Spectral Function of the 1D Hubbard Model in the $U \to +\infty$ Limit

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We show that the one-particle spectral functions of the one-dimensional Hubbard model diverge at the Fermi energy like $|\omega - \varepsilon_F|^{-3/8}$ in the $U \to +\infty$ limit. The Luttinger liquid behavior $|\omega - \varepsilon_F|^{\alpha}$, where $\alpha \to 1/8$ as $U \to +\infty$, should be limited to $|\omega - \varepsilon_F| \sim t^2/U$ (for U large but finite), which shrinks to a single point, $\omega = \varepsilon_F$, in that limit. The consequences for the observation of the Luttinger liquid behavior in photoemission and inverse photoemission experiments are discussed.

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Because of large quantum fluctuations, the low-energy physics of interacting electrons in 1D is not of the Fermi liquid type, but can be described by the Luttinger liquid theory [1–3]. According to that theory, the momentum distribution function should have no step at k_F but should behave like $n_k - n_{k_F} \propto \mathrm{sgn}(k_F - k)\,|k - k_F|^{\alpha}$, where α is a nonuniversal exponent that depends on the interaction. This has been confirmed for the Hubbard model by Ogata and Shiba [4] in the $U \to +\infty$ limit, in which case $\alpha = 1/8$ [5]. Similarly, the local (momentum averaged) one-particle spectral functions $A(\omega)$ (inverse photoemission spectrum) and $B(\omega)$ (photoemission spectrum) defined by

$$A(\omega) = \sum_{f,\sigma} |\langle f, N+1 | a^{\dagger}_{0,\sigma} | 0, N\rangle|^2 \delta(\omega - E_f^{N+1} + E_0^N),$$
$$B(\omega) = \sum_{f,\sigma} |\langle f, N-1 | a_{0,\sigma} | 0, N\rangle|^2 \delta(\omega - E_0^N + E_f^{N-1}) \tag{1}$$

are expected to behave like $|\omega - \varepsilon_F|^{\alpha}$ close to the Fermi energy. In recent photoemission experiments, the function $B(\omega)$ has been measured over a large energy range with a resolution of several meV [6]. Under these conditions, is it possible to detect the Luttinger liquid behavior? The Luttinger liquid theory itself does not predict how far the power-law behavior will hold, and to answer this crucial question a determination of the spectral function for microscopic lattice models is necessary. This is a very difficult problem. Even for the Hubbard model, which is soluble by Bethe ansatz [7] and whose low-energy properties are reasonably well understood [8,9], an exact calculation of the spectral functions has not been possible so far, although much has been done in this direction, both analytically using bosonization [10], canonical transformation [11], and Bethe ansatz [12], and numerically with Monte Carlo calculations [13].

In this Letter, we present a calculation of these spectral functions for the Hubbard model in the $U \to +\infty$ limit. The Hubbard model is defined by

$$H = -t \sum_{i,\sigma} (a^{\dagger}_{i+1,\sigma} a_{i,\sigma} + \text{H.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \tag{2}$$

where t is the hopping integral and U is the on-site repulsion. We will denote by N the number of fermions and by L the number of sites (we choose L even); the site index i runs from $i = 0$ to $L - 1$. Furthermore, we take N to be of the form $4n + 2$ (n integer) so that the ground state is nondegenerate. In the $U \to +\infty$ limit, it has been shown, using the Bethe ansatz solution, that the eigenstates can be written as a product of a spinless fermion wave function and a squeezed spin wave function [4]:

$$|N, f\rangle = |\psi^N_{L,Q}(\{I\})\rangle \otimes |\chi^{N_\downarrow}_N(Q, \tilde{f}_Q)\rangle. \tag{3}$$

The spin wave function $|\chi\rangle$ is characterized by the number of down spins $N_\downarrow$, the total momentum Q, and the quantum number $\tilde{f}_Q$ within the subspace of momentum Q. The spinless fermion part $|\psi\rangle$ is an eigenfunction of N spinless fermions on L sites with momenta $k_j L = 2\pi I_j + Q$, where the I_j, $j = 1, \ldots, N$, are integer quantum numbers. The two components of the wave function are coupled through the momentum Q of the spin wave function, which imposes a twisted boundary condition on the spinless fermion wave function (each fermion hopping from site $L - 1$ to site 0 will acquire a phase e^{iQ}).

In the limit $U \to +\infty$, all the states with different spin configurations are degenerate and the energy is equal to $-2t \sum_j \cos k_j$; i.e., it does not depend on the quantum numbers $\tilde{f}_Q$. In the ground state, the spinless fermion wave function $|\psi^N_{\mathrm{GS},L}\rangle$ is described by the quantum numbers $Q = \pi$ and $\{I\} = \{-N/2, \ldots, N/2 - 2, N/2 - 1\}$ so that the distribution of the k_j's is symmetric around the origin, the spin part being the ground state of the Heisenberg model according to Ogata and Shiba's prescription [4].

For a less than half-filled model, the spectral function $A(\omega)$ has contributions from both the lower and upper Hubbard bands [11] and $A(\omega) = A^{\mathrm{LHB}}(\omega) + A^{\mathrm{UHB}}(\omega)$. If we use the Ogata-Shiba wave function in Eq. (1), we get $A^{\mathrm{LHB}}(\omega)$ and $B(\omega)$. To do this, we just write operator $a^{\dagger}_{0,\sigma}$ entering Eq. (1) as $b^{\dagger}_0 \hat{Z}^{\dagger}_{0,\sigma}$, where $b^{\dagger}_j$ creates a spinless fermion at site j and $\hat{Z}^{\dagger}_{j,\sigma}$ inserts a spin σ after skipping the first j spins. $A^{\mathrm{UHB}}(\omega)$ can actually be obtained in that framework by a minor modification of the wave function [14]. The summation over the different

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spin configurations ($\tilde{f}_Q$) can then be performed because the energy depends only on the quantum numbers $\{I\}$ and Q, and we get

$$A^{\mathrm{LHB}}(\omega) = \sum_{Q,\sigma} C_{\sigma,N}(Q) A_Q(\omega),$$

$$A^{\mathrm{UHB}}(\omega) = \frac{1}{L - N + 1} \sum_{Q,\tilde{Q},\sigma} D_{N,-\sigma}(Q) B_{Q-\tilde{Q}}(U - \omega),$$

$$B(\omega) = \sum_{Q,\sigma} D_{\sigma,N}(Q) B_Q(\omega), \tag{4}$$

where $\tilde{Q} = 2\pi j/(L - N + 1)$, $j = 0, \ldots, L - N$. Furthermore $C_{\sigma,N}(Q)$ and $D_{\sigma,N}(Q)$ are given by

$$C_{\sigma,N}(Q) = \sum_{\tilde{f}_Q} |\langle \chi_{N+1}(Q, \tilde{f}_Q) | \hat{Z}^{\dagger}_{0,\sigma} | \chi_N(\pi, 0) \rangle|^2, \tag{5}$$

with $Q = 2\pi j/(N + 1)$ (j integer) and

$$D_{\sigma,N}(Q) = \sum_{\tilde{f}_Q} |\langle \chi_{N-1}(Q, \tilde{f}_Q) | \hat{Z}_{0,\sigma} | \chi_N(\pi, 0) \rangle|^2, \tag{6}$$

with $Q = 2\pi j/(N - 1)$, while $A_Q(\omega)$ is given by

$$\sum_{\{I\}} |\langle \psi^{N+1}_{L,Q}(\{I\}) | b^{\dagger}_0 | \psi^N_{\mathrm{GS},L} \rangle|^2 \delta(\omega - E^{N+1}_f + E^N_0), \tag{7}$$

and a similar definition holds for $B_Q(\omega)$.

The problem has now been reduced to the calculation of quantities involving only the charge or the spin. A similar approach has already been followed by Sorella and Parola [15] in their calculation of the momentum distribution function. For instance, our $D_{\sigma,N}(Q)$ is equivalent to their $Z(Q)$. However, they could not calculate the spectral function away from half filling because they did not know how to evaluate the charge part in that case. In the following, we show how to calculate these quantities for any band filling.

Let us start with $C_{\sigma,N}(Q)$ and $D_{\sigma,N}(Q)$. These quantities satisfy the sum rules $\sum_Q C_{\sigma,N}(Q) = 1$ and $\sum_Q D_{\sigma,N}(Q) = N_\sigma/N$, and they have a singularity at $Q_\sigma = \pi N_\sigma/N$. We have calculated them for small clusters (Fig. 1), and we found that for $N_\uparrow = N_\downarrow$, in which case $Q_\uparrow = Q_\downarrow = \pi/2 \equiv Q_0$, they behave like $\sim |Q - Q_0|^{-\eta}$ with $\eta = 0.49 \pm 0.01$ if $Q > Q_0$ and $\eta = 0.14 \pm 0.01$ if $Q < Q_0$ for C_Q and $\eta = 0.49 \pm 0.01$ if $Q < Q_0$ and $\eta = 0.34 \pm 0.02$ if $Q > Q_0$ for D_Q. Let us note that, although they are very small, $C_{\sigma,N}(Q)$ and $D_{\sigma,N}(Q)$ do not vanish identically for $Q < Q_0$ and $Q > Q_0$, respectively, contrary to what was claimed in Ref. [15]. The exponents of the main singularities are consistent with the theoretical value 1/2. In Fig. 1, the solid lines are fits to the numerical results that have been used in the following.

Let us now turn to the charge part. For $Q = \pi$, the only excited states that contribute are those with

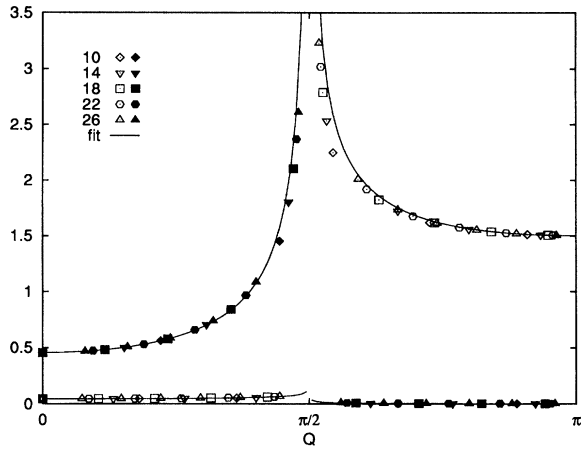

FIG. 1. $(N + 1)C_{\sigma,N}(Q)$ (open symbols) and $(N - 1) \times D_{\sigma,N}(Q)$ (solid symbols) for cluster sizes $N = 10$, 14, 18, 22, and 26.

one particle-hole pair, and $A_\pi(\omega)$ is just the spinless fermion density of states $1/\pi\sqrt{4t^2 - \omega^2}$. The problem is not so simple for $Q \neq \pi$ because we have to evaluate matrix elements between states with different boundary conditions. Let us suppose that k and k' correspond to boundary conditions with Q and Q', respectively. Then one can easily show that

$$[b^{\dagger}_{k'}, b_k]_+ = \frac{1}{L} e^{-i(k'-k)/2} e^{i(Q'-Q)/2} \frac{\sin([Q' - Q]/2)}{\sin([k' - k]/2)}. \tag{8}$$

Clearly, we are faced with Anderson's orthogonality catastrophy [16], and states with many particle-hole excitations will contribute. More generally, the matrix element $\langle 0 | b_{k_N} \cdots b_{k_2} b_{k_1} b^{\dagger}_{k'_1} b^{\dagger}_{k'_2} \cdots b_{k'_N} | 0 \rangle$ is given by

$$L^{-N} e^{i(Q'-Q)N/2} \prod_j e^{-i(k'_j - k_j)/2} \sin^N \frac{Q' - Q}{2} \times \begin{vmatrix} \sin^{-1} \frac{k'_1 - k_1}{2} & \sin^{-1} \frac{k'_1 - k_2}{2} & \cdots & \sin^{-1} \frac{k'_1 - k_N}{2} \\ \sin^{-1} \frac{k'_2 - k_1}{2} & \sin^{-1} \frac{k'_2 - k_2}{2} & \cdots & \sin^{-1} \frac{k'_2 - k_N}{2} \\ \vdots & \vdots & & \vdots \\ \sin^{-1} \frac{k'_N - k_1}{2} & \sin^{-1} \frac{k'_N - k_2}{2} & \cdots & \sin^{-1} \frac{k'_N - k_N}{2} \end{vmatrix}.$$

The central observation is that this determinant is very similar to the Cauchy determinants [17] and that it can be expressed as a product:

$$\pm \prod_{j>i} \sin \frac{k_j - k_i}{2} \prod_{j>i} \sin \frac{k'_j - k'_i}{2} \prod_{i,j} \sin^{-1} \frac{k'_i - k_j}{2},$$

where the sign is + for $N = 1, 4, 5, 8, 9, \ldots$ and − for $N = 2, 3, 6, 7, \ldots$. After a straightforward calculation one finally gets

$$|\langle \psi^{N+1}_{L,Q}(\{I\}) | b^{\dagger}_0 | \psi^N_{\mathrm{GS},L} \rangle|^2 = \frac{1}{L^{2N+1}} \cos^{2N} \frac{Q}{2} \prod_{j>i} \sin^2 \frac{k_j - k_i}{2} \prod_{j>i} \sin^2 \frac{k'_j - k'_i}{2} \prod_{i,j} \sin^{-2} \frac{k'_i - k_j}{2}. \tag{9}$$

For the matrix element entering $B_Q(\omega)$, a similar expression holds with N replaced by $N-1$. With such an expression, it becomes possible to calculate the spectral functions numerically. To do that, we generate the quantum numbers I_j and calculate the energy and the product of Eq. (9). It turns out that the sum rules $\int_{-\infty}^{\infty} A_Q(\omega)\,d\omega = 1 - N/L$ and $\int_{-\infty}^{\infty} B_Q(\omega)\,d\omega = N/L$ hold separately for each Q. Moving from $Q=\pi$ to $Q=0$, the effect of the many-particle excitations becomes important. The weight of the Van Hove singularity decreases; a power-law singularity appears near the Fermi energy and a tail appears beyond the Van Hove singularity. This tail comes from the incoherent part of $A_Q(k\sim\pi,\omega)$ and $B_Q(k\sim 0,\omega)$, and its weight increases when Q decreases. Including up to three particle-hole excitations, we already get almost all the spectral weight. For instance, for $L=60$ we get 99.993% of the total weight in the worst case, namely, for $Q=0$. So, for all practical purposes, we can limit ourselves to three particle-hole excitations. This is an important observation because the number of states grows exponentially with the size, and to take into account all the states is possible only for smaller systems ($L\approx 30$).

We are now in a position to calculate numerically $A(\omega)$ and $B(\omega)$, and a typical result is presented in Fig. 2. Note that the following sum rules are satisfied [18,11]: $\int_{-\infty}^{\infty} A^{\mathrm{LHB}}(\omega)\,d\omega = 2(1-N/L)$ and $\int_{-\infty}^{\infty} A^{\mathrm{UHB}}(\omega)\,d\omega = \int_{-\infty}^{\infty} B(\omega)\,d\omega = N/L$.

The most interesting and surprising result is that, instead of going to zero, as the Luttinger liquid theory predicts, the spectral functions increase when $\omega\to\varepsilon_F$, where $\varepsilon_F = -2t\cos 2k_F$ is the Fermi energy of the spinless fermions and $k_F=\pi N/2L$ is the Fermi momentum of the fermions with spin. In fact, using the same framework, we can prove analytically that they diverge in that limit. To do that, we first use the fact that the low-energy spectrum consists of towers of excitations centered at momenta $(N+1)Q/L + 4pk_F$, $p=0,\pm1,\pm2,\ldots$, to write $A_Q(\omega)$ as the sum of the contributions coming from each tower $\tilde{A}_Q^p(\omega)$. The lowest excitation in tower p corresponds to a set of densely packed quantum numbers I_j shifted by p. From the definition of the momenta k_j, this is equivalent to imposing a twist of wave vector $Q+2p\pi$, so that $\tilde{A}_Q^p(\omega)=\tilde{A}_{Q+2p\pi}^0(\omega)$. So all we have to do is calculate $\tilde{A}_{\tilde{Q}}^0(\omega)$, where $\tilde{Q}$ can take values inside and outside the first Brillouin zone. Now, $\tilde{A}_{\tilde{Q}}^0(\omega)$ has peaks at energies $\varepsilon_0 + ju_c 2\pi/L$, $j=1,2,\ldots$, where ε_0 is the energy of the lowest peak in the tower. This energy is equal to $E_0^{N+1}(\tilde{Q}) - E_0^N = \varepsilon_F + \pi u_c(1+\alpha_{\tilde{Q}})/L$, where

$$\alpha_{\tilde{Q}} = \frac{1}{2}\left(\frac{\tilde{Q}}{\pi}\right)^2 - \frac{1}{2}. \tag{10}$$

So $\tilde{a}_{\tilde{Q}}^0(\omega)$ can be written as $\sum_j \tilde{a}_{\tilde{Q}}^j \delta(\omega - \varepsilon_0 - ju_c 2\pi/L)$. From Eq. (9), one can show that

$$\tilde{a}_{\tilde{Q}}^j = \frac{(1+\alpha_{\tilde{Q}})(2+\alpha_{\tilde{Q}})\cdots(j+\alpha_{\tilde{Q}})}{j!}\,\tilde{a}_{\tilde{Q}}^0 + O(1/L)$$
$$\approx \frac{(j+1/2+\alpha_{\tilde{Q}}/2)^{\alpha_{\tilde{Q}}}}{\Gamma(\alpha_{\tilde{Q}}+1)}\,\tilde{a}_{\tilde{Q}}^0 \tag{11}$$

and

$$\tilde{a}_{\tilde{Q}}^0 = \frac{1}{L}(L\sin\pi n)^{-\alpha_{\tilde{Q}}} f(\tilde{Q}) + O(1/L), \tag{12}$$

where the dependence on size and filling is taken care of. If we put it all together, we get

$$\tilde{A}_{\tilde{Q}}^0(\omega) \approx \frac{1}{2\pi u_c}\,\frac{1}{\Gamma(\alpha_{\tilde{Q}}+1)}\left(\frac{\omega-\varepsilon_F}{2\pi u_c \sin\pi n}\right)^{\alpha_{\tilde{Q}}} f(\tilde{Q}). \tag{13}$$

The function $f(\tilde{Q})$ for $\tilde{Q}\ll L$ satisfies the recursion relation

$$f(\tilde{Q}+\pi) = f(\tilde{Q}-\pi)\,\frac{\Gamma(\tilde{Q}/2\pi)^2}{\Gamma(-\tilde{Q}/2\pi)^2}\,\pi^{2\tilde{Q}/\pi}, \tag{14}$$

where $f(\pi)=1$, and in the interval from $=0$ to π it can be approximated within 0.01% by

$$\ln f(\tilde{Q}) \approx -0.3047 + 0.3248\tilde{Q}^2/\pi^2 - 0.0201\tilde{Q}^4/\pi^4.$$

Finally, because of the divergence of $C_{\sigma,N}(Q)$ and $D_{\sigma,N}(Q)$ at $Q=\pi/2$, $A^{\mathrm{LHB}}(\omega)$ is dominated close to ε_F by $A_{\pi/2}(\omega)$. This function is itself dominated by $\tilde{A}_{\pi/2}^0(\omega)$, which diverges with the exponent $\alpha_{\pi/2} = -3/8$ at ε_F. So, $A^{\mathrm{LHB}}(\omega)\propto|\omega-\varepsilon_F|^{-3/8}$ near ε_F. The whole proof can be reproduced for $B(\omega)$ which also diverges as $|\omega-\varepsilon_F|^{-3/8}$. Let us note that this power law cannot be clearly identified numerically with large but finite systems because there are other subdominant diverging contributions.

This divergence of $A^{\mathrm{LHB}}(\omega)$ with exponent $-3/8$ is different from the prediction of the Luttinger liquid theory according to which $A^{\mathrm{LHB}}(\omega)$ should vanish as $|\omega-\varepsilon_F|^{\alpha}$, where α, the exponent that also enters the

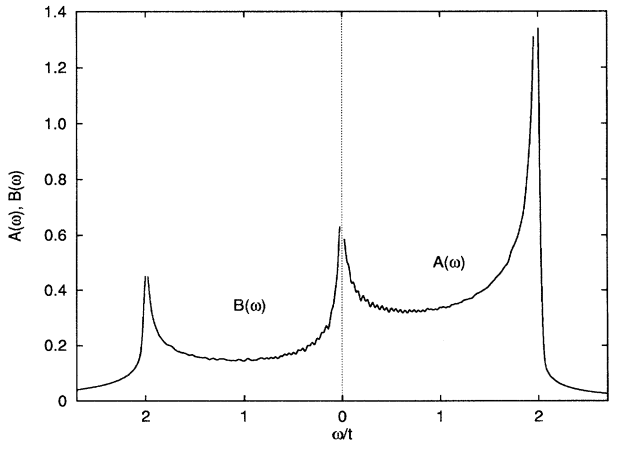

FIG. 2. $A^{\mathrm{LHB}}(\omega)$ and $B(\omega)$ for the quarter-filled $U\to+\infty$ Hubbard model with $L=260$ and $N=130$.

momentum distribution function, is known to be equal to $1/8$ in the $U \to +\infty$ limit. This apparent contradiction can be lifted as follows. First, we note that the exponent $-3/8$ can be explained very simply on the basis of the Green's function of the large-U Hubbard model [9] which is given by

$$G(x,t) \sim \frac{e^{i(k_F x - \varepsilon_F t)}}{(x - u_c t)^{1/2}(x - u_s t)^{1/2}} \frac{1}{(x^2 - u_c^2 t^2)^{1/16}}.$$

If we set $u_s = 0$, then $A(\omega)$ behaves like

$$\int dt\, G(x = 0, t) e^{i\omega t} \sim \int dt \frac{e^{i(\omega - \varepsilon_F)t}}{t^{5/8}} \sim |\omega - \varepsilon_F|^{-3/8},$$

while, if u_s is finite, it behaves like

$$\int dt\, G(x = 0, t) e^{i\omega t} \sim \int dt \frac{e^{i(\omega - \varepsilon_F)t}}{t^{9/8}} \sim |\omega - \varepsilon_F|^{1/8}.$$

However, in both cases, n_k behaves like

$$\int dx\, G(x, t = 0) e^{ikx} \sim \int dx \frac{e^{i(k - k_F)x}}{x^{9/8}} \sim |k - k_F|^{1/8}.$$

So, as long as spin velocity $u_s > 0$, or equivalently $U < +\infty$, the behavior very close to ε_F is given by $|\omega - \varepsilon_F|^{1/8}$, but this behavior is limited to frequencies $|\omega - \varepsilon_F| < u_s \sim t^2/U$. In the limit $U \to +\infty$, this domain shrinks to a single point, $\omega = \varepsilon_F$, and the spectral function diverges as $|\omega - \varepsilon_F|^{-3/8}$. If U is large but finite, there will be a peak in the spectral function at $\omega \sim t^2/U$ reminiscent of this divergence. This seems to be consistent with the Monte Carlo results of Preuss *et al.* [13], which show an increase of the spectral functions close to the Fermi level.

The implications for the experimental observation of the Luttinger liquid behavior are rather dramatic. To be able to see a difference from a step function in spite of the finite resolution, α should be large enough, which means one should consider strongly correlated systems. But the present calculation shows that the range of validity of the asymptotic law $(\omega - \varepsilon_F)^\alpha$ becomes very small if the correlations are too big. Whether realistic models of one-dimensional conductors with intermediate values of the repulsion terms can lead to measurable effects remains to be seen.

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