Shadow Band in the One-Dimensional Infinite-U Hubbard Model

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We show that the factorized wave function of Ogata and Shiba can be used to calculate the k dependent spectral functions of the one-dimensional, infinite-U Hubbard model, and of some extensions to finite U. The resulting spectral function is remarkably rich: In addition to low energy features typical of Luttinger liquids, there is a well defined band, which we identify as the shadow band resulting from $2k_F$ spin fluctuations. This band should be detectable experimentally because its intensity is comparable to that of the main band for a large range of momenta.   [S0031-9007(96)00898-8]

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The calculation of the spectral functions of models of correlated electrons is one of the most challenging and largely unsolved issues of condensed matter theory. Although a number of numerical techniques can be used, e.g., exact diagonalization of finite clusters [1] or quantum Monte Carlo simulations [2], exact results are available only in very special cases, mostly for one-dimensional spin models [3]. As far as one-dimensional electron models are concerned, most of the well established results have been obtained in the framework of the Luttinger liquid theory [4–7], which is believed to be the correct description of the low energy properties of a large class of Hamiltonians. However, an accurate determination of the dynamical properties for all frequencies is so far still lacking.

In this paper we perform such a calculation for the following one-dimensional models. (i) The Hubbard model defined by the Hamiltonian

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

in the infinite-U limit, which is also equivalent to the $J \rightarrow 0$ limit of the standard t-J model. (ii) An extension of the t-J model first proposed by Xiang and d'Ambrumenil [8] defined by the Hamiltonian

$$\mathcal{H} = -t \sum_{i,\sigma}(\tilde{c}_{i,\sigma}^{\dagger}\tilde{c}_{i+1,\sigma} + \text{H.c.})$$
$$+ \sum_{i,j} \sum_{\alpha=x,y,z} J^{\alpha}(S_i^{\alpha}S_{i+j}^{\alpha} - \tfrac{1}{4}\delta_{\alpha,z}n_i n_{i+j})\mathcal{P}_{i,j}, \quad (2)$$

where $\tilde{c}$ are the usual projected operators and $\mathcal{P}_{i,j} = \prod_{j'=1}^{j-1}(1 - n_{i+j'})$ in the exchange part of the Hamiltonian, ensures that two spins interact as long as there is no other spin between them. The motivation to study this model is that, unlike the infinite-U Hubbard model, there is an energy J associated to spin fluctuations, and this will give us useful indications about the $1/U$ corrections in the case of the finite-U Hubbard model.

Although the Hamiltonians of the two models are different, they share the remarkable property that in both

cases the eigenstates can be factorized [8–12] as

$$|f,N\rangle = |\psi_L^N(Q,\{I\})\rangle \otimes |\chi_N(Q,\tilde{f}_Q)\rangle, \quad (3)$$

where $|\psi_L^N(Q,\{I\})\rangle$ is an eigenfunction of N noninteracting spinless fermions on L sites with momenta $k_j L = 2\pi I_j + Q$ (I_j are integers, $j = 1,\ldots,N$) and $|\chi_N(Q,\tilde{f}_Q)\rangle$ is an eigenfunction of the one-dimensional spin-$\frac{1}{2}$ Heisenberg model with N spins (we choose N as even integer, not multiple of four) and momentum $Q = 2\pi J/N$, J integer. This momentum imposes a twisted boundary condition with phase e^{iQ} to the spinless fermions [8,9,13]. For more details, see Ref. [14]. This wave function has already been used by Ogata and Shiba [10] to calculate the momentum distribution function and by Penc, Mila, and Shiba to calculate the local spectral function of the infinite-U Hubbard model [14].

In the following, we will determine the full momentum dependence of the photoemission and inverse photoemission spectral functions defined by

$$A(k,\omega) = \sum_{f,\sigma}|\langle f,N+1|c_{k,\sigma}^{\dagger}|0,N\rangle|^2$$
$$\times \delta(\omega - E_f^{N+1} + E_0^N),$$

$$B(k,\omega) = \sum_{f,\sigma}|\langle f,N-1|c_{k,\sigma}|0,N\rangle|^2$$
$$\times \delta(\omega - E_0^N + E_f^{N-1}).$$

As a result of the factorized form of the wave functions, the spectral functions can be obtained as a convolution:

$$A^{\text{LHB}}(k,\omega) = \sum_{\omega',Q,\sigma}C_{\sigma}(Q,\omega')A_Q(k,\omega - \omega'),$$
$$B(k,\omega) = \sum_{\omega',Q,\sigma}D_{\sigma}(Q,\omega')B_Q(k,\omega - \omega'). \quad (4)$$

A similar expression holds for the spectral function in the upper Hubbard band [15] $A^{\text{UHB}}(k,\omega \approx U)$, which we will not discuss here. In these expressions, $A_Q(k,\omega)$ and

$B_Q(k, \omega)$ involve only the spinless fermion part of the wave function and are defined as

$$
\begin{aligned}
A_Q(k, \omega) = L \sum_{\{I\}} &|\langle \psi_L^{N+1}(Q, \{I\})|b_0^\dagger|\psi_{L,\pi}^{N,GS}\rangle|^2 \\
&\times \delta(\omega - E_f^{N+1} + E_0^N)\delta(k - P_f^{N+1} + P_0^N),
\end{aligned}
$$

$$
\begin{aligned}
B_Q(k, \omega) = L \sum_{\{I\}} &|\langle \psi_L^{N-1}(Q, \{I\})|b_0|\psi_{L,\pi}^{N,GS}\rangle|^2 \\
&\times \delta(\omega - E_0^N + E_f^{N-1})\delta(k - P_f^{N-1} + P_0^N),
\end{aligned}
\tag{5}
$$

where the momentum and energy of the states are given by $P^{N'} = \sum_{j=1}^{N'} k_j$ and $E^{N'} = -2t \sum_{j=1}^{N'} \cos k_j$, and where b and $b^\dagger$ are spinless fermion operators. $C_\sigma(Q, \omega)$ and $D_\sigma(Q, \omega)$ depend on the spin wave function only and are given by

$$
\begin{aligned}
C_\sigma(Q, \omega) = \sum_{\tilde{f}_Q} &|\langle \chi_{N+1}(Q, \tilde{f}_Q)|\hat{Z}_{0,\sigma}^\dagger|\chi_N^{GS}\rangle|^2 \\
&\times \delta(\omega - E_f^{N+1} + E_0^N),
\end{aligned}
$$

$$
\begin{aligned}
D_\sigma(Q, \omega) = \sum_{\tilde{f}_Q} &|\langle \chi_{N-1}(Q, \tilde{f}_Q)|\hat{Z}_{0,\sigma}|\chi_N^{GS}\rangle|^2 \\
&\times \delta(\omega - E_0^N + E_f^{N-1}),
\end{aligned}
\tag{6}
$$

where $\hat{Z}_{0,\sigma}^\dagger$ appends a spin σ to the beginning of the spin wave function $|\chi_N\rangle$ making it $N + 1$ sites long, and $\hat{Z}_{0,\sigma}$ is the Hermitian conjugate of $\hat{Z}_{0,\sigma}^\dagger$.

To evaluate the charge contribution, one needs matrix elements between states with different boundary conditions (e^{iQ} for the final state, $e^{i\pi}$ for the ground state [14]). For $Q \neq \pi$ the overall phase shift $(Q - \pi)/L$ due to momentum transfer $Q - \pi$ to the spin degrees of freedom gives rise to Anderson's orthogonality catastrophe [16], and the matrix elements $|\langle \psi_{N+1}(Q, \{I\})|b_0^\dagger|\psi_N^{GS}\rangle|^2$ can be shown to be equal to

$$
L^{-2N-1} \cos^{2N} \frac{Q}{2} \prod_{j>i} \sin^2 \frac{k_j - k_i}{2}
$$
$$
\times \prod_{j>i} \sin^2 \frac{k_j' - k_i'}{2} \prod_{i,j} \sin^{-2} \frac{k_i' - k_j}{2},
\tag{7}
$$

where k_j (k_j') are wave vectors with phase shift Q/L (π/L). The restriction imposed by $\delta(k - P_f^{N\pm1} + P_0^N)$ is then implemented by restricting the sum over $\{I\}$ to states which have the correct momentum.

The calculation of the spin contribution is based on the spin-$\frac{1}{2}$ Heisenberg Hamiltonian with N' sites

$$
\mathcal{H}_{\text{spin}} = \sum_{i=1}^{N'} \sum_{\alpha=x,y,z} \tilde{J}^\alpha (S_i^\alpha S_{i+1}^\alpha - \tfrac{1}{4}\delta_{\alpha,z}),
\tag{8}
$$

with $N' = N$ for the ground state and $N \pm 1$ for the final states. The model of Eq. (2) corresponds to $\tilde{J}^\alpha =$

J^α. For the infinite-U Hubbard model, one has to consider the isotropic case and to take the limit $\tilde{J} \to 0$. In that case, there is no energy associated to spin excitations, and we can write $C_\sigma(Q, \omega) = C_\sigma(Q)\delta(\omega)$ and $D_\sigma(Q, \omega) = D_\sigma(Q)\delta(\omega)$. The functions $C_\sigma(Q)$ and $D_\sigma(Q)$ have already been studied earlier [13,14]. They can be calculated numerically with exact digonalizations (up to 26 sites) or with DMRG [17] (up to 130 sites, keeping 300 states per block). It turns out that there is a very strong singularity $(\pi/2 - Q)^{-1/2}$ for $Q < \pi/2$ and a small contribution coming from the higher order excitation towers for $Q > \pi/2$ in the case of $D_\sigma(Q, \omega)$. For $C_\sigma(Q, \omega)$ the situation is reversed and both are symmetric with respect to $Q = 0$.

Using these results, it is straightforward to get the spectral functions for the infinite-U Hubbard model. One just has to generate the quantum numbers for the charge part, calculate the corresponding energy, momentum, and matrix elements, and perform the convolution in Q. The results are presented in Figs. 1 and 2 for a quarter-filled system. There are several interesting features to notice. In the low energy region near k_F we can identify three
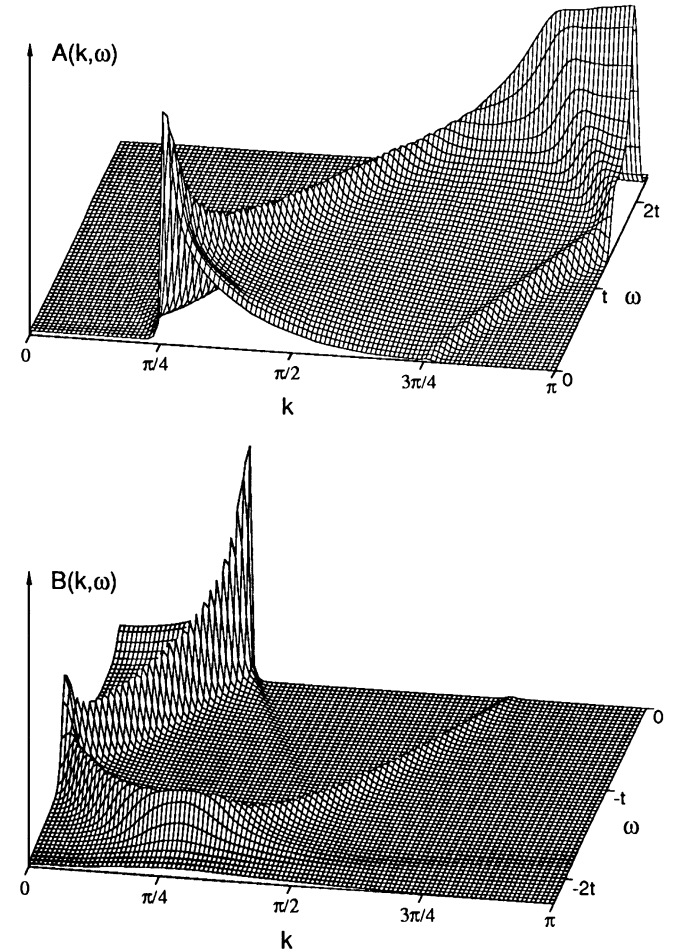

FIG. 1. One particle spectral functions of the $U \to +\infty$ Hubbard model for $L = 228$ sites and $N = 114$ electrons with Fermi momentum $k_F = \pi/4$.
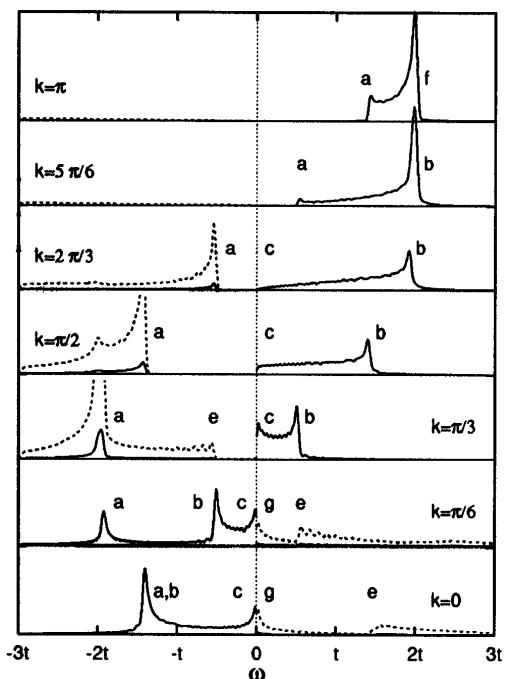
FIG. 2. The same as Fig. 1, but for some selected momenta. Some parts of the spectra are multiplied by 10 and are shown with dashed lines.

structures: There are divergences at $\omega = u_c(k - k_F)$ and $\omega = 0$ and a lot of spectral weight between them (peaks "b" and "c" in Fig. 2). There is also a small weight ("e") appearing on the other side of the Fermi energy at $\omega = -u_c(k - k_F)$. If we remember that the spin velocity u_s vanishes for the infinite-U Hubbard model, all these features are consistent with the Luttinger liquid calculations of Meden and Schönhammer [7] and of Voit [7]. The small peak "g" comes from higher harmonics. The dispersion of the charge part (b) is given exactly by $E(k) = -2t \cos(|k| + k_F)$, in agreement with the observation of Preuss et al. [2] based on Monte Carlo results for $U/t = 4$.

However, the Luttinger liquid picture does not exhaust the features of the spectral function of Figs. 1 and 2. For larger energies, or away from k_F, there is a well defined bandlike structure ("a") with considerable spectral weight and a dispersion given by $E(k) = -2t \cos(-|k| + k_F)$. We interpret this feature as a shadow band [18] coming from the spin fluctuations which diverge at $2k_F$. The scattering of the charges by these fluctuations produces an image of the main spectrum at $k + 2k_F$. This is very similar to the mechanism of the shadow bands proposed for the two-dimensional model with strong antiferromagnetic fluctuations. This shadow band is responsible for the singularity at $3k_F$ present in the momentum distribution function [10,19,20]. Finally, there is a Van Hove singularity at $\pm 2t$ which gives rise to a clear peak for wave vectors close to the extrema of the bands ("f").

Let us now turn to the model of Eq. (2). To get the spectral function, we need $C_\sigma(Q, \omega)$ and $D_\sigma(Q, \omega)$ for the Heisenberg model. This can be done numerically for the isotropic case ($J^{x,y,z} = J$) using Lánczos diagonalization of small clusters or DMRG [21]. We find that $C_\sigma(Q, \omega)$ is zero for $\omega < -\tilde{J} \ln 2 + u_\sigma |\sin(k - \frac{\pi}{2})|$, where $u_\sigma = \frac{\pi}{2} \tilde{J}$ is the spin velocity in the squeezed system, that it has an inverse square root singularity at $Q = \pi/2$, and that the largest contributions come from the lower edge of the excitation spectrum. The main difference with the infinite-U case is that the spin fluctuations have an energy of order J, so that the spin velocity $u_s = u_\sigma L/N$ does not vanish anymore. The low energy part of the spectrum then has exactly the form predicted by the Luttinger liquid theory.

For the XY case ($J^{x,y} = J$, $J^z = 0$) one can give a closed expression for $C_\sigma(Q, \omega)$ and $D_\sigma(Q, \omega)$ after mapping the problem onto noninteracting spinless fermions by a Jordan-Wigner transformation. After some algebra, the matrix elements $|\langle \chi_{N+1}(Q, \tilde{f}_Q)|Z_{0,\sigma}^\dagger|\chi_N^{GS}\rangle|^2$ of Eq. (6) can be obtained as

$$[N(N+1)]^{-M} \prod_{j=1}^{M} \sin^2 \frac{q_j'}{2} \prod_{j>i} \sin^2 \frac{q_j - q_i}{2}$$

$$\times \prod_{j>i} \sin^2 \frac{q_j' - q_i'}{2} \prod_{i,j} \sin^{-2} \frac{q_i' - q_j}{2}, \quad (9)$$

where q_j and q_j' are the momenta of the M spinless fermions representing the $-\sigma$ spins on the N and $N +$
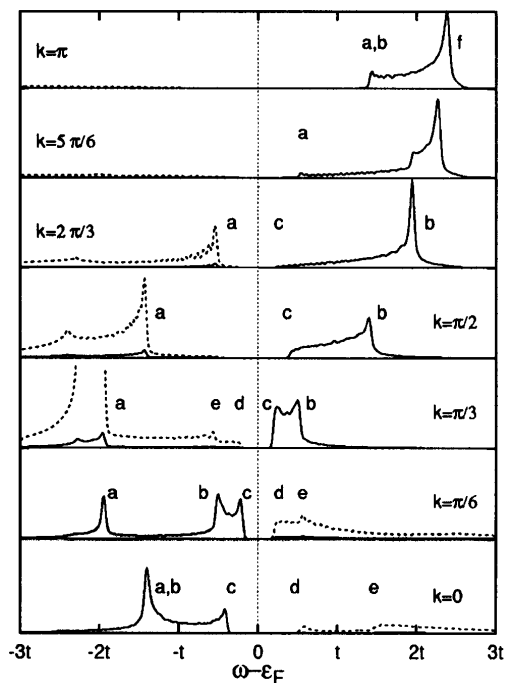

FIG. 3. Spectral function for the model of Xiang and d'Ambrumenil with XY exchange, $J = 0.4t$, $L = 228$, $N = 114$, and $\varepsilon_F = -J/\pi$. Some parts of the spectra are multiplied by 10 and are shown with dashed lines.

1 site lattice. They are quantized according to $q' = 2\pi J'_j/(N+1)$ and $q = 2\pi J_j/N$, where J_j and J'_j are integer quantum numbers, and $\tilde{f}_Q \equiv \{J'_j, j = 1, \ldots, M\}$. The total momentum and energy of $|\chi_{N+1}(Q, \tilde{f}_Q)\rangle$ are given by $Q = \sum_j q'_j$ and $E^{N+1} = J \sum_j \cos q'_j$. Details will be given elsewhere [15]. A similar expression holds in the case of $D_\sigma(Q, \omega)$. This formulation also allows one to derive analytical results. For instance, the static function $\omega(0 \to j, \sigma)$ introduced by Ogata and Shiba [10] can be shown to have the asymptotic behavior $\propto j^{-5/8} \cos(\frac{\pi}{2} j + \frac{\pi}{4})$. Thanks to this mapping, one can calculate the spectral function with the same accuracy as for the infinite-U Hubbard model. The results are shown in Fig. 3 for a quarter-filled system. It is essentially the same as that of the Hubbard model, except that at low energies an extra peak "d" accounting for the extra exponents in the spin part of the XY model has appeared (this peak has nothing to do with peak g in Fig. 2). Because of finite J, both "c" and "d" follow the $\omega = u_\sigma \cos \frac{\pi}{2} \frac{k}{k_F}$ dispersion. Furthermore, we can see that the shadow band ("a") and the Van Hove–like singularity ("f") are broadened by the spin fluctuations.

Finally, let us comment on the experimental implications of the present results. It would be most interesting to observe the shadow band in angular-resolved photoemission or inverse photoemission experiments on quasi-one-dimensional conductors. The intensity of that band in the previous calculations is certainly big enough for it to be detected. What about the experimentally more relevant case of the Hubbard model with finite U? In that case the factorized wave functions are no longer eigenfunctions of the Hubbard model, and there are two types of $1/U$ corrections to the spectral functions. The first type is due to the energy coming from the spin part with an effective coupling $\tilde{J} \approx \frac{4t^2}{U}(n - \frac{\sin 2\pi n}{2\pi})$. We expect these corrections to be very similar to those of the model of Eq. (2), and the main effect is to give a finite velocity to the spin excitations. However, there are also $1/U$ corrections entering the matrix elements of the spinless part of the wave function. We can anticipate that they will have two effects on the spectral function. They will produce a transfer of spectral weight to the upper Hubbard band which, according to Eskes and Oleś [22], will be small, except very close to half filling, and they will modify the power laws of the singularities. So, at least not too close to half filling, the shadow band seems to be robust against $1/U$ corrections. Whether this remains true for small values of U is not clear yet. Let us just mention that, according to recent numerical results obtained by Maekawa, Tohyama, and Yunoki [23] in a study of the spectral function of the Hubbard model for $U/t = 10$ based on Lánczos diagonalization of finite clusters, there seems to be a structure in addition to the Luttinger liquid features, suggesting that $U/t = 10$ is already large enough to guarantee the presence of a well defined shadow band.

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