Correlations in the one-dimensional almost-half-filled band Hubbard model in the large-U limit

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By a numerical study of finite-size lattices a picture is presented of the spin correlations around a hole in the almost-half-filled band Hubbard model. Using an effective Hamiltonian in the large-U limit, systems with up to 15 sites have been studied. In the same limit the two-hole correlation has been calculated and a weak attraction found between the two holes at finite, compared to infinite U.

I. INTRODUCTION

Numerical diagonalization of the Hamiltonian matrix for finite-size lattice systems has been used to study the correlations in the Hubbard model.[1] Recently there has been renewed interest in this model for the case of the almost-half-filled band,[2] partly due to the proposal of the two-dimensional model as candidate for the explanation of high T_c superconductivity.[3] The calculation, however, of correlation functions of the full Hubbard model by exact diagonalization has been limited to lattices of the order of six sites by the large dimension of the basis set.

In this work, by using an effective Hamiltonian in the large-U limit,[4] the problem reduces to one of dimension similar to the calculation of spin-$\frac{1}{2}$ chains and systems up to 15 sites can be studied. In the same limit Takahashi[5] has previously explored the spin of the ground state for some two- and three-dimensional lattices. The results presented here form a qualitative picture of the spin correlations in the one-dimensional (1D) model. Presumably this picture is particular to the 1D lattice as the topology of the lattice is crucial. From the work of Lieb and Mattis[6] it is known that the spin in the ground state of the 1D Hubbard model is quite generally the minimum allowed, while by Nagaoka's[7] work, for many three-dimensional lattices at the infinite U limit and almost-half-filled band, it is the maximum allowed. On the other hand, the nature of the ground state in two dimensions is still under discussion.[3]

In the following I first discuss the effective Hamiltonian used in the numerical calculation, its symmetries, and range of validity. Then the spin correlations around a hole are shown and compared to the spin correlations of the Heisenberg spin-$\frac{1}{2}$ chain. Finally the hole-hole correlation function is presented.

II. EFFECTIVE HAMILTONIAN AND METHOD

I consider the Hubbard model on a one-dimensional lattice with periodic boundary conditions

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

where $c_{i\sigma}(c^\dagger_{i\sigma})$ are annihilation (creation) operators of a fermion with spin $\sigma=\uparrow,\downarrow$, $n_{i\sigma}=c^\dagger_{i\sigma}c_{i\sigma}$, M the number of fermions, and N the number of sites. In the cases studied $M<N$. In the large-U limit an effective Hamiltonian can be derived[4] to order (t/U) acting only between states with M singly occupied sites and $N-M$ empty sites. Within it the number of empty sites (called holes) is well defined as in the large-U limit double occupancy of sites is only virtually allowed. The effective Hamiltonian consists of three terms: the kinetic energy of the hole

$$T_{\text{h}}=-t\sum_{i,\sigma}c^\dagger_{i\sigma}c_{i+1,\sigma}+\text{H.c.}\ ,$$

a Heisenberg spin-$\frac{1}{2}$ chain-type term

$$H_{\text{s}}=(t^2/U)\sum_i(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+1}-1)\ ,$$

where the sum over sites excludes the empty sites ($\boldsymbol{\sigma}_i$ are Pauli spin matrices), and two terms involving next-nearest-neighbor hopping of the hole, with and without flip of the intermediate spin

$$T_2=-(t^2/U)\sum_{i,\sigma}(c^\dagger_{i-1,\sigma}c_{i\sigma})n_{i,-\sigma}(c^\dagger_{i\sigma}c_{i+1,\sigma})+(c^\dagger_{i-1,-\sigma}c_{i,-\sigma})n_{i,-\sigma}(c^\dagger_{i\sigma}c_{i+1,\sigma})+\text{H.c.}$$

For even number of sites the Hamiltonian is electron-hole symmetric and the results are valid for the doubly occupied sites if $M>N$. This effective Hamiltonian preserves the translational and rotational symmetry of the Hubbard model and so the eigenstates are characterized by their total momentum K and spin S. Using the translational symmetry, the Hamiltonian matrix is diagonalized in every K momentum subspace separately. The lattices studied are divided in two sets: up to 15 sites with $N-1$ fermions (one hole) to calculate the spins correlations around the hole and up to 12 sites with $N-2$ fermions (two holes) to calculate the hole-hole correlation function. In the first set the maximum dimension of the reduced basis set is 3432 (for 15 sites) while in the second set it is 1386 (for 12 sites). Standard routines were used to diagonalize the Hamiltonian matrix for small size lattices and the Davidson method[8] for the largest size ones.

To check the range of validity of the calculation I compared the energy levels obtained from the effective Hamiltonian to the ones from the full Hubbard model for lattice sizes up to six sites. In the range of coupling $0<t/U<0.25$, the error is found to be of order $(t/U)^2$ or less than 10%. The results presented are in this range and all the quantities are calculated for the ground state.

III. CORRELATION FUNCTIONS

The first set of results are for lattices with $N=7$, 11, 15 sites and $N-1$ fermions. They are chosen because they have a nondegenerate ground state with spin $S=0$ and total momentum $K=0$ for all t/U. In other cases, having a degenerate ground state for $U=0$, there is sometimes crossing between ground states with different spin and momentum, cases not included in the Lieb and Mattis[6] analysis. Qualitatively, however, the correlation functions behave similarly.

In Fig. 1 the ground-state expectation value of the hole kinetic energy operator is presented for $N=11$ in the range $0<t/U<0.25$. In this range there is a reduction of the order of 5% in the kinetic energy of the hole due to spin fluctuations. It is remarkable, however, that this reduction is practically independent of the size of the system (of the order of one in a thousand between $N=7$ and 15 sites) suggesting that the screening of the hole is a local effect.

Next, in Fig. 2, the spin-spin correlation

$$g_1(n)=\langle \hbar_i \sigma^z_{i+1}\sigma^z_{i+n}\rangle$$

as a function of distance n from the hole for $N=15$ is shown. The operator $\hbar_i=(1-n_{i\uparrow})(1-n_{i\downarrow})$ determines if the site i is empty. Again, as for the hole kinetic energy, the results are, within a few percent, independent of the size of the system. Also plotted is the $\langle \sigma^z_i\sigma^z_{i+n-1}\rangle$ correlation for the Heisenberg spin-$\frac{1}{2}$ chain with periodic boundary conditions[9] and $\langle \sigma^z_1\sigma^z_n\rangle$ with open ends for a lattice with 14 sites. The latter can be simply obtained by setting the matrix elements of the hole kinetic energy and next-nearest-neighbor hopping equal to zero. There is short-range antiferromagnetic order with the spin correlations almost identical to that of a spin chain with periodic boundary conditions for $t/U\rightarrow 0$. As is shown in the Appendix, the two systems would have identical correlations in this limit if the next-nearest hopping was not included. For $t/U>0$ the hole becomes heavier and the spin correlations resemble those of the spin chain with open ends. They can be closely reproduced by a Heisenberg spin chain model where the spins at the ends, corresponding to $i-1$ and $i+1$, are linked with a bond of strength $J'\approx J[1-\alpha(t/U)]$ for small t/U, with $\alpha\approx 2.8$.

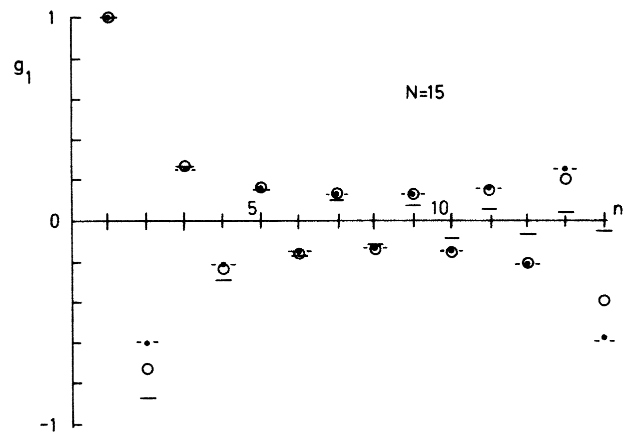

FIG. 2. Spin correlation $g_1(n)=\langle \hbar_i\sigma^z_{i+1}\sigma^z_{i+n}\rangle$ for the lattice with $N=15$ sites. The symbols are ● for $t/U=0.01$; ○ for $t/U=0.25$; – – –, — for a Heisenberg spin chain with periodic boundary conditions and open ends, respectively.

This effect can also be probed by looking at the nearest-neighbor spin correlation

$$g_2(n)=\langle \hbar_i\sigma^z_{i+n}\sigma^z_{i+n+1}\rangle$$

as a function of the distance n from the hole. In Fig. 3 this correlation is shown for the lattice with 11 sites and compared with the value for the Heisenberg spin-$\frac{1}{2}$ chain:

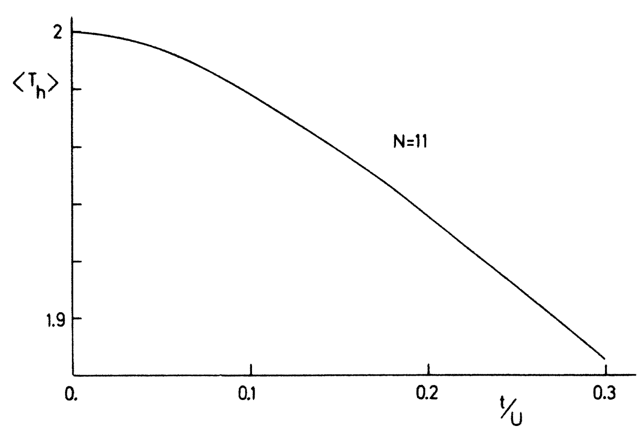

FIG. 1. Hole kinetic energy (in arbitrary units) as a function of coupling t/U for the lattice with $N=11$ sites ($t=1$).

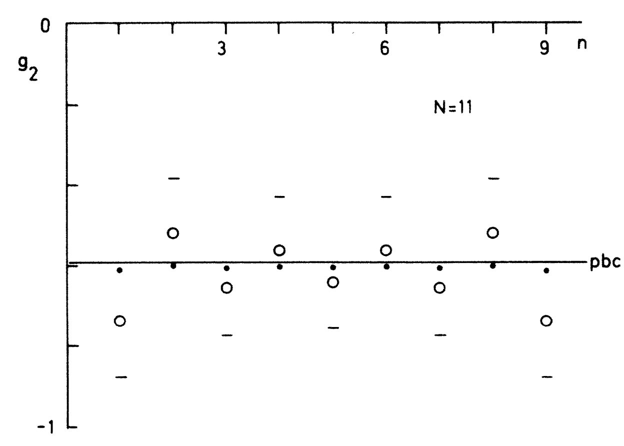

FIG. 3. Spin correlation $g_2(n)=\langle \hbar_i\sigma^z_{i+n}\sigma^z_{i+n+1}\rangle$ for the lattice with $N=11$ sites. The symbols are ● for $t/U=0.01$; ○ for $t/U=0.25$; — for a Heisenberg spin chain with open ends and the straight line for periodic boundary conditions (pbc).

$-(\frac{4}{3})(\ln 2-\frac{1}{4})$. For $t/U \to 0$ the values coincide while for finite t/U deviations develop which decay away from the hole. Increased antiferromagnetic order appears in every second-neighbor pair. If the lattice was deformable a distortion probably would appear favoring the formation of spin singlets around the hole and increasing the hole mass.

The question arises if the antiferromagnetic order observed is favored by the even number of spins in the lattices presented. For odd number of fermions the z component of the spin in the ground state is $\frac{1}{2}$ and maybe a ferromagnetic configuration is favorable for the spins neighboring the hole. In Fig. 4 the correlation function $g_1(n)$ is plotted for the lattice with ten sites and nine electrons. The spin in the ground state is $S=\frac{1}{2}$ and the momentum $K=2(2\pi/N)$. The correlation between the two spins neighboring the hole remains antiferromagnetic, while the nonzero z component of the total spin is accounted for by a gradual turning of the spins around the chain.

These results can be discussed in the context of the theorem by Nagaoka[7] that the ground-state spin configuration is ferromagnetic for many two- and three-dimensional lattices in the limit $t/U \to 0$. This is also the argument for the formation of magnetic polarons around vacancies[10] in solid ^{3}He, for instance. The basis of the proof is that all spin configurations in two and three dimensions can be reached by moving the hole around the lattice. For a 1D lattice this is not possible. Although a local ferromagnetic polarization around the hole is not excluded, the numerical calculations above and the argument in the Appendix show that antiferromagnetic correlations are favored.

Finally, in Fig. 5, I present the hole-hole correlation function

$$g_{hh}(n)=\langle \hbar_i \hbar_{i+n} \rangle$$

for the 12-site lattice with ten fermions and coupling in the range $0<t/U<0.25$. For $t/U=0$ the two holes

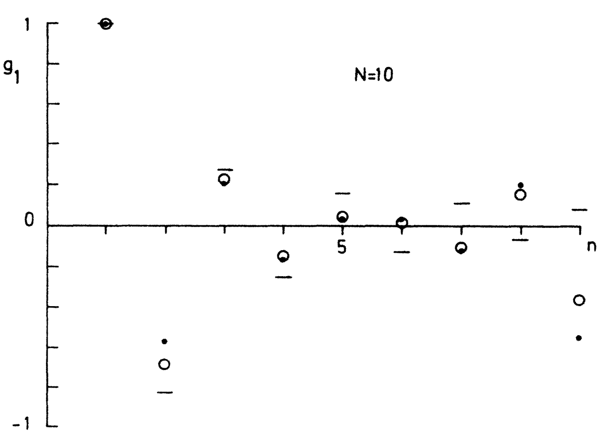

FIG. 4. Spin correlation $g_1(n)=\langle \hbar_i \sigma_{i+1}^z \sigma_{i+n}^z \rangle$ for the lattice with $N=10$ sites. The symbols are ● for $t/U=0.01$; ○ for $t/U=0.25$; — for a Heisenberg spin chain with open ends.

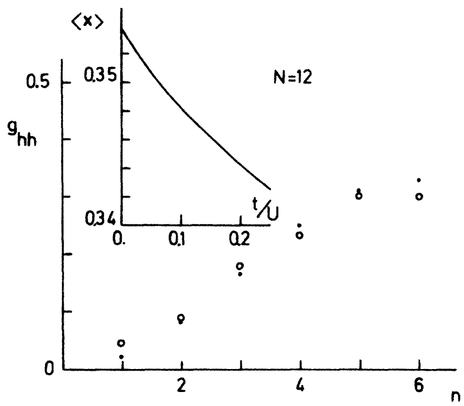

FIG. 5. Hole-hole correlation $g_{hh}(n)=\langle \hbar_i \hbar_{i+n} \rangle$ for the lattice with $N=12$ sites. The symbols are ● for $t/U=0$; ○ for $t/U=0.25$. In the inset the mean-hole distance $\langle x \rangle$ (in arbitrary units) as a function of coupling t/U for the same lattice.

behave as spinless fermions and the correlation function g_{hh} is given by

$$g_{hh}(n)=\left[\frac{2}{N}\right]\left[1-\cos\frac{2\pi}{N}n\right].$$

There is a weak attraction between the holes due to spin fluctuations which can be quantified by plotting (in the inset) the mean distance of the two holes

$$\langle x \rangle=\left[\frac{1}{N}\right]\sum_n n g_{hh}(n), \quad n=1,\ldots,N/2$$

as a function of t/U, normalized to the number of sites N. For $N\to\infty$ and $t/U=0$, $\langle x \rangle \to \frac{1}{4}+1/\pi^2$. I should note that turning off the third term in the effective Hamiltonian, the next-nearest-neighbor hopping, reduces the attraction between the holes. Because of the limited size of the lattices studied in these numerical calculations it is difficult to conclude if, at finite density, the holes form bound states or what the properties of the hole liquid may be.

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APPENDIX

In this section an argument is presented that shows that the spin correlation $g_1(n)$, for a lattice with N sites in the limit $t/U \to 0$ and neglecting next-nearest-neighbor hopping, is equal to the spin correlation of the Heisenberg spin-$\frac{1}{2}$ chain on $N-1$ sites. It is as if the spins on sites $i-1$ and $i+1$, around a hole on site i, are connected with the same coupling as the rest of the spins around the ring. The argument holds for $(N-1)/2$ odd which is the case for the lattices studied.

The starting point is the observation by Brinkman and Rice[11] that the hole kinetic energy operator T_h repeatedly applied, starting from some arbitrary parent state (with one hole and $N-1$ spins), moves the hole around the ring and creates a subspace of $M \times N$ distinct states with $M = N-1$ in general. Every N applications, the hole returns to the original position but the spins are in a configuration translated by one site. This remark will be used later in the argument. If the parent state has some symmetry then $M < (N-1)$; M is an integer. The complete basis set is therefore divided in a number m of subspaces by this procedure. The structure of the Hamiltonian in each subspace is like that of a 1D tight-binding model of dimension $M \times N$, with energy spectrum $\epsilon = -2t \cos k$, $k = 2\pi\lambda / MN$; λ is an integer. Therefore, for $t/U = 0$, the hole kinetic energy Hamiltonian has, in the ground state m, degenerate eigenfunctions of momentum $k = 0$ and energy $-2t$.

To proceed, degenerate perturbation theory to order t/U must be applied between these m states for the second term H_s in the effective Hamiltonian. It should be noted again that H_s is a Heisenberg-type Hamiltonian but on an N-site lattice with one empty site. The main point of the argument is that H_s, in the space of the m degenerate ground-state eigenfunctions, has identical matrix elements to the $k = \pi$ irreducible representation of an $(N-1)$-sites Heisenberg spin-$\frac{1}{2}$ chain for $(N-1)/2$ odd. [12] To construct the basis states in the $k = \pi$ irreducible representation the translation operator is repeatedly applied on a parent state. The number of states so created is again m and by construction similar in structure to the T_h eigenstates, which concludes the argument.

For $(N-1)/2$ even, the ground-state momentum of the corresponding spin chain is $k = 0$. In this case the spin correlations between the two systems are different for $t/U \to 0$, the effective Hubbard Hamiltonian having stronger antiferromagnetic spin correlations. For $(N-1)/2$ noninteger, the spin correlations resemble, in magnitude, those of $(N-1)/2$ odd but there exists no study for the corresponding spin chain.

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