Brief Reports

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Correlation functions and dynamical properties of the one-dimensional Hubbard model

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The oscillating behaviors of correlation functions in real space are determined for the one-dimensional Hubbard model with various electron densities and arbitrary values of U by the exact-diagonalization technique. Of them, the oscillation of density-density correlation function depends drastically on the value of U and doping: The oscillation occurs at $2k_F$ for small U or large doping and at $4k_F$ for large U or small doping. The pairing susceptibility in the singlet channel shows $2k_F$ oscillations while there are no oscillations in the triplet channel. The hole spectral function is also calculated, and it is found that in the large-U limit the dynamical property of a single hole depends strongly on the background with doping.

The Hubbard model is one of the simplest Hamiltonians for studying a strongly correlated electron system and is considered as a possible candidate to describe high-T_c superconductivity. Although high-T_c oxide materials are two-dimensional (2D) systems, it is interesting to study the one-dimensional (1D) model since some properties in the 1D case are believed to be shared by the 2D system.[1]

Interacting 1D electron systems generally behave as Luttinger liquids[2] in which the correlation functions have power-law decays with the critical exponents which depend on the interacting strength. For the 1D Hubbard model, the exact solution was obtained some time ago by Lieb and Wu[3] and the thermodynamics was clarified by many authors.[4,5] Many important properties, such as correlation functions and the corresponding critical exponents in some limits (e.g., weak coupling and large U), have also been studied recently by both analytical and numerical approaches.[6-10] However, these quantities as well as the dynamical property at arbitrary U still need to be investigated by a systematic method.

The purpose of this paper is to calculate various correlation functions in real space and study the dynamical properties of holes for the 1D Hubbard model with various electron densities and arbitrary U by using the exact-diagonalization technique. Because of the limitation of finite sites, the critical exponents which govern the asymptotics of the correlation function cannot be calculated directly with our method. But, the oscillating behavior of the correlation in real space corresponding to the singularity in momentum space can be determined. In addition, through the calculation of the spectral function, we find that the hole dynamical property depends strongly on the dopant concentration: In the large-U limit, when a hole moves in a high doping background, the quasiparticle peak at the bottom of the spectrum always shows up, while when it moves in a half-filling background, the low-lying excitation peak is smeared out.

The 1D Hubbard model is given by

$$H=-\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where the hopping matrix element has been taken as unity for convenience. Here we use the Lanczos method[11,12] to obtain the energy and the wave function of the ground state of a finite-site system. By examining the convergence of the results, we confirm that the ground-state energy and wave function are accurately determined (about 12 and 6 decimals, respectively). In order to treat the sign caused by the exchange of electrons properly, we choose a periodic boundary condition for $N=4m+2$ and an antiperiodic boundary condition for $N=4m$, with N being the electron number and m an integer. For any electron density n ($=N/N_a$, N_a is the site number) and U, we have compared our results of the ground-state energy and the local moment $L_0=(1/N_a)\sum_i\langle \mathbf{S}_i^2\rangle$, where $\mathbf{S}_i$ is the spin operator at the ith site, with those of the Bethe-ansatz exact solution at the thermodynamical limit,[5] and found that for $N_a=8$ our results are already very close to the Bethe-ansatz solution.

With the ground-state wave function obtained by the Lanczos method, we can easily calculate various physical quantities in real space. First we consider the distribution function defined in real space by

$$\bar{C}_j=\frac{1}{N_a}\sum_{i,\sigma}\langle c_{i\sigma}^{\dagger}c_{i+j\sigma}\rangle\ , \tag{2}$$

which has been computed on different Hubbard chains from $N_a=8$ to 12 sites. It is found that for small U, $\bar{C}_j$ shows a k_F oscillation, which means the behavior of fermions favors free electrons, while for large U, in addition to the k_F oscillations, $\bar{C}_j$ has a weak modulation at $3k_F$. These results correspond exactly to the singularities of distribution functions at k_F and $3k_F$ in momentum space in the large-U limit, which have been found by both analytical[8,10] and numerical[9] approaches. By increasing the value of U, we find that although weak $3k_f$ oscillations can be enhanced, the k_F oscillations of the distribution function cannot be removed, from which we can see how the dynamics of an electron is affected by spin background. For example, one might expect that in the large-U limit, electrons should behave like spinless fermions, so their distribution in real space may have an oscillation at $2k_F$. As we have shown above, the rearrangement of spin configurations in the hopping process plays a very important role in smearing out the $2k_F$ singularity, leading to a singularity at k_F and a weak oscillation at $3k_F$ instead.

Another interesting quantity is the spin-spin-correlation function:

$$\bar{S}_j=\frac{1}{N_a}\sum_i \langle S_i^z S_{i+j}^z \rangle \ . \tag{3}$$

We have performed the calculation for $\bar{S}_j$ with various electron densities and values of U and found that a $2k_F$ oscillation always shows up from weak-coupling region to the large-U limit. At half-filling, this result is equivalent to that of the 1D $S=\frac{1}{2}$ Heisenberg model since in this case $k_F=\pi/2$. With the increase of the distance x_j, the amplitude of $\bar{S}_j$ is decreased. This result indicates that there is no long-range antiferromagnetic order in a 1D model, which is different from that of the higher-dimensional system. When the system is away from half-filling, the oscillation of the spin-spin correlation is incommensurate. The increase of U can only enhance the amplitude of $\bar{S}_j$, which results in increasing the spin-spin correlation length. Doping also leads to a decrease of the amplitude of $\bar{S}_j$, but the $2k_F$ oscillation cannot be smeared out by varying the electron density. In this sense, the effect of doping on $\bar{S}_j$ is equivalent to the decrease of U. The $2k_F$ singularity of the spin-spin correlation in momentum space has been also observed by other approaches.[6-10]

Now we present the results of the density-density correlation and the pairing susceptibility. The density-density correlation function in real space is defined by

$$\bar{N}_j=\frac{1}{N_a}\sum_i \langle n_i n_{i+j} \rangle \ . \tag{4}$$

Figure 1 shows the results of density-density correlation function with various values of U at quarter filling for $N_a=12$. We find a noteworthy result, namely that the oscillating behavior of $\bar{N}_j$ depends drastically on the value of U. It can be seen from this figure that for $U=0$, $\bar{N}_j$ has an obvious oscillation at $2k_F$ ($k_F=\pi/6$ in the present case). However, when we turn on U, the oscillation is shifted gradually away from $2k_F$. For $U\geq 5$, $2k_F$ oscillations are smeared out and oscillations show up at $4k_F$. The inset of Fig. 1 shows more clearly how the oscillating behavior of the density-density correlation changes with varying values of U. We have done the same calculation for different electron densities and found that the smaller the doping, the larger U is needed to create an oscillation at $4k_F$ and eliminate that at $2k_F$. Near half-filling, as U is increased, this correlation function is rapidly suppressed because the number of doubly occupied sites is reduced. Our results support the idea that in the large-U limit, the description of the charge dynamics of the system is possible in terms of noninteracting spinless fermions, where k_F has to be replaced by $2k_F$. Hence the oscillation at $2k_F$ has to be modified correspondingly in this limit and the leading contribution to the density-density correlation function is the oscillations at $4k_F$.

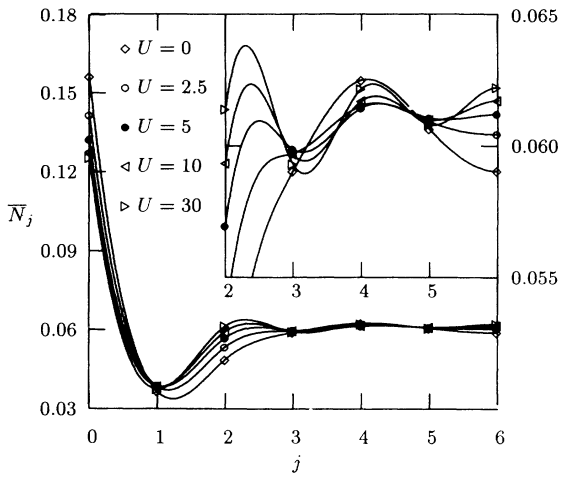

FIG. 1. Real-space density-density correlation function $\bar{N}_j$ (see text) at quarter filling for a 12-site system. The inset shows more clearly that the oscillating behavior of $\bar{N}_j$ changes with U. Here the solid lines are drawn as guides to the eyes.

Another important quantity is the pair susceptibility:

$$\bar{B}_j^{S,T}=\frac{1}{N_a}\sum_i \langle (b_i^{S,T})^\dagger b_{i+j}^{S,T} \rangle \ , \tag{5}$$

where superscript S (T) stands for the singlet (triplet) channel and the operators $b_i^{S,T}$ are defined by

$$b_i^{S,T}=\frac{1}{\sqrt{2}}(c_{i\uparrow}c_{i+1\downarrow} \mp c_{i\downarrow}c_{i+1\uparrow}) \ . \tag{6}$$

Figures 2(a) and 2(b) show $\bar{B}_j^{S,T}$ for a 12-site system with four holes and six holes at different values of U. It is clear that for all values of U (from $U=0$ to 30) the pair susceptibility in singlet channel has $2k_F$ oscillations, which means that the oscillating behavior of $\bar{B}_j^S$ does not depend on U. This behavior is very similar to that of the spin-spin correlation. The $2k_F$ oscillations in $\bar{B}_j^S$ have also been obtained by the bosonization approach for the whole region of U.[7,8] However, a surprising result is found, namely that there does not exist any oscillation in $\bar{B}_j^T$ for all values of U and its magnitude is much smaller

compared to that of $\bar{B}_j^S$.

From Fig. 2 we see that $\bar{B}_j^{S,T}$ are the smooth function of U and have similar oscillating behaviors for all values of U. At $U=0$, $\bar{B}_j^{S,T}$ can be expressed analytically as

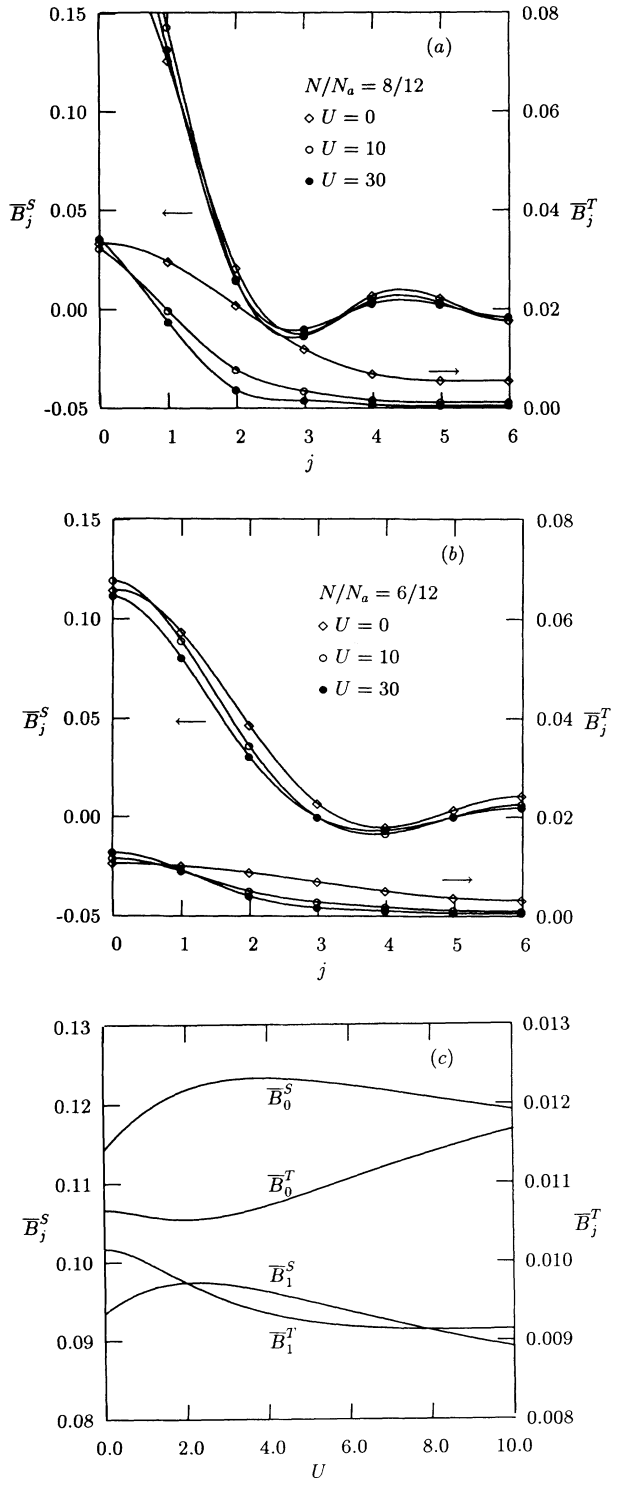

FIG. 2. Real-space pairing susceptibilities $\bar{B}_j^{S,T}$ (see text) for 12-site systems with (a) $N/N_a=8/12$ and (b) $N/N_a=6/12$. (c) shows how $\bar{B}_j^{S,T}$ at $j=0$ and 1 change with U for quarter filling. The solid lines are simply guides to the eyes.

$$\bar{B}_j^{S,T}=\frac{1}{2\pi^2}\left[\frac{1-\cos(2k_F x_j)}{x_j^2} \pm\frac{1}{x_j^2-a^2}[\cos(2k_F a)-\cos(2k_F x_j)]\right], \quad (7)$$

where a is the lattice constant. It is obvious that for large x_j, $\bar{B}_j^S \propto x_j^{-2}[1+\cos(2k_F a)-2\cos(2k_F x_j)]$ shows $2k_F$ oscillations while $\bar{B}_j^T \propto x_j^{-2}[1-\cos(2k_F a)]$ has no oscillations, which is consistent with our numerical calculations. The same behavior of $\bar{B}_j^{S,T}$ has also been found for the so-called supersymmetric t-J model with $J=2t$ based upon the Bethe-ansata solution.[13]

Another point that should be made here is that $\bar{B}_j^{S,T}$ is not a monotonic function of U. The on-site and the nearest-neighbor pair susceptibilities as functions of U at quarter filling for 12 sites are shown in Fig. 2(c). The on-site correlation in the singlet channel $\bar{B}_0^S$ has a maximum value around $U=4$, while the maximum of the nearest-neighbor correlation $\bar{B}_1^S$ is located at $U=2$. The opposite situation is found in the triplet channel. Comparing their magnitude, only the pair correlation in the singlet channel is important. From Fig. 2(c) we can see that $\bar{B}_j^S$ (with $j=0,1$) has a maximum correlation in intermediate U.

Now we present the results for the hole spectral function $A(k,\omega)$ with momentum k and energy ω (with respect to the ground state of N electrons). The spectrum can be expressed as

$$A(k,\omega)=-\frac{1}{\pi}\,\mathrm{Im}G(k,\omega+E_0) \quad (8)$$

and the hole Green's function is defined by

$$G(k,\omega)=\int dt\, e^{i\omega t}\langle\psi_0|c_{k\sigma}^{\dagger}(t)c_{k\sigma}(0)|\psi_0\rangle\ , \quad (9)$$

where $c_{k\sigma}=\sum_i c_{i\sigma}e^{ikx_i}$. $\psi_0(E_0)$ is the ground-state wave function (energy) of an N_a-site system with N electrons, which we have obtained using the Lanczos approach. The momentum k should be chosen according to the boundary condition, which depends on the site and electron number. We have evaluated the spectral function by performing the Lanczos procedure on a wave function $|\Phi_0\rangle \propto c_{k\sigma}|\psi_0\rangle$ and by employing the Lanczos coefficients in the continued fraction representation of Eq. (8).[14]

In Figures 3(a)–3(d) we show how the density of states $D(\omega)$ $[=\sum_k A(k,\omega)]$ changes with the electron density and the value of U. At $U=0$, $D(\omega)$ shows δ-like peaks, which is consistent with the free-hole picture. In this case, the different peak can be identified with a particular given momentum $k \le k_F$. The lowest-energy peak in the figures corresponds to the lowest-lying excitation at k_F, while other peaks come from the allowed k below k_F. According to previous discussion, $D(\omega)$ in Figs. 3(a) and 3(c) are calculated in terms of the periodic boundary condition with allowed momenta $k=2\pi l/N_a$, $l=0,\pm1,\ldots,N_a/2$, while in Figs. 3(b) and 3(d) the antiperiodic boundary condition is used with allowed momenta $k=\pi(2l-1)/N_a$, $l=0,\pm1,\ldots,N_a/2$. We can see from the figures that the behavior of the spectral functions changes drastically with the increase of the

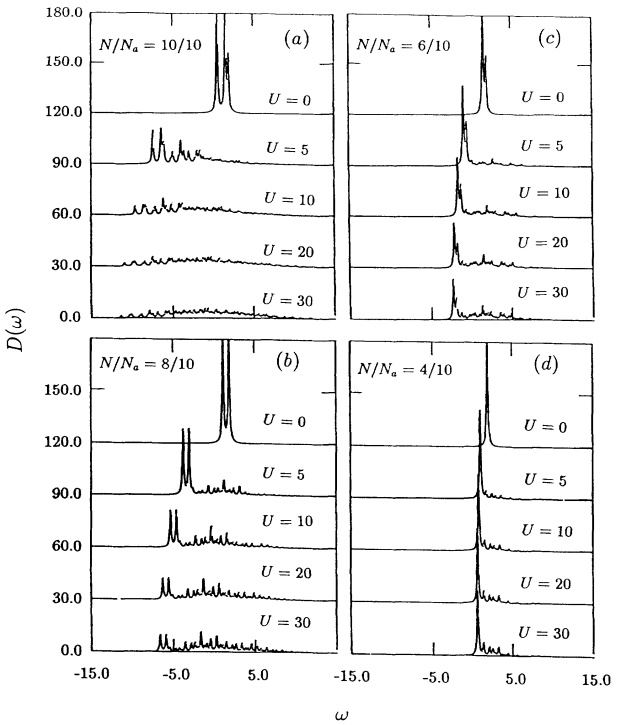

FIG. 3. Hole density of states $D(\omega)$ for 10-site systems with various U and electron densities with (a) $N/N_a=10/10$, (b) $N/N_a=8/10$, (c) $N/N_a=6/10$, and (d) $N/N_a=4/10$. $D(\omega)$ has been calculated with a hole lifetime of 0.1. From bottom to top the curves are shifted by 0, 30, 60, 90, and 120 on the vertical scale.

doping concentration. It is clear from Figs. 3(c) and 3(d) that when a hole moves in the four-hole and six-hole backgrounds (both cases are close to the quarter filling), the quasiparticle peak at the bottom of the spectrum still remains even at $U=30$, which means that the effect of U is not a crucial issue at high doping. This result is reasonable because the number of the doubly occupied sites is reduced at high doping, which causes U to be less important. The spectrum in Fig. 3(b) shows similar behavior except that at the large-U limit (say $U=20$ and 30) the low-lying peaks have almost equal weight with the high-energy excitations.

The interesting results have been found at half-filling. From Fig. 3(a) it can be seen that when $U \geq 10$ the low-lying peak at k_F almost disappears. This indicates that the conventional quasiparticle picture does not work in this case, which is very different from the 2D Hubbard model where the quasiparticle peak at the bottom of the spectrum always shows up regardless of how large U is. Here we attribute this disappearance of the quasiparticle peak to the singularity of the spectrum at k_F.

Another point we should note is that in Figs. 3(a)–3(d) the spectrum at $U=20$ is almost the same as that at $U=30$. This means that our results already reach the large-U limit at $U=20$. Thus we can convince that the spectrum at $U=20$ and 30 can represent the large-U behavior.

Summarizing, we have studied the oscillating behavior of various correlation functions in real space for the 1D Hubbard model by a numerical study of finite sites. Particularly, we have also calculated the hole spectral function and found that the hole dynamical properties depend strongly on the doping background.

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