(J\)) is expected, at half-filling this splitting does not occur since the kinetic energy is suppressed.
due to the constraint of no double-occupancy. In this case the bonding and the antibonding bond lie on top of each other (indicated by the thick solid line), and the single-particle states below the Fermi-momentum are shown as solid circles while the unoccupied states are denoted by open circles. In this case the highest occupied level is completely filled, and this constitutes a closed shell configuration. Upon doping with two holes a splitting into a bonding and an antibonding band occurs. Also, the highest occupied energy levels which belong to the antibonding band (at momenta $(\pi/4, \pi)$ and $(-\pi/4, \pi)$) are only half-filled. Then, we have an open shell for this case. Finally, for 4 holes only the lowest state in the antibonding band is filled, while the bonding band is half-filled for all of the above cases.

In the following, it will become apparent that the presence of exchange interactions modifies this simple picture by introducing additional features into the naively expected electronic occupation structure predicted by the non-interacting limit. For example, the presence of strong antiferromagnetic (AF) correlations in the system favors the formation of a magnetic superstructure, i.e. “shadow bands” which were first suggested by Kampf and Schrieffer in the context of the two-dimensional cuprates close to half-filling. In subsequent numerical studies it has been shown that an antiferromagnetic correlation length of about 2-3 lattice spacings - as it is realized e.g. in Bi2212 - is sufficient to produce a shadow Fermi surface that is barely resolvable by current PES techniques. On the other hand, at half-filling and T=0 there is long-range antiferromagnetic order in two dimensions, and thus a strong shadow signal is expected for this case, as it was observed for Sr$_2$CuO$_2$Cl$_2$. In the two-leg ladder the situation differs slightly since only short-range order with a correlation length of roughly 3.19 lattice spacings is found at half-filling.

Nevertheless, as is shown in Fig. 2, there is a clear shadow signal for momenta $|k| > |k_F|$ ($k_F = (\pi/2, 0)$) in the bonding band of 2-leg ladders. In analogy to the two-dimensional case, a sharp peak at the lower end of the PES is observed. It disperses with a bandwidth of order $J$ as can be seen by varying the ratio $J/t$. Also, this feature becomes sharper as $J/t$ is increased which implies that it is associated mainly with the spin degrees of freedom in the system. Furthermore a broader high-energy band located at binding en-
ergies of order $t$ is observed, corresponding to incoherent excitations of the hole. As $J/t$ is increased much of the weight from the incoherent band is transferred to the low-energy band. ARPES experiments in undoped 2-leg ladders should be able to observe considerable weight above the naive Fermi momentum, as shown in Fig. 2.

The introduction of a hole into the half-filled system leads to the splitting of the final states in $A_{\mathbf{h}}(\mathbf{p}, \omega)$ into a bonding and an antibonding band. The hole goes into the antibonding band distorting the staggered spin order of the half-filled system. Thus, shadow band features are more visible in the bonding band especially at large values of $J/t$.

Upon doping the system with two holes, a main Fermi surface consistent with the occupied sites indicated in Fig. 1 is observed. A Fermi surface crossing of a sharp band dispersing as $-2t_{\text{eff}} \cos(k)$ can be seen. The effective hopping $t_{\text{eff}}$ is smaller than $t$, as observed also in two-dimensional clusters. However, as the doping level is increased $t_{\text{eff}} \rightarrow t$. The Fermi momenta lie between $(\pi/2, 0)$ and $(3\pi/4, 0)$ for the bonding band and at $(\pi/4, \pi)$ for the antibonding band.

In the bonding band, a sharp peak is observed at low binding energy at momenta $(3\pi/4, 0)$ and $(\pi, 0)$, very similar to the shadow features found at half-filling in Fig. 2. Note that by increasing the ratio $J/t$, an interesting feature occurs at momentum $(\pi/2, \pi)$ in the PES, just above the antibonding $k_F$ for this filling: while there is little coherent low-energy spectral weight at this momentum for $J/t=0.5$, a sharp peak emerges as $J/t$ is increased. It is hence dynamically generated by correlations that increase with $J/t$. As suggested recently by Hayward et al. a $d_{x^2-y^2}$ resonant valence bond (RVB) phase may become stable in this parameter regime. We thus tentatively associate the PES weight which appears at $(\pi/2, \pi)$ with increased $d_{x^2-y^2}$ RVB correlations. It may correspond to a Bogoliubov quasiparticle excitation made of an electron and a hole $(\alpha_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k} \uparrow} + v_{\mathbf{k}} c_{-\mathbf{k} \downarrow})$.

In principle, all holes and electrons close to $k_F$ can contribute to the formation of the superconducting (SC) condensate. Then, the following question arises: how much of the spectral weight seen in the $(3\pi/4, 0)$ and $(\pi, 0)$ PES peak is due to pairing and how much is due to short-range AF correlations along the chains? To distinguish these two contributions
to the spectral weight at \((3\pi/4, 0)\) and \((\pi, 0)\) we include into the Hamiltonian (Eq. 1) a nearest-neighbor interaction term along the rungs, \(V \sum_j n_1(j) n_2(j)\), which disfavors a bound state of two holes on a rung if \(V\) is repulsive. For either sign of \(V\), the \(d_{x^2-y^2}\) character of the bound state is destroyed if the magnitude of \(V\) is chosen to be large enough. From an explicit calculation of the spin-spin correlation functions (shown in Fig. 4) we observe that in the presence of the nearest neighbor interaction term AF correlations are increased in the chains when \(V\) is negative and decreased for positive \(V\). This is consistent with the observation that the two-hole rung state is destroyed for a large enough positive \(V\), spreading the second hole into the chains and thus smearing out the background staggered short-range spin order at short distances. However, the addition of a repulsive \(V\)-term with \(V\) as large as \(5t\) only reduces the AF correlation length from 3 (at \(V=0\)) to about 2 lattice spacings. Then, the main effect of the rung density-density repulsion is to destroy the d-wave bound state, not altering much the staggered spin-spin correlations. This is important for our discussion below on the interpretation of some of the PES features observed in our calculations.

In Fig. 5 PES are shown for a two-hole ground state at fixed \(J/t=1.0\) for various values of \(V/t\). Indeed the peak located at \((\pi/2, \pi)\) for \(V/t=0\) disappears when the magnitude of \(V/t\) is large, indicating the suppression of pairing. However, the peak at \((3\pi/4, 0)\) increases for negative \(V\) and decreases for positive \(V\) having thus the same qualitative dependence on \(V/t\) as the AF correlation length of the system. Certainly it cannot be ruled out that there are small contributions from the now very weakly bound 2-hole state to the low-energy spectral weight in the bonding band above \(k_F\). However, our calculation suggests that the superstructure observed in the bonding band is dominated by backscattering processes characteristic of AF correlations. Note that at \(V=-5t\) the bonding band is shifted away from the chemical potential by a substantial amount reflecting the fact that an attractive interaction across the rungs increases the band splitting.

The strength of backscattering processes in the bonding band (with characteristic momentum \(Q_b = (\pi, 0)\)) and in the antibonding band (with characteristic momentum \(Q_a = (\pi, \pi)\)) is reflected in the relative spectral intensities of the low-energy peak in
$A_h(Q_b, \omega)$ and $A_h(Q_a, \omega)$ respectively. While the coherent part in $A_h(Q_a, \omega)$ is reduced with negative $V/t$, it is enhanced in $A_h(Q_b, \omega)$ and vice versa.

Before turning to higher hole-filling levels let us discuss the Inverse Photoemission Spectra (IPES) shown in Fig. 3. While for small values of $J/t$ a rather coherent IPES band is observed, for $J/t=2.0$ higher energy excitations carry considerable spectral weight. To understand this behavior we should remember that a hole quasiparticle is made out of an actual hole (empty site) plus a surrounding region where the AF correlations have been altered with respect to those in the absence of carriers. This effect reduces drastically the quasiparticle weight $Z$ in the PES. When a hole is annihilated in an IPES process the spin-excitations of the “dressed” quasiparticle are left behind and form a low-energy band of width $J$ above $k_F$. However, there are a variable number of such spin excitations, i.e. multi-magnon processes which become more dominant at larger $J/t$. Thus, more high-energy spectral weight is observed in the IPES with increasing $J/t$.

Finally let us turn to a higher filling level, i.e. 4 holes. The corresponding PES and IPES are shown in Fig. 6. The Fermi momentum in the antibonding band is now shifted with respect to the 2-hole ground state according to Fig. 1. It lies between $(\pi/4, \pi)$ and $(\pi/2, \pi)$. A shadow peak is observed in the bonding band at $(3\pi/4, 0)$ and $(\pi, 0)$ although considerably weaker than for the case of 2 holes. This corresponds to a shorter AF correlation length for this doping. A feature possibly induced by d-wave pairing correlations which sharpens rapidly with increasing $J/t$ appears at momentum $(\pi/4, \pi)$. An increase in low-energy coherence is also observed at $(\pi/2, \pi)$.

The observation of robust antiferromagnetically induced sharp peaks in two-leg ladder systems is not entirely surprising. Remember that in these systems there is a robust spin-gap that quite likely survives the introduction of a small density of carriers. This spin-gap is caused by the tendency of spins to form rung singlets, which favors hole pair formation in these rungs. Once such pairs are formed, the staggered spin background remains almost intact.

In conclusion, we have studied the Photoemission Spectra for two-leg t-J ladders at
various hole-doping levels. In analogy to the two-dimensional case, sharp peaks induced by remnant short-ranged antiferromagnetic correlations are observed for small hole-doping levels. Such robust peaks should be detectable in ARPES experiments applied to ladder systems. Previous work has also indicated that similar structure clearly appears in undoped spin-1/2 Heisenberg chains even in the presence of spin-Peierls dimerization. Then, it is not necessary to have AF long-range order to observe “shadow bands”. A mild AF correlation length of only 2 or 3 lattice spacings is enough, since the effect is dominated by short-range AF fluctuations. In addition, PES weight for momenta close to $k_F$ is generated by increasing the ratio $J/t$. This dynamically generated weight may signal the onset of $d_{x^2-y^2}$-order.

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Figure Captions

1. Schematic plot of the occupied (solid circles) and unoccupied (open circles) states in a 2×8 ladder system with periodic boundary conditions.

2. Photoemission Spectra for a half-filled 2×8 t-J ladder with periodic boundary conditions. The δ-functions have been given a finite width of $\epsilon = 0.25t$.

3. Photoemission Spectra (solid lines) and Inverse Photoemission Spectra (dashed lines) for a 2×8 t-J ladder with 2 holes. The position of the chemical potential is indicated by the thin solid line.

4. Hole-hole and spin-spin correlations for a 2×8 t-J-V ladder with 2 holes at $J/t=1.0$. The sites on the first chain are labeled with $j=1,...,8$, and the sites on the second chain have $j=9,...,16$.

5. Photoemission Spectra for a 2×8 t-J-V ladder with 2 holes at $J/t=1.0$.

6. Photoemission Spectra (solid lines) and Inverse Photoemission Spectra (dashed lines) for a 2×8 t-J ladder with 4 holes.
bonding
antibonding
0 holes
2 holes
4 holes

(0,0) (π,0)
(0,π) (π,π)

antibonding
bonding
