Spectral Functions of One-dimensional Models of Correlated Electrons

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Using the Ogata-Shiba wave function, the spectral functions of the one-dimensional (1D) infinite $U$ Hubbard model are calculated for various concentrations. It is shown that the “shadow band” feature due to $2k_F$ fluctuations becomes more intense close to half-filling. Comparing these results with exact diagonalization data obtained on finite clusters for the finite $U$ Hubbard model and for the $t – J$ model, it is also shown that this feature remains well-defined for physically reasonable values of the parameters ($U/t \simeq 10, J/t \simeq 0.4$). The “shadow” structure in the spectral functions should thus be observable in angle-resolved photoemission experiments for a variety of quasi-one dimensional compounds.

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The situation is much more favorable in 1D. First of all, it is known that there is no quasi-particle peak in the spectral function but two divergences due to spin-charge separation \cite{4}. Besides, using the Ogata-Shiba wave-function \cite{5}, exact results have been recently obtained \cite{6} for the spectral functions of the infinite $U$ limit of the Hubbard model defined by:

$$\mathcal{H} = -t \sum_{i,\sigma} (\hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i+1,\sigma} + \text{h.c.}) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

or, equivalently, for the $J = 0$ limit of the $t – J$ model defined by:

$$\mathcal{H} = -i \sum_{i,\sigma} (\hat{c}_{i,\sigma}^{\dagger} \hat{\tilde{c}}_{i+1,\sigma} + \text{h.c.})$$

$$+ J \sum_{i} (\hat{S}_{i} \cdot \hat{S}_{i+1} – \frac{1}{4} n_{i} n_{i+1}), \quad (2)$$

where $\hat{c}$ are the usual hole operators, and the rest of the notation is standard. Combining these results with numerical simulations should allow us to reach a precise picture of the spectral functions of one-dimensional systems.

In this paper we will concentrate our efforts on three aspects of the spectral functions of 1D systems: 1. The first one is the extra weight created near the Fermi energy close to half-filling by short-range antiferromagnetic correlations. It is this feature that is usually referred to as “shadow band” in the literature. 2. The second issue presented here is that the “shadow” weight is actually part of an extended band that can be followed in the whole Brillouin zone. 3. The third point is that this extended band still exists away from half-filling due to diverging $2k_F$ fluctuations, although its weight near the Fermi level diminishes rapidly with hole doping. In portions of the paper we will refer to all these features with
the common language of “shadow band”, but it must be clear to the reader that in doing so we are extending the usual meaning of this term to include all the extra interesting features caused by $2k_F$ fluctuations, both close and away from the Fermi energy, that appear in the spectral functions of 1D systems.

The presence of shadow bands in 1D systems was first revealed in studies of the spectral function corresponding to a hole injected into one dimensional Heisenberg models at half-filling\(^7\). They were identified as potentially observable features in photoemission experiments for CuGeO\(_3\) and other undoped compounds where antiferromagnetic fluctuations are important. Other related aspects were first discussed in Ref.\(^8\) where a calculation of the spectral functions in the infinite $U$ limit showed unambiguously that, in addition to the charge and spin features typical of a Luttinger liquid, there is a well-defined structure whose dispersion can be followed in the whole Brillouin zone. This accumulation of weight in the spectral functions originates from diverging spin fluctuations\(^8\) at $2k_F$, the 1D equivalent of the diverging fluctuations at $(\pi/a, \pi/a)$ in the 2D case at half-filling, and by analogy it was also called a shadow band.

A clear identification of these features in photoemission experimental results for quasi-one dimensional systems is still lacking. On the theoretical side, progress can be made along two lines: First, by estimating the evolution of the shadow band features, in particular their intensity, with electron concentration to determine which systems are a priori the best candidates to observe the effect. Second, by extending the calculations to more realistic parameters, i.e. $U < +\infty$ or $J > 0$, to investigate if the band remains a well-defined structure when the on-site repulsion is no longer infinite.

To address the first point, we have calculated the spectral functions for an infinite repulsion along the lines of Ref.\(^4\) for various concentrations $n$. Some results for $B(k, \omega)$ are shown in Figure 1. The evolution between $n = 1/2$ and $n = 1$ is smooth. When $3k_F$ is larger than $\pi/a$, i.e. for $n > 2/3$, the band at finite binding energy discussed in Ref.\(^6\) at $n = 1/2$ is now folded back when it hits the zone boundary and it crosses the Fermi level at $2\pi/a - 3k_F$. This detail is very important since now non-trivial structure in the spectral functions appears near the Fermi energy. The rest of the shadow band evolves smoothly with density becoming more intense close to half-filling. Note, however, that the effect is likely less dramatic as expected in 2D systems for realistic values of $U/t$. This is due to the fact that in 1D there is always perfect nesting, independent of the band-filling, since the Fermi surface consists of only two points. The 1D best candidates to show these shadow band effects are compounds with a concentration close to 1, as anticipated in Ref.\(^6\). However, quarter-filled systems should not be disregarded since the portion of the band that appears at energies between $-2t$ and $-t$ for $0 \leq k \leq \pi/2a$ could be experimentally detectable, unless the usual large spurious backgrounds that contaminate photoemission results as we move away from the Fermi level hide the signal in the noise.

![FIG. 1. Spectral function $B(k, \omega)$ of the $U \rightarrow +\infty$ Hubbard model calculated with the help of the Ogata-Shiba wave-function. a) $n = 3/4$ ($k_F = 3\pi/8$), 200 sites; b) $n = 7/8$ ($k_F = 7\pi/16$), 176 sites; c) $n = 1$ ($k_F = \pi/2$), 190 sites.](image)

The second point, i.e. calculations for realistic parameters, is more difficult to address. Even for models that are integrable, such as the Hubbard model or the super-symmetric $t - J$ model ($J/t = 2$), a calculation of the spectral functions for large systems remains an open problem. The only available methods are numerical\(^\[11\]\). Relatively large systems can be handled with Monte Carlo simulations\(^\[11\]\), but the results require an analytic continuation which is difficult to control. Thus exact diagonalizations of finite clusters seem to be more appropriate. Such calculations have already been presented for 1D systems\(^\[12\-13\]\). The main limitation of these simulations is the size of the systems - typically 16 to 20 sites close to half-filling. The spectral functions obtained with the exact diagonalization method consist of
a collection of discrete $\delta$ functions, and they are difficult
to interpret without an underlying theory.

The originality of the present work is to use the
essentially exact results obtained for infinite $U$ with the
Ogata-Shiba wave function to interpret the results for fi-
nite clusters. To illustrate how this works, we have com-
pared in Fig. 2 the "exact" results for $n = 7/8$ (Fig. 2a)
with the results obtained for the same model on a 16 site
cluster using exact diagonalizations (Fig. 2b). Details
about the numerical method can be found in Ref. [10].

Clearly, the calculation on 16 sites is not able to repro-
duce a continuum: The true spectral function has a con-
tinuum between the peaks corresponding to the charge
and spin excitations of the Luttinger liquid [4], whereas
the spectral function of Fig. 2b has several peaks in the
same energy interval. This is best observed for $k = 0$,
where the continuum is replaced by a collection of 4
peaks. This proves that detecting the position of the spin and charge excitations corresponding to the Lut-
tinger liquid features is not possible on the basis of ex-
act diagonalizations of small clusters, unless a variety of
boundary conditions is used and a finite size scaling anal-
ysis is carried out. In spite of this problem, the shadow
band is clearly visible on the data of Fig. 2b, and both its
intensity and its dispersion are in good agreement with
the exact results. The continuum that exists between the
Van Hove singularity at $-2t$ and the shadow band around
$k = \pi$ is again poorly described on the finite cluster, but
the main band and the shadow band can be clearly iden-
tified. Thus we believe that discussing the intensity of
the shadow band on the basis of exact diagonalization
results is meaningful.

Let us now turn to more realistic parameters. To make
our analysis below more convincing, we have calculated
the spectral functions for both the Hubbard model and
the $t - J$ model, and we have compared the results us-
ing the relation $J = 4t^2/U$. Some results obtained at
$n = 3/4$ for $U/t = 10$ and $J/t = 0.4$ are depicted on Fig.
3a and 3b, respectively. The results are roughly the same.
In agreement with what was stated before, we will not try to interpret the details of the fine structure around \( \omega/t = 0 \) for small momentum or around \( \omega/t = -2 \) for large momentum. What is clearly observable, although it carries a small weight, are “shadow” features located at the same position as in the infinite \( U \) case. Its intensity is larger in the \( t-J \) case than in the Hubbard case, and this difference grows as \( U \) becomes smaller (since the agreement between Hubbard and \( t-J \) models is expected only at large \( U/t \)). Increasing \( J/t \) does not suppress the spectral weight around the shadow band but simply makes the feature broader, while decreasing \( U/t \) suppresses the intensity of the shadow band quite dramatically close to the zone boundary. The spectral weight which is lost appears around \( \omega = U \), a region not shown on Fig. 3b for clarity. This likely arises from corrections of order \( 1/U \) that are not included in the \( t-J \) model \([14]\). However, we have checked that, for parameters as small as \( U/t = 5 \), the shadow band remains quite intense for small wave vectors.

Upon approaching half-filling, the shadow band becomes quite intense. For instance, we show in Fig. 4 the spectral functions for \( J/t = 0.4 \) at \( n = 7/8 \). A photoemission experiment performed on a compound described by such parameters should be able to detect the portion of the shadow band the closest to the Fermi energy, and actually follow it in a large part of the Brillouin zone.

In conclusion, we have presented a detailed study of the “shadow” band that appears in the spectral functions of 1D systems due to diverging \( 2k_F \) fluctuations \([4]\). First, we have studied its evolution with electron concentration. As anticipated in Ref. \([4]\), its weight near the Fermi level is considerably enhanced close to half-filling. Then, we have shown that this feature is quite robust for realistic values of \( U/t \) (or increasing \( J/t \)). This is true even away from half-filling specially regarding the weight located at a finite binding energy \([4]\). We believe that it should be possible to detect this band experimentally either close to the Fermi level in nearly half-filled systems or at energies of the order of the band width for systems far from half-filling, and it is our hope that the present study will encourage experimentalists to search for this novel feature of the spectral functions of 1D correlated electron systems.

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FIG. 4. Spectral functions for the \( t-J \) model at \( n = 7/8 \) obtained on a 16 site cluster using exact diagonalizations and periodic boundary conditions. Solid lines: \( B(k, \omega) \); Dashed lines: \( A(k, \omega) \).

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