Bond-charge interaction in the extended Hubbard chain

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We study the effects of a bond-charge interaction (or correlated hopping) on the properties of the extended [i.e., with both on-site (U) and nearest-neighbor (V) repulsions] Hubbard model in one dimension at half-filling. Energy gaps and correlation functions are calculated by Lanczos diagonalization on finite systems. We find that, irrespective of the sign of the bond-charge interaction, X, the charge-density-wave (CDW) state is more robust than the spin-density-wave (SDW) state. A small bond-charge interaction term is enough to make the differences between the CDW and SDW correlation functions much less dramatic than when $X=0$. For $X=t$ and fixed $V<2t$ (t is the uncorrelated hopping integral), there is an intermediate phase between a charge ordered phase and a phase corresponding to singly occupied sites, the nature of which we clarify: it is characterized by a succession of critical points, each of which corresponds to a different density of doubly occupied sites. We also find an unusual slowly decaying staggered spin-density correlation function, which is suggestive of some degree of ordering. No enhancement of pairing correlations was found for any X in the range examined. [S0163-1829(96)02325-9]

I. INTRODUCTION

Over recent years bond-charge interactions between fermions have been invoked to explain a variety of phenomena, such as lattice stiffening in polyacetylene,[1,2] and high-temperature superconductivity.[3–5] This kind of interaction had already appeared in the study of magnetism of narrow d-band electrons as discussed by Hubbard:[6] the Coulomb interaction matrix elements are expressed in terms of Wannier states $|i\rangle$ localized at sites i, giving rise not only to the well-known on-site repulsion, $U=\langle ii|1/r|ii\rangle$, and nearest-neighbor repulsion $V=\langle ij|1/r|ij\rangle$, but also to $X=\langle ii|1/r|ij\rangle$. The Hamiltonian then becomes

$$\mathcal{H}=-\sum_{\langle ij\rangle,\sigma}[t-X(n_{i-\sigma}+n_{j-\sigma})](c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.})$$
$$+U\sum_{i}n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle ij\rangle,\sigma\sigma'}n_{i\sigma}n_{j\sigma'}, \quad (1)$$

where $\langle ij\rangle$ stands for nearest-neighbor sites, $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) a fermion at site i in the spin state $\sigma=\uparrow$ or $\downarrow$, and $n_i=n_{i\uparrow}+n_{i\downarrow}$, with $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. The second-quantized form of the interaction justifies calling this extra term a bond-charge interaction, also referred to as correlated- or density-dependent-hopping: it favors (hinders) hopping involving sites with nonzero charge if $X<0$ ($X>0$). While in the original problem the parameters were such that $U\gg V\gg X$, in more recent applications[3] one may have $U\gg V\sim X$, or even $U\sim V\sim X$, such as in an effective model for the CuO_2 planes in high-temperature superconductors.[5]

For the case of on-site repulsion only (i.e., $X=V=0$, $U\neq 0$) an exact solution in one dimension based on the Bethe ansatz has been known for some time.[7] For a half-filled band and for strong repulsion, the ground state is reminiscent of a Néel state, but differing in a fundamental way: the staggered spin correlations are *critical*, corresponding to an algebraic spatial decay; this is commonly referred to as a spin-density-wave (SDW) state. When nearest-neighbor repulsion (V) is included, no exact solution has been found, even in one dimension. For nearest-neighbor repulsion in the absence of both hopping and on-site repulsion, the ground state displays charge ordering (CO), since it is more favorable for the electrons to doubly occupy alternate sites, leaving their neighbors empty. As the hopping is switched on, quantum fluctuations disturb this ''static'' ordering, turning into a charge-density-wave (CDW) state. Different approximations have been used in order to obtain the phase diagram for intermediate values of both U and V; the picture that emerges is that there is a CDW-SDW phase transition at zero temperature, along a critical curve slightly displaced from the strong-coupling prediction $V_c=U/2$.[8–13]

The information on the effects brought about by the bond-charge interaction in the presence of *repulsive* on-site and intersite interactions (i.e., U, $V>0$) is somewhat limited. (For either U or V attractive, see, e.g, Refs. 4 and 14). On the one hand, mean-field-type calculations[15] predict that a bond-charge interaction gives rise to superconductive pairing for $4zX^2>UV$ (z is the coordination number); though very interesting, the validity of this result in one and two dimensions should be questioned. On the other hand, when $X=t$ the total number of doubly occupied sites, $N_2\equiv\Sigma_i n_{i\uparrow}n_{i\downarrow}$, becomes a conserved quantity, allowing exact statements to be made[16–18] for the model defined by (1) at half-filling ($\langle n\rangle=1$), and for any lattice dimensionality d: (i) For $U<2zV-z\max(2t,V)$, the ground state corresponds to a nonmagnetic charge ordered metal.[17,18] (ii) For $U>z\max(2t,V)$, the ground state corresponds to a paramagnetic insulator, with exactly one fermion at every site[16] [singly occupied (SO) sites], leading to a very high degeneracy with respect to the total spin value.[17] Further, Ovchinnikov[17] also argues that as U decreases below the SO boundary, $U=4t$ when $V<2t$, the appearance of doubly occupied sites (henceforth referred to as the DO region) is favored. Also for $X=t$, but in one dimension with $V\equiv 0$, one finds three regimes, differing by the allowed site occupancy: (i) no doubly

occupied sites (no empty sites) for $\langle n\rangle<1$ ($\langle n\rangle>1$); (ii) no singly occupied sites; (iii) all possibilities.[17,19]

In view of the wide range of applications of bond-charge interaction, a clear understanding of the zero-temperature phase diagram is clearly in order. In particular, the behavior with X of the boundary between the CDW and the SDW phases is of interest, together with any indication of superconducting correlations becoming dominant. When $X=t$ most of the definite statements made in relation to the intermediate (DO) phase concern the location of the boundaries with the CO and SO phases, while a precise understanding of its nature and of its properties is still lacking. With this in mind, here we consider the half-filled model in one dimension and discuss the phase diagram; from now on, energies will be expressed in units of the usual hopping, t.

The layout of the paper is as follows. In Sec. II we briefly outline the procedure used to determine the phase-transition boundaries and several correlation functions, which will be useful in interpreting the nature of the phases involved. In Sec. III we present our results for the case without double occupancy conservation, i.e., for $-1\leqslant X<1$; the case $X=1$ is discussed in Sec. IV. And finally, Sec. V summarizes our findings.

II. ENERGY GAP AND CORRELATION FUNCTIONS

The Hamiltonian (1) for chains with N_s sites and $N_e=N_s$ fermions (half-filled band) is diagonalized through the Lanczos algorithm;[20–22] periodic (antiperiodic) boundary conditions are used for $N_s=4,8,12$ ($N_s=6,10$).[10] We obtain the lowest eigenvalues and corresponding eigenvectors, from which the energy gap, defined as

$$\Delta=E_1-E_0 \tag{2}$$

is calculated, where E_0 and E_1 are the two lowest energy eigenvalues. The gap defined above is at constant number of particles, unlike the charge gap Δ_c used in Ref. 10, which is related to a finite-difference approximant to the inverse compressibility. At zero temperature, and in the thermodynamic limit (TDL), a phase transition is marked by a change in the ground state; one therefore expects the energy difference between the two lowest states to vanish at the transition point. While in many quantum systems the energy gap, defined as in Eq. (2), only vanishes at the transition in the TDL,[23] in the present case Δ vanishes for finite-sized systems, and it will be used to estimate the location of CDW-SDW transition points. For a given X, we fix V and determine U_c, the value of U where Δ vanishes. In principle, the location of the transition point, $U_c(V,X)$, depends on the system size, N_s, and we have to perform extrapolations towards $N_s\rightarrow\infty$.

As a test of this procedure, we show in Fig. 1 our results for the CDW-SDW transition line for $X=0$. We have found excellent agreement with other estimates,[10–13] including the deviation of the phase boundary from the strong-coupling prediction $V_c=U/2$ for $U\gtrsim 1$, confirming that the gap defined by Eq. (2) is indeed appropriate.

In addition to the energy gap, the nature of the different phases is probed by the staggered spin-spin correlation function,

$$\mathcal{F}_S(\ell)=(-1)^{\ell}\langle m_i m_{i+\ell}\rangle, \tag{3}$$

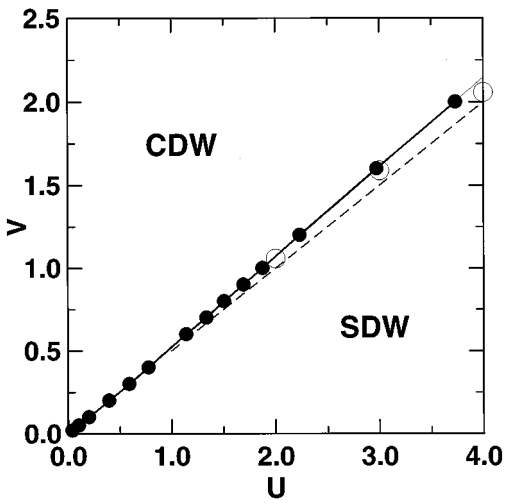

FIG. 1. Phase diagram V vs U for the usual (i.e., $X=0$) extended Hubbard model at half-filling. CDW and SDW denote charge- and spin-density-wave ground states. The dotted line is the strong-coupling prediction $V_c=U/2$, and the solid line guides the eye through our extrapolated results, shown as solid circles. For comparison, some results from Ref. 11 are shown as empty circles.

by the charge-density correlation function,

$$\mathcal{F}_C(\ell)=\frac{1}{4}\langle n_i n_{i+\ell}\rangle, \tag{4}$$

by the singlet superconductor correlation function,

$$\mathcal{F}_{SS}(\ell)=\langle c_{i+\ell\downarrow}c_{i+\ell\uparrow}c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle, \tag{5}$$

and by the triplet superconductor correlation function,

$$\mathcal{F}_{TS}(\ell)=\langle c_{i+\ell\downarrow}c_{i+\ell+1\uparrow}c^{\dagger}_{i+1\uparrow}c^{\dagger}_{i\downarrow}\rangle, \tag{6}$$

where

$$m_i=n_{i\uparrow}-n_{i\downarrow}, \tag{7}$$

and

$$n_i=n_{i\uparrow}+n_{i\downarrow}. \tag{8}$$

One should note that with the above definitions the $\ell\rightarrow\infty$ limit of the charge correlations is 1/4, whereas all others go to zero.

As further tests of our calculations, the dotted lines in Fig. 2 represent the behavior of spin and charge correlations in the absence of bond-charge interaction. Figure 2(a) shows that in the CDW phase, charge correlations are slowly decaying with the distance, while spin correlations are rapidly decaying, indicating that the former are dominating. In the SDW phase the roles are inverted, as shown in Fig. 2(b). As is well known, the system is far from a superconducting instability in this case, which is reflected by the singlet and triplet correlations falling off with the distance much faster than their spin or charge counterparts. We have also tested for any crucial size dependence of the above correlation functions, and found that the results for $N_s=12$ are hardly different from those for $N_s=10$ or 8. These procedures will now be used in the analysis of the role played by bond-charge interaction.

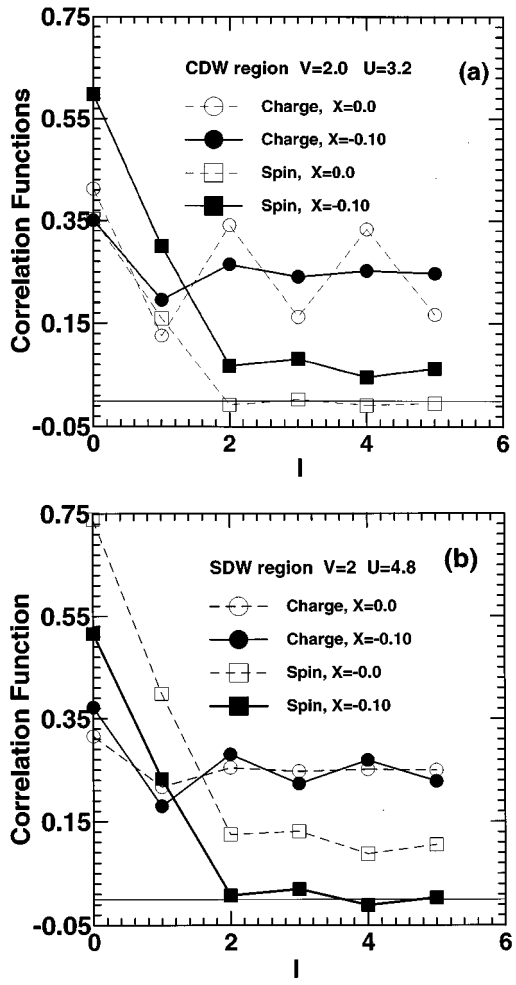

FIG. 2. Charge-density (circles) and spin-density (squares) correlation functions vs intersite distance, for a 10-site chain with $V=2$, in (a) the CDW phase ($U=3.2$), and (b) the SDW phase ($U=4.8$); dotted lines and open symbols correspond to $X=0$ and solid lines and solid symbols to $X=-0.1$.

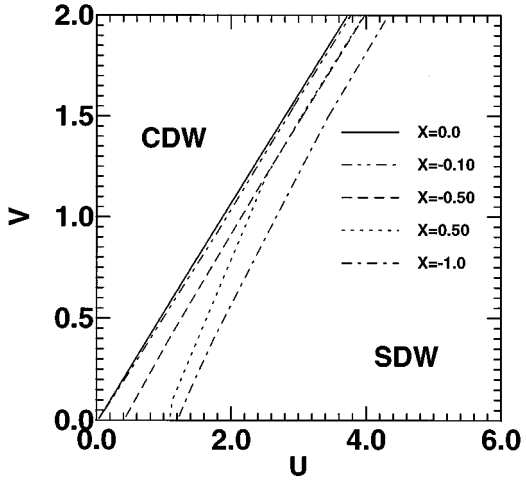

FIG. 3. Extrapolated phase diagram V vs U for the extended Hubbard model at half-filling. The solid line represents the system without bond-charge interaction, and the other lines correspond to $X=-0.1$ (dotted), $X=-0.5$ (dashed), $X=0.5$ (long-dashed), and $X=-1$ (dot-dashed).

III. RESULTS FOR $-1\leqslant X<1$

We now discuss the effects of correlated hopping on the phase-diagram and correlation functions. Using the procedure outlined in Sec. II, the vanishing of the gap locates a phase transition point. Figure 3 shows constant-X sections of the phase diagram. For nonzero X, the CDW-SDW phase boundary is displaced to the right of that corresponding to $X=0$; that is, the CDW region grows with $|X|$, at the expense of the SDW region; see Fig. 3. The case $X=\pm 0.5$ illustrates that while for large U (and V) the location of the phase boundary is independent of the sign of X, this is not so for $U\lesssim 2.5$: the CDW region is larger for $X>0$ than for $X<0$. A rough picture can be used to explain this sign dependence, as follows. The dominant contribution to the ground state in the CDW phase is from a charge-ordered state ($|\cdots\uparrow\downarrow\ 0\ \uparrow\downarrow\ 0\ \uparrow\downarrow\cdots\rangle$). For small V, a spin resonating between two sites would typically lower the energy by $\sim U$ for breaking the ''pair,'' and add $\sim X$ due to the correlated hopping (in order to stress the role of the bond-charge energy, we do not consider the t hopping). Since one can think of hopping-induced ''pair'' breaking as the mechanism by which the CDW state becomes an SDW state, a smaller U_c is needed when $X<0$.

In Fig. 2(a) we show the effect of bond-charge interaction on the correlation functions in the CDW region, by comparing the results for $X=0$ (dotted lines) with the corresponding ones for $X=-0.1$ (solid lines). Charge correlations, which are slowly decaying in the absence of a bond-charge interaction, become strongly damped when $X\neq 0$. Spin correlations, on the contrary, are enhanced when the bond-charge interaction is present. Turning into the SDW phase, we see from the data shown in Fig. 2(b) that the behavior is exactly the opposite of that in the CDW phase: charge correlations are enhanced, while spin correlations are depressed. Though with somewhat smaller amplitudes of charge oscillations, the behavior is qualitatively the same as V is decreased. Therefore, the differences between CDW and SDW phases, which are very pronounced when $X=0$, become quite smooth already for a small value of X. Since when $X=0$ the CDW-SDW transition is expected to be of first order for $U>1.5$ (see, e.g., Ref. 13), this may be indicative that bond-charge interaction weakens the first-order character of this transition.

This fact has other consequences. In a standard strong-coupling perturbation theory analysis,[11] the critical curve would be given by

$$V_c=\frac{U}{2}+1.545\frac{(t-X)^2}{U}, \tag{9}$$

which would indicate a growth of the SDW phase into the CDW, contrary to the behavior shown in Fig. 3. The results displayed in Fig. 2 reflect the fact that the contribution of SDW-like states to the ground state in the CDW region is much more important in the presence of a bond-charge interaction than when $X=0$; a similar statement holds for the contribution of CDW-like states in the SDW region. Since the standard strong-coupling analysis neglects these contributions altogether, quantum fluctuations other than those present in Eq. (9) could account for the above discrepancy.

As far as superconducting correlations are concerned, they are not enhanced by the presence of a bond-charge interaction in either phase, meaning that no tendency towards pairing has been detected at half-filling.

IV. RESULTS FOR $X=1$

The case $X=1$ shows remarkable features due to the conservation of the number of doubly occupied sites.[16] This regime can therefore be considered as quasiclassical, in the sense that fluctuations brought about by the uncorrelated hopping term are limited by the conservation of the number of doubly occupied sites. Computationally, this considerably restricts the Hilbert space, accelerating the Lanczos algorithm; we were able to consider lattices up to $N_s=24$ in this case.

The energy spectrum in the intermediate region deserves a closer look. One finds three different regimes as U is varied. For $U<U_{c_1}(N_s,V)$, the ground state corresponds to full charge ordering (CO), with energy per fermion $E_{\mathrm{CO}}/N_s=U/2$. At the other extreme, $U>U_{c_2}(N_s,V)$, the ground state corresponds to singly occupied (SO) sites, with energy $E_{\mathrm{SO}}/N_s=V$. In between those limits, the number of doubly occupied (DO) sites plays a dominant role in selecting the ground states. The calculated energy (per fermion) of the lowest state with one doubly occupied (DO) site, for a given system size, corresponds to a straight line with slope $1/N_s$. Since the regime $X=1$ can be considered as quasiclassical, this is the strong-coupling result, where the energy cost of having one doubly occupied site ($N_2=1$) is U. Similar analyses for the cases $N_2=2,3,\ldots$, indicate that the slopes of the lowest energy levels are given by N_2/N_s, if $N_2\leqslant(N_s/2-1)$; recall that $N_2=N_s/2$ corresponds to having all sites doubly occupied, which is the CO state. It is interesting to note that the dominant contributions to the ground state comes from states where the DO sites are farthest apart, so they are evenly distributed throughout the chain, and singly occupied sites surround both sides of the DO ones. For instance, when $N_2=4$ on a 12-site ring, the dominant contributions to the ground state are

$$|0\ \uparrow\ \uparrow\downarrow\ \downarrow\ 0\ \uparrow\downarrow\ 0\ \uparrow\ \uparrow\downarrow\ \downarrow\ 0\ \uparrow\downarrow\rangle+\text{C.p.},$$

where C.p. stands for circular permutations.

When the lowest energies corresponding to different number of DO sites are compared, several regimes can be clearly distinguished. For a given system size, as U decreases below U_{c_2}, the lowest states correspond in succession to one, two, three, etc., doubly occupied sites. On the other hand, since the energy densities extrapolate to horizontal lines in the thermodynamic limit (see the discussion above), one may be misled to think that all energies should merge in that limit, amounting to a macroscopic degeneracy of states. The proper way to analyze the DO region is therefore in terms of *densities* of DO sites, in a situation analogous to that of occupancy. That is, for a given ratio N_2/N_s we calculate the lowest energies for chains with $N\cdot N_2$ DO sites out of $N\cdot N_s$ sites, with $N=1$, 2, 3, and so forth. The energy levels thus obtained extrapolate as $N_s\rightarrow\infty$ to the ones shown in Fig. 4. Though for finite systems the densities do not vary continuously, the following trend can be inferred from Fig. 4:

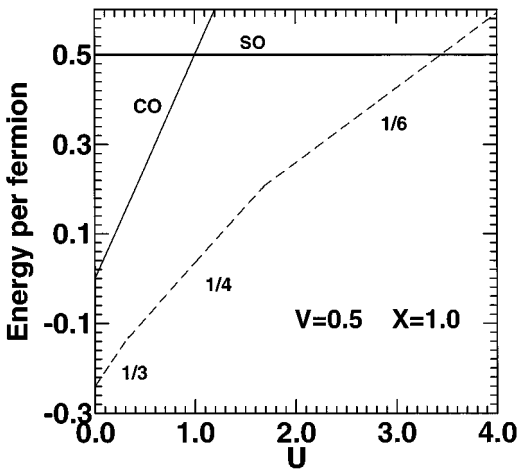

FIG. 4. Extrapolated lowest energy levels per fermion for different densities of doubly occupied sites, $\rho_2\equiv N_2/N_s$, which label the curves.

Below U_{c_2} the ground state suffers a succession of transitions to states with continuously increasing density of DO sites. In a renormalization group language, for fixed V, the DO region consists of a line of fixed points between the CO and the SO regions; each fixed point corresponds to a density of DO sites. As V is varied, this line of fixed points is displaced accordingly, and we may view the DO region in the phase diagram of Fig. 5 as a critical region made up of fixed points.

Another remarkable feature of the $X=1$ region is that states with $S^z\equiv\Sigma_i\langle m_i\rangle=N_s-2N_2$, corresponding to the maximum S^z compatible with the number of DO sites, are degenerate with those with $S^z=0$. In Ref. 17 it was shown that if one assumes the stability of the ferromagnetic state (similarly to the Nagaoka[24] problem), then there is a full degeneracy in S^z at the transition point $V=0$, $U=4$. Our results show that this degeneracy is partially lifted for $V\neq0$.

Further insight is obtained by examining the correlation functions defined by Eqs. (3)–(6). In the CO region, the

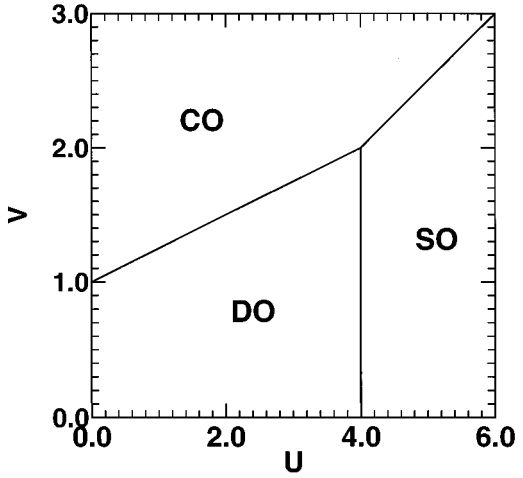

FIG. 5. Phase diagram V vs U for the extended Hubbard model at half-filling and $X=1$. CO, SO, and DO stand for charge-ordered, singly occupied, and doubly occupied states, respectively.

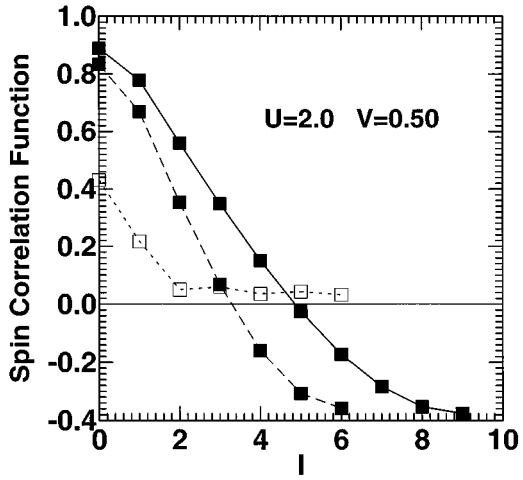

FIG. 6. Staggered spin-density correlation function vs intersite distance in the $S^z=0$ sector, for $U=2$ and $V=0.5$. Short-dashed lines represent data for $X=0$ in the SDW region with $N_s=12$ sites. Long-dashed (solid) lines represent data for $X=1$ with a ground state corresponding to one DO site on a chain with $N_s=12$ ($N_s=18$) sites.

charge correlation function alternates between 1/2 and 0, without any decaying with the distance; similarly, the spin-density correlations vanish identically, while superconducting correlations are zero for $\ell \neq 0$. This clearly confirms the static picture. In the SO region, the charge-density correlation function is uniform, sticking to the value 1/4, the usual asymptotic value corresponding to one fermion per site. Since all singly occupied states are degenerate, irrespective of S^z and of the spin arrangement for a given S^z, the specific form of a spin-density correlation function depends on the ground state one is considering, though the magnitude is always 1. Again, no relevant superconducting correlations were observed.

We now turn to the analysis of correlations in the more interesting DO region. First we consider the case of one DO site. While charge correlations attain their limiting value 1/4 for any $\ell > 1$, the staggered spin-density correlations display a decreasing monotonic behavior, as shown in Fig. 6. The ground state in this case is dominated by states such as

$$|0 \uparrow \downarrow \uparrow \downarrow \uparrow\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow\rangle + \text{C.p.},$$

for $N_s=12$ and similarly for $N_s=18$. Note that the DO site is located in the ring exactly opposite to the empty site, and that the alternating sequence of up and down spins is displaced by one site whenever one goes through either an empty or a DO site; this explains the sign change in $\mathcal{F}_S(\ell)$ in Fig. 6 near $\ell = N_s/4$. For comparison, we also show in Fig. 6 the staggered spin-density correlation function in the absence of bond-charge interaction in the SDW region. The ''kinked'' correlations obtained when $X=1$ are quite robust, and their slower spatial decay is suggestive of some degree of ordering. In the region where the ground state corresponds to two DO sites the behavior is qualitatively the same, and this may be a trademark of the DO region.

The degeneracy of the state with $S^z=0$ with that having maximum S^z is also manifested when comparing the spin-density correlation functions: Apart from the slightly larger value at $\ell=0$ (i.e., essentially the local moment), the amplitude does not decay with the distance, reflecting the strong pinning of the quasiferromagntic state.

Similarly to $|X|<1$, superconducting correlations are not enhanced by bond-charge interaction.

V. CONCLUSION

The effects of bond-charge interaction on the extended Hubbard model have been inferred from the analysis of a particular gap function to locate the transition points, and from various correlation functions; in the absence of bond-charge interaction, i.e., $X=0$, this procedure reproduces the known results quite accurately. For fixed $X \neq 1$, we find that this term causes the charge-density-wave region to grow at the expense of the spin-density-wave phase; this growth increases with $|X|$ and is more pronounced for $X>0$ than for $X<0$. As far as correlations are concerned, bond-charge interaction smooths the CDW-SDW transition, possibly driving them to second order or, at least, weakening their first-order nature; this point is surely worth being pursued further.

For $X=1$, we have presented evidence indicating that the intermediate phase, between the charge ordered and singly occupied states, comprises a succession of ground states corresponding to a continuous variation of the density of doubly occupied sites. Further, these $S^z=0$ states are degenerate with those having maximum S^z compatible with the density of doubly occupied sites. Associated with these doubly occupied states, the staggered spin-density correlation functions corresponding to $S^z=0$ develop ''kinks,'' while those corresponding to a maximum S^z display pinning behavior.

As far as the possibility of bond-charge interaction favoring a superconducting state, we have found no enhancement of pairing correlations, for the values of X considered here. This does not rule out the possibility of pairing for larger values of $|X|$, for higher dimensions or for other band fillings; we are currently investigating the possibilities of other fillings and higher dimensions.

Upon completion of this work, we received a preprint by Arrachea *et al.*,[25] in which the model discussed in Refs. 16–19 is studied by several methods; their model reduces to the one presented here in some special cases, for which the overall results agree with ours.

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