Spectral Properties of the One-Dimensional Hubbard Model

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The spectral properties of the 1D Hubbard model are obtained from quantum Monte Carlo simulations on large systems ($N = 84$) using the maximum entropy method. It is shown for the first time that the one-particle excitations are characterized by dispersive cosinelike bands, in extremely good agreement with slave-boson mean-field ones. Velocities for spin and charge excitations are obtained that lead to a conformal charge $c = 0.98 \pm 0.05$. An exact sum rule for spin and charge excitations is fulfilled accurately with deviations of at most 10% only around $2k_F$.

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Since Anderson [1] proposed that the high-T_c superconductors (HTS) should be considered as Luttinger liquids [2], a great deal of interest was focused on such systems. The best known Luttinger liquids are the Luttinger and the Hubbard model (HM), both in one dimension (1D). In spite of the fact that both models can be solved exactly [3,4], very little was known about their dynamical properties until recently.

In the case of the Luttinger model, the spectra for collective excitations can be easily obtained by bosonization [3], whereas the one-particle properties were calculated only recently [5,6]. However, since lattice effects are neglected in this model, the results obtained give only the asymptotic behavior for vanishing excitation energy. Since this region is the most difficult to be accessed by photoemission experiments, further progress is necessary in order to clarify the situation for the HTS.

Lattice effects are contained in the 1D HM, that has an exact solution by Bethe ansatz (BA) [4]. A number of authors succeeded in extracting from BA information about spectral properties [7–11], however, many of these results are limited to special situations (e.g., half filling, $U \to \infty$ and/or one-hole doping, or $\omega = 0$). Only recent progress achieved in the frame of conformal field theory [12] led to the asymptotic properties of correlation functions irrespective of the coupling constant and doping. Complementary to these achievements, a Landau-Luttinger liquid theory was advanced in order to describe the low-energy properties of the 1D HM [13]. In spite of the importance of these developments, a general description of spectral properties at finite frequencies is still lacking.

We present in this Letter spectra for one-particle, spin- and charge-density excitations obtained with the maximum entropy method (MEM) [14] from quantum Monte Carlo (QMC) simulations of the 1D HM. These spectra were obtained for system sizes up to 84 sites, allowing for a precise identification of finite-size effects. One particle spectra are presented for the first time that lead to a clear determination of a dispersion relation, in contrast with previous methods. For half filling, two bands appear that agree extremely well with the slave-boson mean-field (SBMF) [15] dispersion obtained in the antiferromagnetic state. The spectral weight, however, is not evenly spread between the two bands. When the system is doped, a depression appears in the density of states at the Fermi energy, in sharp contrast to results obtained recently by similar methods on the two-dimensional (2D) HM [16], where a peak develops near that region. A single band is observed, again in very close agreement with SBMF results in the paramagnetic state. Thus, it appears as a general feature that the SBMF bands are able to accurately describe the dispersion of the one-particle excitations in spite of the Luttinger-liquid character of the system. This situation is reminiscent of the HTS, where band-structure calculations [17] agree well with angle-resolved photoemission results [18], while other measurements seem to signal a departure from a Fermi liquid [1]. The accuracy of the method is tested by comparison with known exact results for spin- and charge-density excitations. At half filling, both the "spinon" velocity and the full dispersion relation for spin excitations agree with results extracted from BA [7]. In the doped case, the spinon and holon velocities obtained lead to a value of the conformal charge of $c = 0.98 \pm 0.05$ for $N = 84$ sites, in very good agreement with the exact value $c = 1$ [12]. The spectrum for spin and charge excitations fulfills excellently a frequency sum rule [19] for each k point except for those close to $2k_F$, where departures of at most 10% are observed. This is to our knowledge the most extensive test of the MEM in connection with QMC simulations for the HM.

We consider the 1D HM described by the following Hamiltonian:

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

where $c^{(\dagger)}_{i,\sigma}$ are annihilation (creation) operators for an electron at site i with spin σ, and $n_{i\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$. Systems with a number of sites N ranging from 12 to 84 with periodic boundary conditions were simulated for inverse temperatures $\beta = 1/k_B T$ up to $\beta = 20/t$ and interaction strength $U = 4t$. The simulations were performed with the grand

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canonical algorithm [20], where the smallest values of $\Delta\tau$, i.e., the time slice, was between 0.1 and 0.125. The analytic continuation of the data to real frequencies was performed with the MEM [14], when the only "prior knowledge" used was the positivity of the spectral functions. We have chosen an uninformative default model $m_i = \varepsilon$, where ε is a small quantity that merely suppresses noise in regions of insufficient information. The regularization parameter has been determined self-consistently by classical MEM. For further technical details we refer to previous applications of the MEM to the single impurity Anderson model [21], the 1D [22] and 2D [23] Heisenberg antiferromagnet, and the 2D HM [16,24].

We first compare the density of states $D(\omega)$ of a ring with 12 sites between data from QMC simulations and exact diagonalization (ED), both for half filling [Fig. 1(a)] and for the doped case [Fig. 1(b)] with $\langle n\rangle = 0.833 \simeq 5/6$. Although the MEM is not able to resolve the rich structure obtained in ED, there is a good agreement in the shape and distribution of weight in the half-filled case. In the doped case, the MEM can reproduce well the structures close to the Fermi energy but has the general tendency of shifting weight to lower energies as one goes to higher energies due to the Laplace-transformation kernel. In particular, the pseudogap observed in ED between those states, stemming from the upper Hubbard band (UHB) brought down by doping to the top of the lower Hubbard band (LHB) [25], and the remaining of the UHB, does not appear in the MEM data. We remark here that no structure in the following spectra are related to ringing. A coarse graining of the data and subsequent use of the MEM do not show appreciable change in the observed features. Details will be presented elsewhere.

In the following the data obtained for our largest system ($N = 84$) well beyond the capability of ED are shown [26]. We discuss first the spectral properties at half filling. Figure 2(a) shows $D(\omega)$ and the spectral function $A(k,\omega)$ is shown in Fig. 2(b), where a dispersion can be clearly seen. Figure 2(c) shows the location of the maxima of $A(k,\omega)$ with the errors assigned by the MEM. These errors give the uncertainty in the location of those maxima. The full curve is the result of a SBMF calculation, where antiferromagnetic order is assumed. A remarkable coincidence is obtained. However, the spectral weight is shared quite differently, since although most of the weight of the LHB appears for $k \lesssim \pi/2$, and the weight of the UHB is mostly concentrated in the region $k \lesssim \pi/2$, around $k = \pi/2$ weight is split between the two bands.

Figure 3 shows the imaginary part of the spin susceptibility $\chi_S(k,\omega)$ and the dispersion extracted from the maxima of Fig. 3(a). From the slope of the dispersion around $k = 0$, we calculate a spinon velocity $v_s/t = 1.23 \pm 0.11$. The exact value extracted from BA [7] $v_s^{\mathrm{BA}} = 2tI_1(2\pi/U)/I_0(2\pi/U)$, where I_0 and I_1 are modified Bessel functions, is for $U/t = 4$, $v_s^{\mathrm{BA}}/t = 1.2263$ [27], that compares remarkably well with our value. The full line in Fig. 3(b) corresponds to the dispersion extracted from Bethe ansatz [7] showing that the agreement with the exact results in the thermodynamic limit is not limited to $\omega \to \infty$ but extends to finite frequencies. For reasons of space, the equivalent quantities to those in Fig. 3 but now for charge-density excitations, are not displayed. We observe a rather broad structure with most of the weight around U, with a gap for $k \to 0$ that agrees within the errors with the one obtained in the one-particle spectrum.

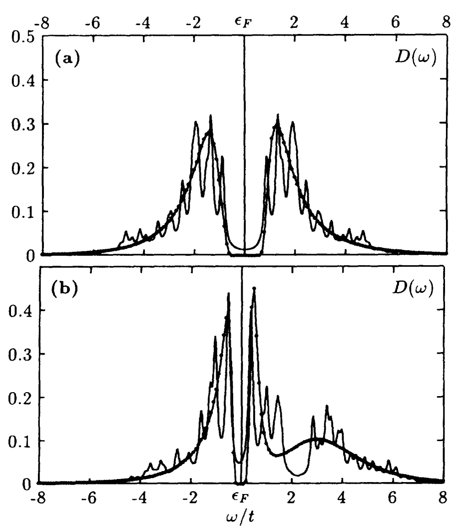

FIG. 1. A comparison between QMC and MEM (lines with dots) and ED (full line) of the density of states for $N = 12$ sites: (a) Half filling; (b) $\langle n\rangle = 5/6$ ($\beta = 16, U = 4$).

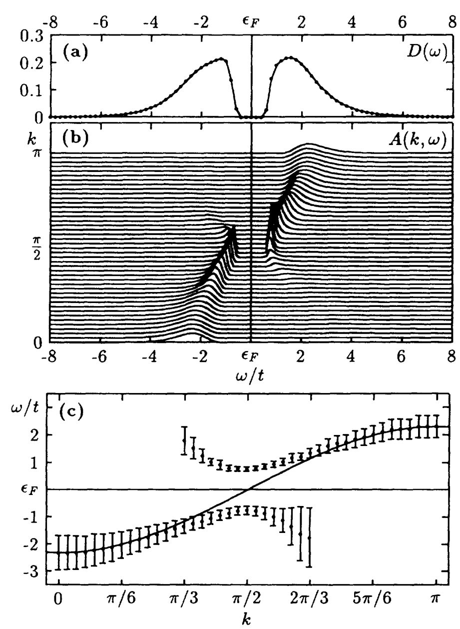

FIG. 2. One-particle excitation for 84 sites at half filling: (a) Density of states; (b) $A(k,\omega)$; (c) maxima of $A(k,\omega)$, the solid line is a cosine function adjusted to the bandwidth ($\beta = 20, U = 4$).

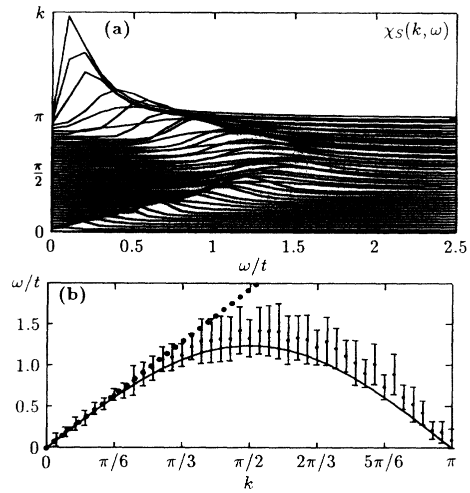

FIG. 3. Spin excitations at half filling: (a) $\mathrm{Im}\chi_S(k,\omega)$; (b) maxima of $\mathrm{Im}\chi_S(k,\omega)$, the dotted line gives the slope at $k = 0$ ($v_s/t = 1.23 \pm 0.11$), and the full line stems from Bethe ansatz.

Now we consider the doped case, where for definiteness we have chosen a hole doping $\delta \simeq \frac{1}{6}$. Figure 4 shows $D(\omega)$, $A(k,\omega)$, and the dispersion of the maxima in $A(k,\omega)$. A depression in $D(\omega)$ is observed at the Fermi energy ϵ_F, that we assign to the fact that a Luttinger liquid has a density of states $D(\omega) \sim |\omega|^\alpha$. The vanishing of $D(\omega)$ at the Fermi energy cannot be seen in the simulation, since due to the small power α ($\alpha \simeq 0.038$ for $U/t = 4$ [28]), an unrealistically high resolution would be necessary. The observed behavior of $D(\omega)$ is opposite to the one obtained in recent simulations of the 2D HM [16], where a peak develops near the Fermi level, as in the infinite-dimensional HM [29]. Again, the "band structure" obtained from $A(k,\omega)$ can be very well described by the SBMF paramagnetic band for $U = 4t$ within the error bars. At $U = 4$ we still do not observe significant weight in $A(k,\omega)$ due to the UHB. However, as was discussed in connection with ED, this can be due to the shifting of weight to lower frequencies by the MEM.

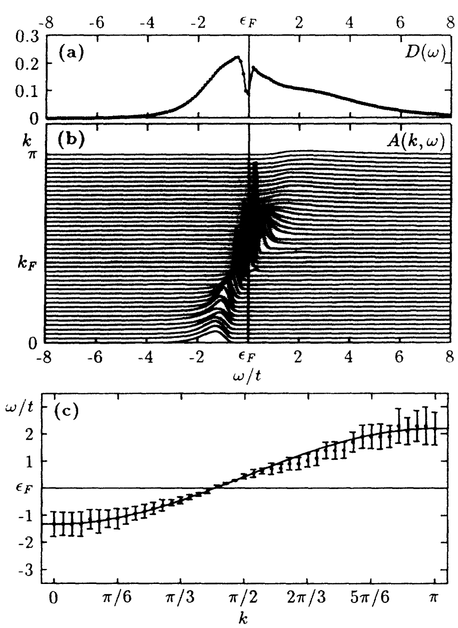

FIG. 4. The same as Fig. 2, but now for $\langle n\rangle = 5/6$.

The spectra for spin excitations are shown in Fig. 5. Again, a linear dispersion appears for low energies around $k = 0$ (inset of Fig. 5). Unfortunately the same resolution is not obtained around $2k_F = 5\pi/6$. However, these data can be combined with the corresponding ones for charge-density excitations (Fig. 6) where features appear around $2k_F$ and $4k_F$ as expected. With the values of spinon and holon velocities extracted from the dispersion curves, it is possible to obtain the conformal charge of the HM, that is known exactly to be $c = 1$. Such a relationship stems from the conformal invariance of the model and has the following form [12]:

$$\frac{E_0(N)}{N} - \epsilon_0 = -\frac{\pi}{6N^2}(v_s + v_c)c + \mathcal{O}\left(\frac{1}{N^2(\ln N)^3}\right), \tag{2}$$

where $E_0(N)$ is the ground-state energy of the system with N sites, ϵ_0 is the ground-state energy per site in the thermodynamic limit, v_s and v_c are the spinon and holon velocities, respectively, and c is the conformal charge of the model. The value obtained for $N = 84$ is $c = 0.98 \pm 0.05$, where E_0 and ϵ_0 were determined from Bethe ansatz [4]. Such a stringent test shows that QMC together with the MEM are able to give reliable real frequency data for low-lying excitations of the HM. It should be stressed, that the insets in Figs. 5 and 6 make manifest charge-spin separation in the model, since $v_c > v_s$. This is clearly seen in all system sizes simulated. Finally, we consider an exact sum rule for the first frequency moment of $\mathrm{Im}\chi_S(k,\omega)$ [19]:

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\omega\,\mathrm{Im}\chi_S(k,\omega) &= -\langle[[H,S^z(k)],S^z(-k)]\rangle \\ &= -2t(1-\cos k)\langle H_{\mathrm{kin}}\rangle, \end{aligned}\tag{3}$$

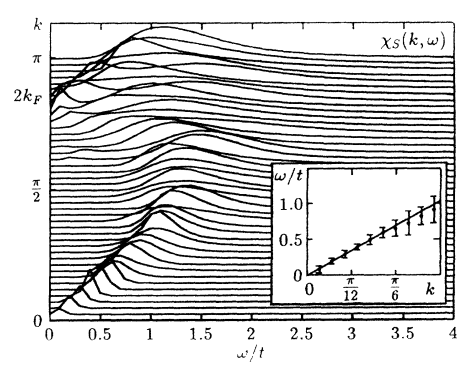

FIG. 5. $\mathrm{Im}\chi_S(k,\omega)$ for $\langle n\rangle = 5/6$. The inset shows the linear part of the dispersion around $k = 0$. The slope gives $v_s/t = 1.33 \pm 0.09$.

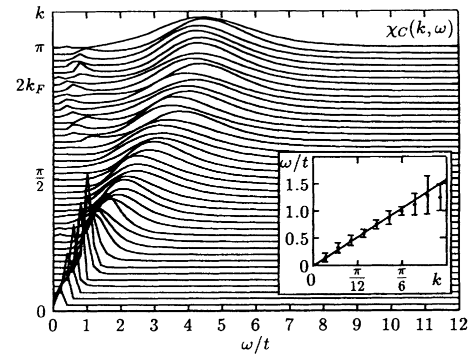

FIG. 6. The same as Fig. 5 but for the charge susceptibility ($v_c/t = 2.02 \pm 0.14$).

[for $\mathrm{Im}\chi_C(k,\omega)$ the same holds] where $S^z = \frac{1}{2}(n_\uparrow - n_\downarrow)$ and $\langle H_{\mathrm{kin}}\rangle$ is the expectation value of the kinetic energy, that can be accurately calculated by QMC. We find [26] that the sum rule is fulfilled accurately over most of the Brillouin zone (deviations of less than 1%), with the exception of $k \gtrsim 2k_F$, where deviations ($\sim$10%) are obtained. They are probably due to a broad continuum similar to the one present in the 1D Heisenberg antiferromagnet around $k = \pi$ [13,30]. This result together with the conformal charge obtained demonstrate the degree of reliability of the numerical data from low to intermediate frequencies and for very large systems that are well beyond the capability of other methods like ED.

Summarizing, we have presented real-frequency spectra for one-particle, spin- and charge-density excitations in the 1D Hubbard model both in the insulating and in the metallic phases. The dispersion of the one-particle excitations is obtained for the first time. It agrees remarkably well with SBMF bands both at half filling and in the doped case in spite of the non-Fermi-liquid character of the system. The density of states in the doped case shows a depression at the Fermi energy as expected for a Luttinger liquid but in sharp contrast to recent results in two dimensions [16]. The dispersion obtained for the spin excitations at half filling agrees with results from BA within the error bars. In the doped case, charge-spin separation is obtained, where the spinon and holon velocities lead to an excellent agreement with the exact value for the conformal charge of the Hubbard model. The quality of the spectral data at intermediate frequencies is checked by an exact sum rule, showing that only around $2k_F$, a departure of around 10% is present. The comparison with such a broad spectrum of exact results demonstrates the reliability of QMC in conjunction with the MEM for the HM.

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