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#### Charge-order transition in the extended Hubbard model on a two-leg ladder

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We investigate the charge-order transition at zero temperature in a two-leg Hubbard ladder with additional nearest-neighbor Coulomb repulsion  $V$  using the density matrix renormalization group technique. We consider electron densities between quarter and half filling. For quarter filling and  $U=8t$ , we find evidence for a continuous phase transition between a homogeneous state at small  $V$  and a broken-symmetry state with “checkerboard” [wave vector  $\mathbf{Q}=(\pi, \pi)$ ] charge order at large  $V$ . This transition to a checkerboard charge-ordered state remains present at all larger fillings, but becomes discontinuous at sufficiently large filling. We discuss the influence of  $U/t$  on the transition and estimate the position of the tricritical points.

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The competition between kinetic energy and Coulomb repulsion in electronic systems can lead to a variety of interesting phenomena, one of them being charge ordering. A periodic charge order, i.e., a modulation of the charge density, can be described as charge density wave. One possible mechanism for charge ordering is the crystallization of electrons due to their long-range Coulomb repulsion as proposed by Wigner.<sup>1</sup> The Wigner lattice of electrons forms *without* the underlying lattice structure at low densities when the system is dominated by the effect of the Coulomb repulsion. Charge ordering may also occur at higher electron densities if the kinetic energy is reduced due to small hybridization of orbitals, or due to the interaction with lattice or spin degrees of freedom. Charge-ordered states have been observed in, for example, rare earth manganites, which have attracted attention recently due to their “colossal” magnetoresistance. Several of these compounds (e.g.,  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  for  $x \geq 0.5$ ) show a charge-ordered ground state for a certain range of doping.<sup>2</sup> Another material showing charge order is  $\text{NaV}_2\text{O}_5$ . It undergoes a phase transition at  $T_c=34\text{ K}$  that is

characterized by the opening of a spin gap and a doubling of the unit cell. While this transition was originally thought to be spin Peierls, recent studies have found evidence for charge order.<sup>3–5</sup> It has been proposed that this material is well-described as a quarter-filled ladder.<sup>6,7</sup> Two-leg ladder models are also thought to be relevant to a number of other materials containing ladderlike structures, such as the vanadates  $\text{MgV}_2\text{O}_5$  and  $\text{CaV}_2\text{O}_5$ , and the cuprates  $\text{SrCu}_2\text{O}_3$  and  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ . For a more detailed description of ladder materials and models, we direct the reader to a recent review<sup>8</sup> and the references contained therein.

One of the simplest models of interacting electrons that allows for charge ordering is the Hubbard model extended with an additional nearest-neighbor (NN) Coulomb repulsion,  $V$ . The charge-order transition in this model has been studied in the one-dimensional (1D) model in the strong-coupling limit,<sup>9</sup> at quarter filling,<sup>10</sup> at half filling,<sup>11,12</sup> in the 2D system at half filling,<sup>13,14</sup> and within the dynamical mean field theory (the limit of infinite dimensions) at quarter<sup>15</sup> and half filling.<sup>16</sup> A variety of techniques, such as mean-field

approximations, perturbation theory, and numerical methods such as the quantum Monte Carlo and the density matrix renormalization group method (DMRG) have been employed in these studies. Their results can be summarized as follows: At the mean-field level, the transition between a homogeneous state and a charge-density wave (CDW) state at half filling in a hypercubic lattice occurs at  $V_c = U/z_0$ , where  $z_0$  denotes the number of nearest neighbors ( $z_0 = 2d$ ). Numerical studies<sup>12</sup> indicate a slightly higher value of  $V_c$ , at least in 1D. Interestingly, in 1D at half filling the transition has been found to be second order at small  $U/t$  and first order at large  $U/t$ , with the tricritical point located at  $U_c/t \sim 4-6$ .<sup>12</sup> Here we use the term “first order” to denote discontinuous behavior of the charge-order parameter as a function of microscopic parameters such as  $V$  or band filling, and “second order” to denote continuous behavior. At quarter filling in 1D, the situation is more complicated since a number of phases compete for large  $V$ .<sup>10</sup> In higher dimensions, the transition seems to always be first order.<sup>13-16</sup> However, conclusive studies that can reliably distinguish between first- and second-order transitions are lacking. Between quarter and half filling, the existence and nature of a transition is unclear in general. In 1D, the extended Hubbard model undergoes phase separation rather than a transition to a CDW state for  $|U|/t < 4$  and large  $V$ .<sup>17</sup> For  $U/t > 4$ , indications are that the 1D system undergoes a transition to a  $q = \pi$  CDW state for sufficiently large  $V$  at all fillings.<sup>23</sup>

In this paper, we examine the charge-order transition in the extended Hubbard model on the two-leg ladder, considering all values of band filling between quarter and half filling. We shall investigate the nature and location of the charge-order transition in the ladder and compare our results with the 1D as well as higher dimensional models.

The single-band extended Hubbard model has the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} n_i n_j. \quad (1)$$

Here, we consider a lattice consisting of two chains of length  $L$ , i.e., a ladder, and discuss band fillings  $\langle n \rangle = N/(2L)$ , with  $N$  the number of electrons. The summation  $\langle ij \rangle$  then runs over all pairs of nearest-neighbor sites in the ladder. In this work, we take both the hopping and the nearest-neighbor Coulomb repulsion to be isotropic; in general, one could consider the anisotropic case, parameterized by  $t_{\parallel}$ ,  $t_{\perp}$ ,  $V_{\parallel}$ , and  $V_{\perp}$ .

The numerical results shown in this paper have been calculated with the DMRG technique<sup>18</sup> on lattices of up to  $2 \times 64$  sites with open boundary conditions, both between the two chains and at the ends of the chains. We have kept up to 600 states per block, resulting in the discarded weight of the density matrix eigenvalues being typically  $10^{-8}$  or less. The errors in the energies and correlation functions arising from the truncation of the density matrix are always less than a few percent.

We now turn to the discussion of the results. In order to investigate the charge ordering, we consider the static charge structure factor

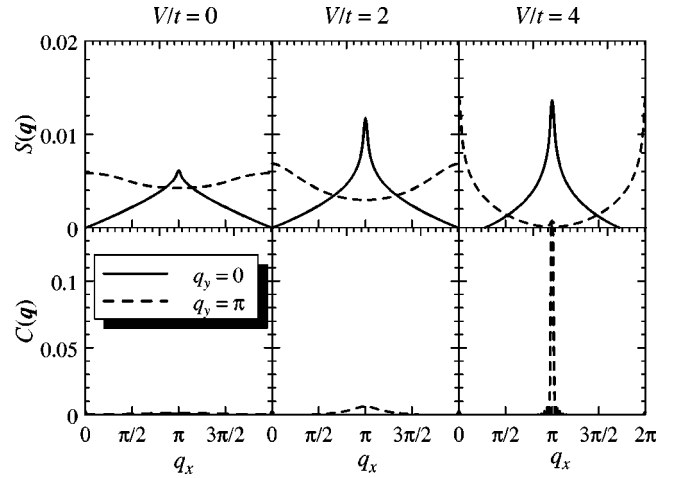


FIG. 1. Charge- and spin-correlation functions for a  $64 \times 2$  ladder,  $U = 8t$ , quarter filling  $\langle n \rangle = 0.5$  (64 electrons), and different values of the nearest-neighbor repulsion  $V$ .

$$C(\mathbf{q}) = \frac{1}{2L} \sum_i e^{i\mathbf{q} \cdot \mathbf{R}_i} \bar{C}(\mathbf{R}_i), \quad (2)$$

where

$$\bar{C}(\mathbf{R}_i) = \frac{1}{N_{\text{av}}} \sum_{\{j\}} \langle \delta n_{j+i} \delta n_j \rangle. \quad (3)$$

$\langle \dots \rangle$  denotes the ground-state expectation value,  $\delta n_j = n_j - \langle n_j \rangle$ , and we average over typically  $N_{\text{av}} = 6$  sites to remove oscillations due to the open boundaries. For checkerboard charge order, which is expected to be the ground state for large values of  $V$ ,  $C(\mathbf{q})$  should show a pronounced peak at  $\mathbf{Q} = (\pi, \pi)$ . The spin order can be studied by looking at the spin structure factor,  $S(\mathbf{q})$ , which is defined similarly in terms of the spin-spin correlation function  $\langle S_{j+i}^z S_j^z \rangle$ .

In Fig. 1, we show the results for  $C(\mathbf{q})$  and  $S(\mathbf{q})$  for a  $2 \times 64$  system at  $U = 8t$  and quarter filling for different values of  $V$ . The transition between a homogeneous state at small  $V$  and an ordered CDW state at large  $V$  can clearly be seen. The DMRG ground state at  $V > V_c$  is fully gapped and has broken translation invariance, i.e., for large  $V$  every second site is empty. [This gapped charge-ordered state with  $(\pi, \pi)$  broken symmetry is present at all fillings from quarter filling to half filling.] In the spin channel, peaks at  $(0, \pi)$  and  $(\pi, 0)$  develop with increasing  $V$ , showing an alternating spin pattern on the *occupied* sites in the CDW state. This spin order arises from virtual hopping processes (fourth order in  $t$ ) which lead to antiferromagnetic couplings between the occupied sites. In the limit of large  $V$  the system can be mapped to a  $J_1 - J_2$  spin- $\frac{1}{2}$  chain, where  $J_1 \gg J_2$  because of the larger number of exchange processes in the diagonal  $(1,1)$  direction.

At half filling, the spin correlations correspond to short-range  $(\pi, \pi)$  order at small  $V/U$ . In the limit of large  $V \gg (t, U)$ , the spin correlations vanish. This behavior is due to the increase in the number of double occupancies in the charge-ordered state at half filling, which leads to a suppression of local magnetic moments. Between quarter and half filling,  $S(\mathbf{q})$  shows peaks at incommensurate wave vectors that correspond to combinations of bonding and antibonding

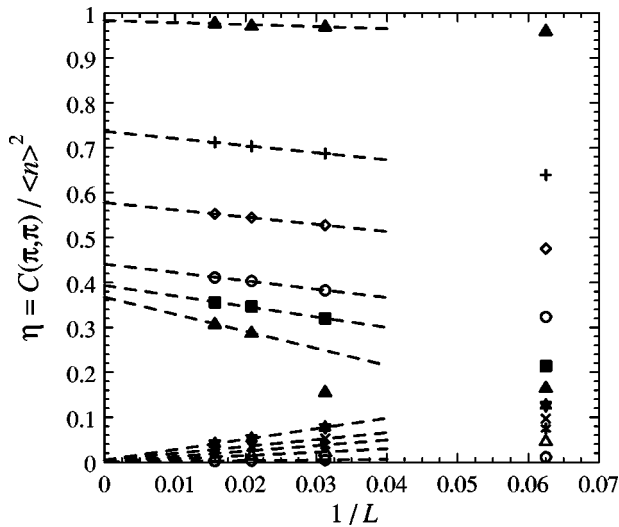


FIG. 2. Finite-size scaling for the staggered charge correlation function at  $U=8t$  and  $\langle n \rangle=0.75$ . The curves correspond to  $V/t = 2.5, 2.8, 2.9, 2.95, 3.0, 3.05, 3.1, 3.2, 3.5, 4.0$ , and  $8.0$  from bottom to top. The dashed lines are linear fits through the data points for  $L=32, 48, 64$ . The irregular behavior at  $V/t=3.05$  may indicate a first-order transition (here the  $L=32$  point was excluded from the fit).

Fermi vectors.<sup>19</sup> Near quarter filling, these peaks tend to be strengthened but also displaced as  $V$  is increased, whereas closer to half filling the peaks tend to be suppressed in the CDW phase. We further note that between quarter and half filling the residual magnetic moments tend to order ferromagnetically in the charge-ordered phase, i.e., the ground-state spin is nonzero.<sup>20</sup> The existence of gapless modes in the homogeneous phase is less clear;<sup>19</sup> at least at half filling both spin and charge gaps are nonzero for any parameters with  $U>0$ .

In order to examine the extent of the charge ordering and the nature of the transition, we calculate the order parameter for a  $\mathbf{Q}=(\pi, \pi)$  charge-ordered state,

$$\eta = \lim_{L \rightarrow \infty} \frac{C(\mathbf{Q})}{\langle n \rangle^2}. \quad (4)$$

We carry out the  $L \rightarrow \infty$  extrapolation by calculating  $\eta(L)$  for  $L=16, 32, 48, 64$ , and performing a linear fit in  $1/L$  through the three largest system sizes (see Fig. 2). (The  $L=16$  point is consistent with the linear extrapolation except in the region of the transition.) This extrapolation is the major source of uncertainty in our results; the error here is typically  $\Delta\eta=0.01$ .

In Fig. 3, we plot  $\sqrt{\eta}$  (which corresponds to the relative difference of the sublattice occupancies in the broken-symmetry charge-ordered state) for  $U=8t$  and different band fillings. For  $U=4t$  as well as  $U=8t$ , we find a transition from a homogeneous state to a charge-ordered state with increasing  $V$  for all values of  $\langle n \rangle$ . Note that the extrapolation with system size is crucial in order to extract the  $V_c$  from our data. Examination of  $\eta(V; L)$  for fixed  $L$ , as used in Ref. 12 to determine  $V_c$  from DMRG results for the 1D system, is not adequate for the ladder system.

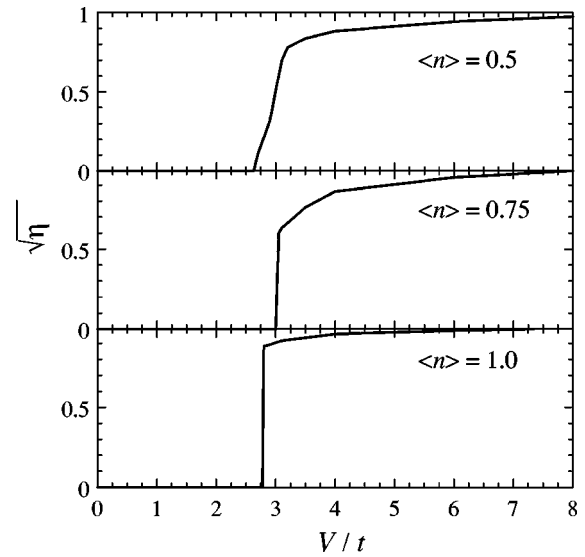


FIG. 3. Order parameter  $\sqrt{\eta}$  versus  $V/t$  for  $U=8t$  and  $\langle n \rangle = 0.5, 0.75$ , and  $1$ . The data indicate a second-order quantum phase transition at  $V_c/t=2.65 \pm 0.1$  between a homogeneous and a charge-ordered state for  $\langle n \rangle=0.5$ . For  $\langle n \rangle=0.75$ , the transition at  $V_c/t=3.05 \pm 0.1$  is weakly first order whereas the transition at half filling at  $V_c/t=2.8 \pm 0.1$  is clearly first order.

An additional, related method to determine  $V_c$  is to examine the scaling of  $LC(\mathbf{Q}; L)$  with  $L$ . This quantity should diverge with  $L$  in the charge-ordered state, but should decrease with  $L$  in the homogeneous state to a value determined by the density correlation length of the system.<sup>11</sup> This method yields the same values of  $V_c$  as that obtained from the extrapolation of  $\sqrt{\eta}$  to within  $\Delta V_c \approx 0.1t$ . Furthermore, we have checked that the compressibility of the system is positive, i.e., there is no tendency to phase separation in the parameter region studied here ( $U/t \geq 4$ ). Note, however, that phase separation occurs for smaller values of  $U/t$ , e.g., for  $U/t=1$  and  $V \gg t$ . A complete investigation of the phase diagram will be published elsewhere.<sup>20</sup>

At  $U=8t$  (Fig. 3) the transition to the charge-ordered state is continuous for small filling (e.g., quarter filling,  $\langle n \rangle = 0.5$ ) whereas for large filling the order parameter clearly shows a jump at a critical value  $V_c$ . This leads to a tricritical point in the  $V$ - $\langle n \rangle$  plane, as can be seen in the phase diagram of Fig. 4. This tricritical behavior seems to be similar to the one observed in the 1D system at half filling.<sup>11,12</sup> The location of the tricritical point depends on the strength of  $U$ , as shown in Fig. 4. For  $U=4t$ , its position is  $\langle n \rangle_{tc} = 0.95 \pm 0.1$ , and at  $U=8t$  we find  $\langle n \rangle_{tc} = 0.65 \pm 0.1$ . The position of the tricritical point (for fixed  $U$ ) has been estimated from the  $\langle n \rangle$  dependence of the magnitude of the jump in  $\eta(V)$ .

Finally, we address the dependence of  $V_c$  on  $U$  and the band filling. At half filling, both weak- and strong-coupling approximations<sup>16,21</sup> for the transition between spin-density wave (SDW) and CDW yield a critical value of  $V_c = U/z_0$  for a system on a hypercubic lattice. However, these Hartree-type approximations assume a SDW phase with true long-range order, which is absent for 1D chains as well as for the ladder system considered here. Nevertheless, the mean-field  $V_c$  is in reasonable agreement with the value of slightly more than  $U/2$  found numerically for a 1D chain.<sup>12</sup> For the ladder

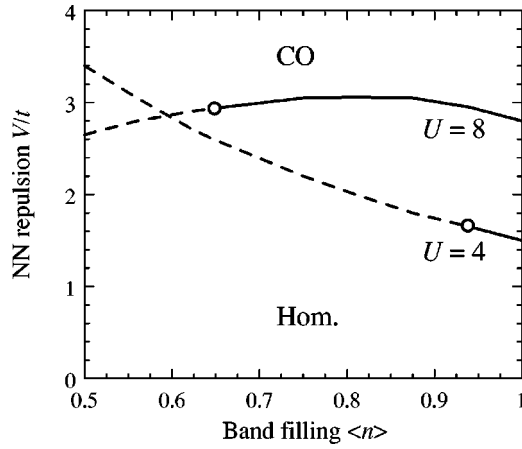


FIG. 4. Phase diagram in the  $V$ - $\langle n \rangle$  plane showing first-order (solid lines) and second-order (dashed lines) transitions between the homogeneous and the charge-ordered state for  $U=4t$  and  $U=8t$ . The boundaries have error  $\Delta V_c \approx 0.1t$  which arises mainly from the  $L \rightarrow \infty$  extrapolation. The circles indicate the estimated positions of the tricritical point with uncertainty  $\Delta \langle n_{tc} \rangle \approx 0.1$ .

systems studied in the present work, the DMRG results for half filling also agree quite well with the predictions of the Hartree approximation. As can be seen in Fig. 5,  $U/V_c$  is consistent with  $V_c = U/3$  in both the weak- and strong-coupling limits.

Below half filling, the behavior is more complicated because it is no longer dominated only by the interplay of  $U$  and  $V$ . Since the average number of double occupancies decreases with decreasing electron density, the kinetic energy becomes important for larger  $U$ . In the region between quarter filling and half filling, we are faced with the interplay of all three energy scales  $t$ ,  $U$ , and  $V$ , and as can be seen in Fig. 4,  $V_c$  varies considerably with  $\langle n \rangle$  and  $U$ .

In summary, our scenario for the charge-order transition in the Hubbard ladder with  $U \geq 4t$  proceeds as follows: At all band fillings, an increasing nearest-neighbor repulsion  $V$  drives a transition from a homogeneous state to a gapped CDW state with  $\mathbf{Q} = (\pi, \pi)$ . At quarter filling, each occupied site in the CDW state carries spin  $\frac{1}{2}$ , and the residual kinetic energy orders these spins “antiferromagnetically” at ordering vectors  $(\pi, 0)$  and  $(0, \pi)$ . A similar charge ordering leading to “zigzag” antiferromagnetic ordering has been found at quarter filling in coupled Hubbard ladders within mean-field theory<sup>7</sup> and in the  $t$ - $J$ - $V$  ladder with adiabatic Holstein phonons.<sup>22</sup> At half filling, the CDW state found at large  $V$

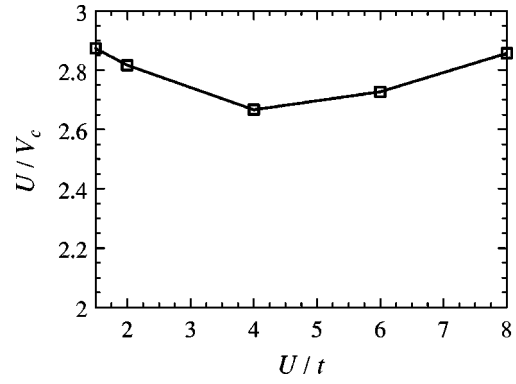


FIG. 5. The ratio  $U/V_c$  at half filling for different values of  $U$ . The data indicate that  $U/V_c$  approaches the value  $z_0=3$  for both weak and strong coupling which is consistent with mean-field arguments.

consists of doubly occupied sites without local moments, so that the spin order is strongly suppressed. The critical  $V_c$  goes asymptotically to the value  $V_c = U/3$  in both the weak- and strong-coupling limits, as predicted by mean-field theory. Between quarter and half filling, there is a mixture of singly and doubly occupied sites in the CDW phase, and the spin order is, in general, incommensurate. The total spin in the CDW phase is nonzero, i.e., charge order co-exists with ferromagnetism. As  $V$  is increased and the system goes into the CDW phase, the incommensurate spin correlations tend to be enhanced closer to quarter filling and suppressed closer to half filling. Note that this suppression of the spin moments within the CDW phase as the filling is increased is in contrast to the behavior in the homogeneous phase at  $V=0$  and  $U \gg t$ , for which the spin moment *increases* with increasing  $\langle n \rangle$ .

An interesting subject for future study would be a more detailed comparison of the phase diagram of the ladder system with that of the 1D chain.<sup>10,17,23</sup> For instance, the phase separation region in the ladder for large  $V/t$  is much smaller<sup>20</sup> than the  $|U|/t < 4$  region found in 1D. The origin of these differences in the charge-ordering process and the role of the nonzero ground-state spin remain to be clarified.

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