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Density-matrix renormalization-group studies of the alternating Hubbard model

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Discrepancies between the single-particle band structure and the exact many-particle behavior are particularly striking in one-dimensional systems. The one-dimensional alternating Hubbard model is especially interesting as a nontrivial model for conjugated polymer chains, such as polyacetelyne. We study this model for chains of 60 sites using the density-matrix renormalization-group method. We obtain the first electronic and magnetic excited-state energies at half filling as a function of an alternating hopping parameter and on-site electron-electron interaction. We also study the effect of the interaction on the dimerization and discuss its relation to the charge gap and spin triplet gap. In addition, we calculate the local spin and charge densities of some excited states, which manifest a clear crossover from bandlike to strongly correlated behavior.

I. INTRODUCTION

The effect of electron-electron interaction is crucial in understanding the properties of conjugated polymers.[1] Although the independent-electron theories such as Su-Schrieffer-Heeger models[2] (or Hückel theory) can explain many experimental features by including the interaction effects within renormalized parameters,[3] it is necessary to use different parametrizations to explain different experiments. There are also some experimental results which cannot be explained at all by the independent-electron theories with any set of parameters. One of them is the level sequence of the excited states. In the independent-electron theories, the dipole-allowed optical $1\,^1B_u$ state is predicted to be the lowest excited state, while in experiment the actual lowest excited state is the optically forbidden (the $2\,^1A_g$ state).[4] Another example is the observation of negative spin densities on some sites, which cannot be explained within independent-electron theories. In models with electron-electron interactions these results are naturally explained.[1] One of the simplest such models is the Peierls-Hubbard model, which has an electron-electron interaction of the form

$$H_{e\text{-}e} = U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{i,j>0} V_j n_i n_{i+j}, \tag{1}$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$. Usually, for simplicity only the first term is considered. The effects of the electron-electron interaction on the ground state properties such as dimerization, solitons, and polarons, and on excited states properties such as the energy gap and the level sequence have been studied by many different methods.[1]

The alternating hopping integral in the Peierls-Hubbard model is $t(1\pm\delta)$ and δ is called the alternating hopping parameter. Recently Soos *et al.* studied the crossover between the excited states $1\,^1B_u$ and $2\,^1A_g$ as a function of δ and the on-site interaction U.[5] This level crossing is one aspect of the crossover from bandlike behavior to strongly correlated behavior. Soos *et al.* also determined the phase boundary by the position of the level crossing. Most previous work on the effects of interaction which produce reliable results come from quantum Monte Carlo or exact diagonalization methods. The limitation of exact diagonalization is that it works only for small system sizes, which is usually less than 12 sites.

Recently a method to study one-dimensional interacting systems, namely, the density-matrix renormalization-group (DMRG) method, has been developed.[6] The DMRG method is especially useful for one-dimensional systems with short range interactions and open boundary conditions. With this method, the energies of the ground state and the lowest few excited states can be obtained with very high precision for fairly large finite systems, especially for a system which has an energy gap.

In this paper we study a simple form of the Peierls-Hubbard model by this method for a system of 60 sites. The model in which the structural energy of the lattice is neglected has the Hamiltonian

$$H = -\sum_{i,\sigma}[t-(-1)^i\delta](c^\dagger_{i\sigma}c_{i+1\sigma} + c^\dagger_{i+1\sigma}c_{i\sigma}) + U\sum_i(n_{i\uparrow}-\tfrac{1}{2})(n_{i\downarrow}-\tfrac{1}{2}), \tag{2}$$

where σ is the spin index of the electron and i is the site index starting from 1. This model is the alternating Hubbard model. It is the same as the Peierls-Hubbard model if we consider homogeneous dimerization of the ground state and assume that the excitations in optical absorption occur where the Born-Oppenheimer approximation is valid. Although there is no technical problem in calculating the ground state energy for inhomogeneous lattice configurations, determining the ground state configuration will take much more computer time. Therefore we will only consider homogeneous dimerization in this paper.

First, we examine the ground state properties, e.g., the effect of interaction on dimerization. We then calculate the first few electronic and magnetic excitation energies as a function of the alternating hopping parameter δ and the on-site interaction U and obtain the optical gap $E_g(\delta, U)$. Finally, we study the local charge and spin densities of some excited states. For one-particle excitation from half filling, the charge and spin densities are similar for a weak interaction, which agrees with the band picture in this region. When the interaction increases the two densities begin to differ from each other more and more. The spin density turns negative at a large interaction, whereas the charge density is always positive. This means that the system has a crossover from bandlike behavior to correlated behavior. Measuring the spin and charge densities of the model directly provides a way of studying the crossover from band to correlated behavior.

II. GLOBAL SYMMETRY OF THE MODEL

In Hamiltonian (2) there is a usual SU(2) symmetry on the spin index. There is also an SU(2) axial charge symmetry which has been found in the Kondo model[7] and the Hubbard model.[8] The axial charge generators are

$$I^z = \frac{1}{2}\sum_i [c^\dagger_{i\alpha} c_{i\alpha} - 1],$$

$$I^- = \frac{1}{2}\sum_i (-1)^i \varepsilon_{\alpha\beta} c_{i\alpha} c_{i\beta},$$

$$I^+_i = (I^-_i)^\dagger, \tag{3}$$

where $\varepsilon_{\alpha\beta}$ is the antisymmetric matrix. The axial charge generators satisfy the same commutation relations as the spin operators:

$$[I^+, I^z] = I^+,\ [I^-, I^z] = -I^-,\ [I^+, I^-] = 2I^z. \tag{4}$$

It is simple to prove that these operators commute with Hamiltonian (2). The particle-hole symmetry is part of the SU(2) axial charge symmetry. The Hamiltonian (2) thus has an SU(2)× SU(2) symmetry group. Actually, the group is SO(4)=SU(2)×SU(2)/Z_2, as pointed out by Yang and Zhang.[9]

III. DEFINITION OF THE GAPS

We chose the total spin in the z direction S_z and total charge Q as good quantum numbers in our DMRG calculations. It is convenient to define the total charge Q to be the difference between the total number of electrons and the number of sites, namely, $Q = 2I^z$. Therefore $Q = 0$ corresponds to half filling. We calculate the energy $E_0(Q, 2S_z)$ of the lowest energy states $|Q, 2S_z\rangle$ for different Q and S_z. The optical gap energy E_g is the sum of the energies required for adding and for removing one electron at half filling,

$$E_g = E_0(1,1) - E_0(0,0) + E_0(-1,1) - E_0(0,0). \tag{5}$$

The triplet axial charge gap E_c and the triplet spin gap E_s are

$$\begin{aligned} E_c &= E_0(2,0) - E_0(0,0), \\ E_s &= E_0(0,2) - E_0(0,0). \end{aligned} \tag{6}$$

Charge and spin densities defined as

$$\begin{aligned} Q(i) &= \langle Q, 2S_z | \left(\sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - 1 \right) | Q, 2S_z \rangle, \\ S_z(i) &= \langle Q, 2S_z | \tfrac{1}{2}(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}) | Q, 2S_z \rangle \end{aligned} \tag{7}$$

can also be calculated within the DMRG method. $Q(i)$ and $S_z(i)$ are zero everywhere for the ground state $|0,0\rangle$ in our DMRG calculation, which is consistent with the Lieb-Mattis theorem that the ground state is a spin and axial charge singlet.[10] Therefore $Q(i)$ and $S_z(i)$ for the one-electron excited state $|1,1\rangle$ are the same as the distributions of charge and spin when an electron is added into the ground state $|0,0\rangle$.

IV. THE DMRG METHOD

In our DMRG calculations we obtain the ground state of chains of length up to 60 sites with open boundary conditions. The hopping integral is set to $t = 1$ and all energies are measured in units of t. 32 states are kept at each iteration of the DMRG calculation and it takes five passes through the 60 sites for the calculation to converge. We use the same program that has been carefully tested in a work on a spinless fermion system.[11] In that work the spinless system is a special case in which all calculations are done in the subspace $2S_z = Q + N$, where N is the number of system sites. We also test the program by comparing the calculated energy with the exact solution for the noninteracting case ($U = 0$). Since there is a spin degree of freedom for electrons, one would expect the precision to be much lower than that for the spinless case, for keeping the same number of states. However, the precision is still very high for our problem because of the energy gap at half filling in the alternating Hubbard model. Table I shows the accuracy of the DMRG method and the weight of the discarded

TABLE I. Comparison of the ground state energies from the DMRG calculations with the exact solution for the non-interacting alternating chain at half filling. The comparison shows that the results of DMRG become more and more accurate as the alternating parameter δ increases, namely, as the energy gap increases. The fifth column in the table is the weight of the discarded states W_d in the DMRG calculations.

δ	E_{exact}	E_{DMRG}	$E_{DMRG} - E_{exact}$	W_d
0.04	-76.077439	-76.044030	0.033409	1.3×10^{-4}
0.08	-76.756269	-76.742580	0.013689	5.1×10^{-5}
0.12	-77.653433	-77.647542	0.005891	2.3×10^{-5}
0.16	-78.729942	-78.727297	0.002645	1.0×10^{-5}
0.20	-79.958046	-79.956835	0.001211	4.7×10^{-6}
0.24	-81.316766	-81.316203	0.000563	2.2×10^{-6}
0.28	-82.789594	-82.789329	0.000264	1.0×10^{-6}
0.32	-84.363173	-84.363049	0.000124	5.1×10^{-7}
0.36	-86.026474	-86.026416	0.000058	2.3×10^{-7}
0.40	-87.770238	-87.770212	0.000026	1.0×10^{-7}

states in the density matrix. In general when $U \neq 0$, the discarded weight varies from 10^{-4} to 10^{-10} depending on the size of the gap. The precision is lower at small δ and small U.

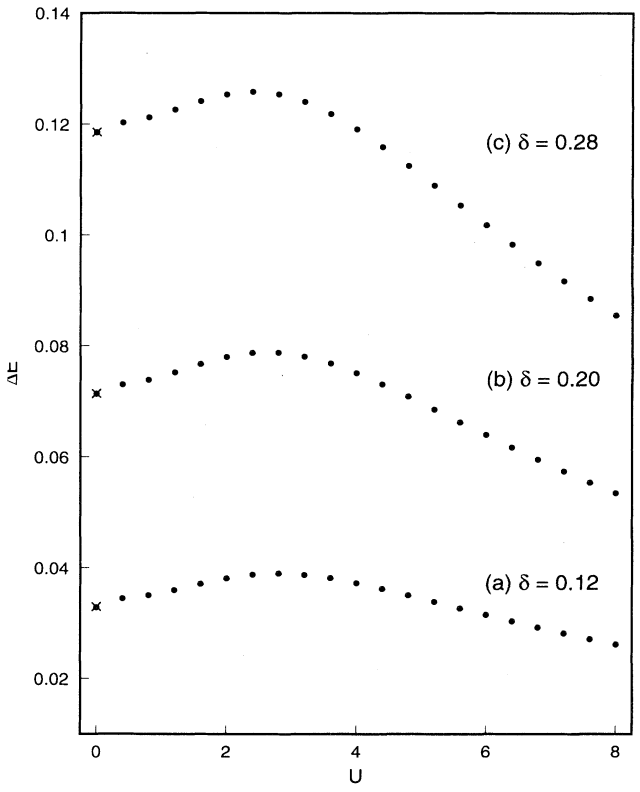

FIG. 1. Magnitude of the electronic energy difference ΔE per site between dimerized and uniform chains versus the on-site Hubbard parameter U. The system has 60 lattice sites and open boundary conditions and δ is the alternating parameter. The dots in the figure are from the density-matrix renormalization-group calculations and the cross at $U = 0$ is obtained from the exact solution.

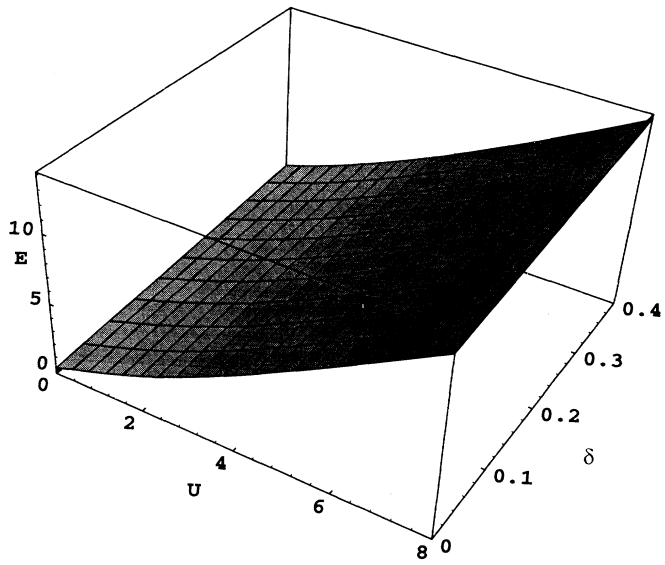

FIG. 2. Energy gap E_c of axial charge triplet excitation versus the alternating parameter δ and the Hubbard interacting parameter U.

V. RESULTS

We examine first the effect of interaction on dimerization. The energy difference between the dimerized ground state $|0,0\rangle$ ($\delta \neq 0$) and uniform ground state ($\delta = 0$) is calculated. In Fig. 1 we show the electronic energy gained per site at fixed dimerization as a function

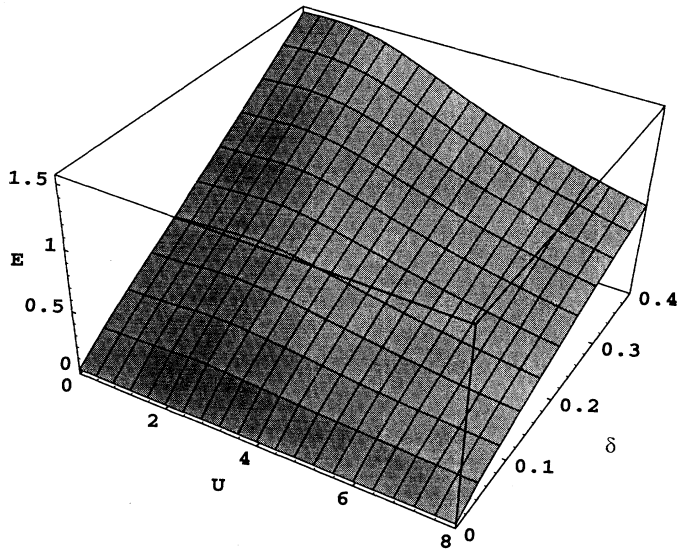

FIG. 3. Energy gap E_s of spin triplet excitation versus the alternating parameter δ and the Hubbard interacting parameter U.

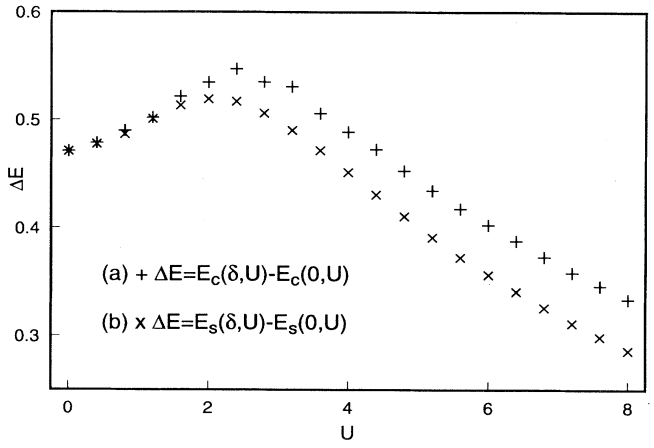

FIG. 4. Difference between the triplet gap of dimerized chain and that of uniform chain at $\delta = 0.12$ as a function of interaction U. (a) The charge triplet gap and (b) the spin triplet gap.

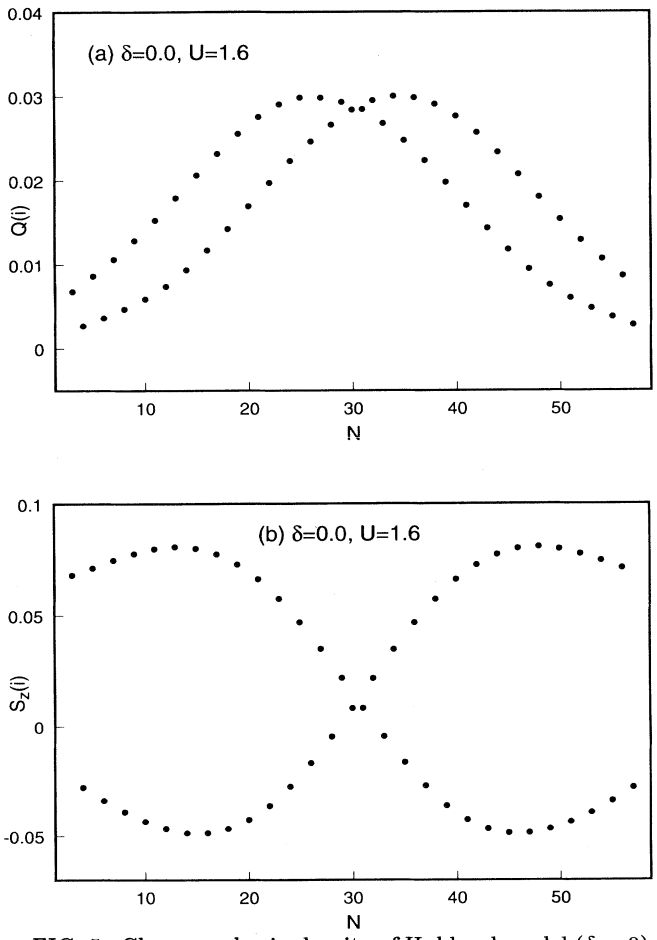

FIG. 5. Charge and spin density of Hubbard model ($\delta = 0$) of the state $|1,1\rangle$. (a) The charge density, which is positive everywhere. (b) The spin density, which can be negative and is very different from the charge density.

of interaction U. The result agrees with calculations by the Monte Carlo method[12] and exact diagonalization,[1] which show that the gain of energy increases in intermediate U. The only difference from previous results is in the magnitude and the position of the peak, which may be caused by the open boundary condition we chose and the length of the chain.

We then calculate the one-particle energy gap E_g, the charge gap E_c, and the spin gap E_s. We find that the difference between E_g and E_c is very small, within the order of one over the system size, which goes to zero in the thermodynamical limit. Therefore we conclude that the one-particle energy gap is mainly determined by the charge part. In Fig. 2 we show the energy gap E_c as a function of δ and U. In Fig. 3 the spin gap E_s is plotted as a function of δ and U. At $\delta = 0$ the model is the Hubbard model and the spin excitation is gapless, which is in agreement with the Bethe ansatz result of the Hubbard model. With a large on-site interaction U, the spin part of the system maps to a Heisenberg model. Unlike the usual Heisenberg model where the exchange coupling is uniform on the whole lattice, this model has an alternating exchange coupling for any nonzero δ. There is no energy gap in the usual Heisenberg model. But the alternating exchange coupling will open an energy gap.

We also calculate the gap difference $E_c(\delta,U)-E_c(0,U)$ and $E_s(\delta,U)-E_s(0,U)$ and plot them as a function of interaction U for a fixed $\delta = 0.12$ (see Fig. 4). We find that the gap difference increases up to intermediate U, which is similar to the energy gain shown in Fig. 1. This similarity can be explained as follows: the energy gain from dimerization is proportional to the sum of the charge gap increased and spin gap opened by dimerization. In Figs. 1 and 4, the peaks are located in the same position, which strongly suggests that there is a relation between them. The charge and spin densities with one added electron are also calculated with the DMRG method. In Fig. 5 we show the results for the ordinary Hubbard model ($\delta = 0$) with $U = 1.6$. It is well known that in the one-dimensional Hubbard model the spin and charge degrees of freedom are separated. We see this clearly in Fig. 5 since the spin density is very different from the charge density. The spin density can be negative, whereas the charge density is positive everywhere. In Fig. 6 (7) the charge (spin) density of one doped electron as a function of position at a fixed $\delta = 0.08$ is shown for several values of the interaction parameter U: (a) $U = 0$, (b) $U = 2.0$, (c) $U = 4.0$, and (d) $U = 8.0$. Comparing Figs. 6(a) and 7(a), it is clear that the charge and spin distributions are the same, as would be expected from the single-particle picture. In a single-particle theory, the electron carries both spin and charge and thus their distributions should be identical. When the interaction increases, the charge and spin distributions become different. The difference increases with the interaction. The behavior at large U is similar to the Hubbard model, except that in the present case the spin excitation has a gap, which makes the spin distribution different. In particular, the spin density can be negative in some places. From Figs. 6 and 7 it is clear that the interaction suppresses the charge density oscillation, but enhances the spin density oscillation.

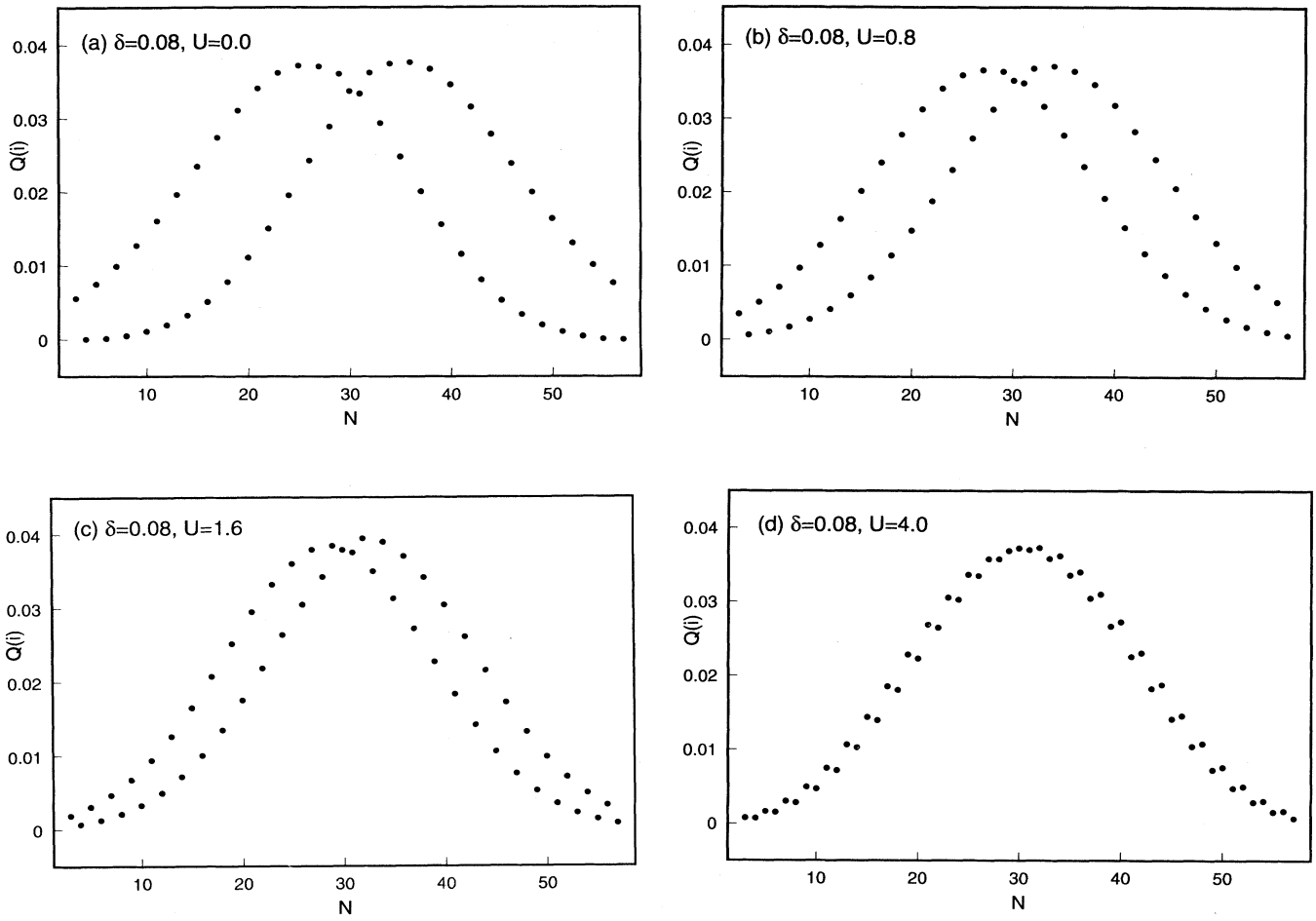

FIG. 6. Charge density of the state $|1,1\rangle$ for $\delta = 0.08$ and several interaction parameters U: (a) $U = 0$, (b) $U = 0.8$, (c) $U = 1.6$, and (d) $U = 4.0$. The charge density is always positive for any U.

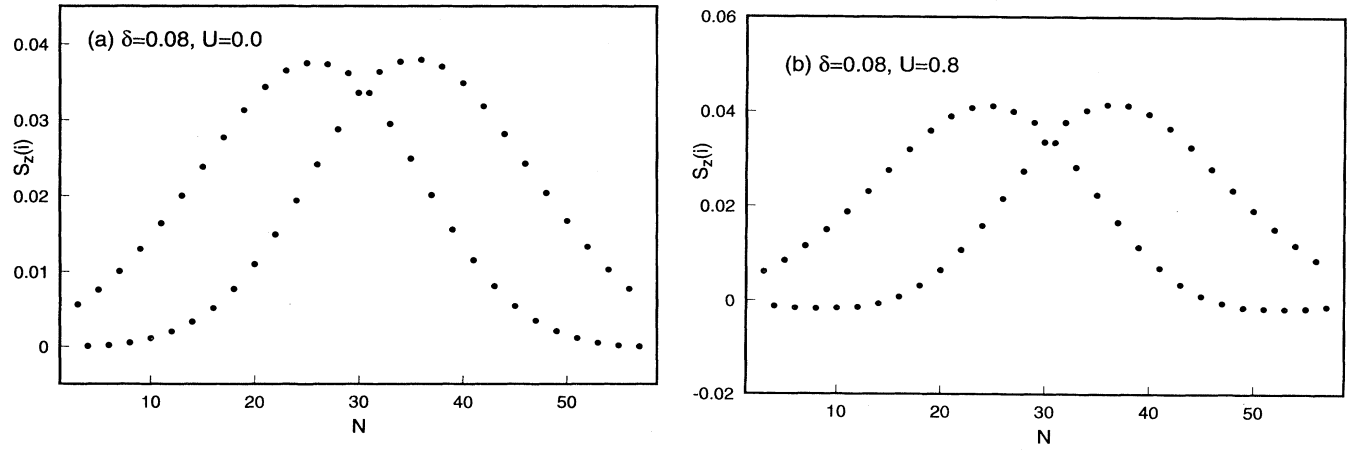

FIG. 7. This plot is identical to Fig. 6, except it is for the spin density of the state $|1,1\rangle$ for $\delta = 0.08$ and several interaction parameters U: (a) $U = 0$, (b) $U = 0.8$, (c) $U = 1.6$, and (d) $U = 4.0$. The spin density demonstrates the crossover from bandlike behavior to strongly correlated behavior as the interaction parameter U increases.

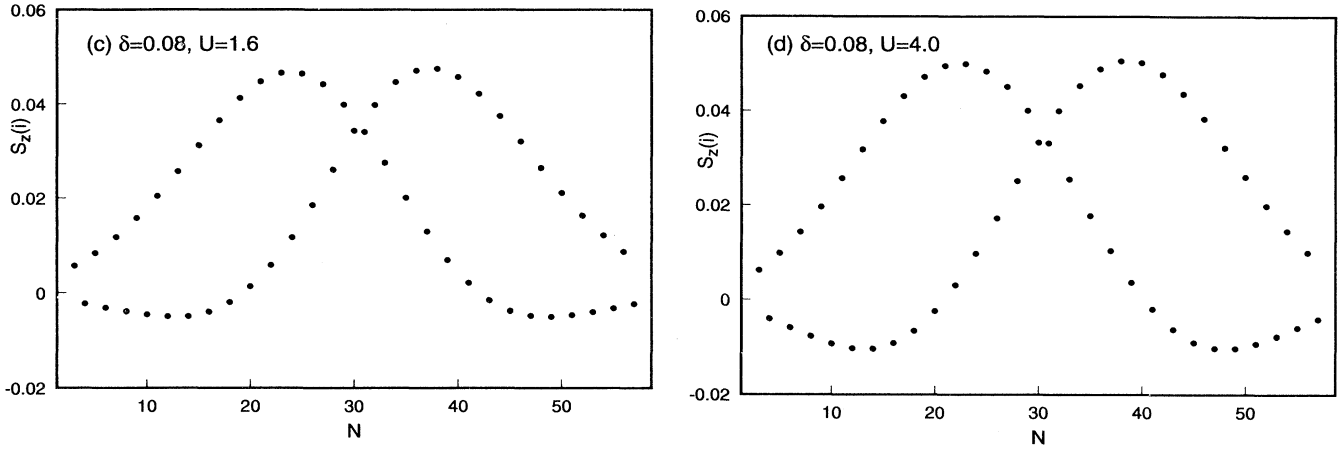

FIG. 7. (*Continued*).

VI. SUMMARY AND CONCLUSION

In summary we have obtained the one-particle, axial charge triplet and spin triplet gaps as a function of δ and U for chains of 60 sites with open boundary conditions. We have found that the one-particle gap is the same as the axial charge triplet gap. The gap difference between a dimerized chain and a uniform chain peaks at an intermediate interaction U. This behavior is the same for the charge triplet gap and for the spin triplet gap and it is similar to the behavior of the energy gain from dimerization. The peaks are located at almost the same value of $U \sim 3t$. We have also studied the crossover from the band picture to the strongly correlated picture by examining the difference in the local charge and spin densities of an extra doped particle.

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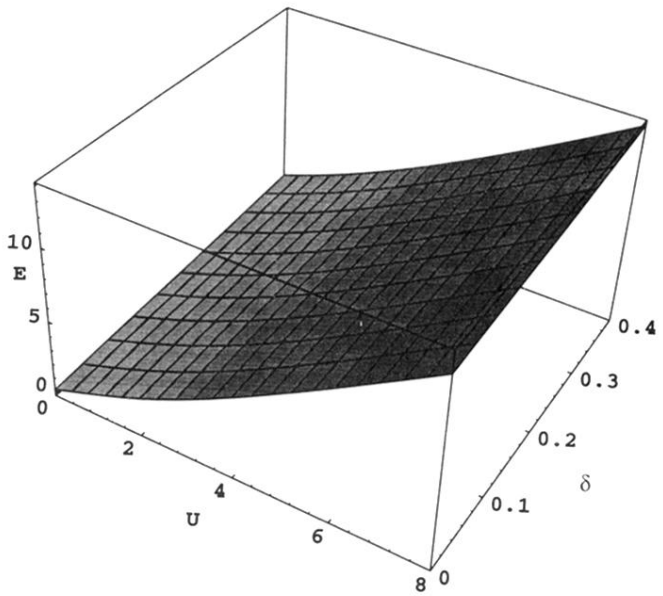

FIG. 2. Energy gap E_c of axial charge triplet excitation versus the alternating parameter δ and the Hubbard interacting parameter U.

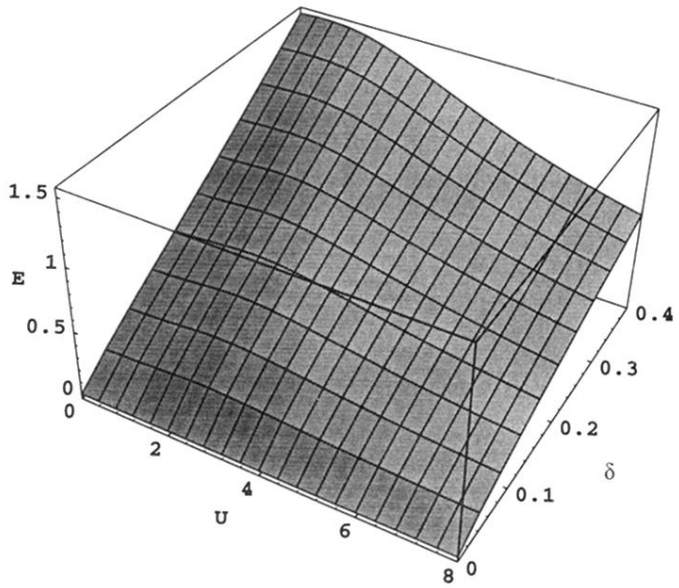

FIG. 3. Energy gap E_s of spin triplet excitation versus the alternating parameter δ and the Hubbard interacting parameter U.