Ground State Phases of the Half-Filled One-Dimensional Extended Hubbard Model

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Using quantum Monte Carlo simulations, results of a strong-coupling expansion, and Luttinger liquid theory, we determine quantitatively the ground state phase diagram of the one-dimensional extended Hubbard model with on-site and nearest-neighbor repulsions U and V. We show that spin frustration stabilizes a bond-ordered (dimerized) state for $U \approx V/2$ up to $U/t \approx 9$, where t is the nearest-neighbor hopping. The transition from the dimerized state to the staggered charge-density-wave state for large V/U is continuous for $U \lesssim 5.5$ and first order for higher U.

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The one-dimensional Hubbard model, which describes electrons on a tight-binding chain with single-particle hopping matrix element t and on-site repulsion U, has a charge-excitation gap for any $U > 0$ at half filling [1]. In the spin sector, the low-energy spectrum maps onto that of the $S = 1/2$ Heisenberg chain; the spin coupling $J = 4t^2/U$ for $U \to \infty$. The spin spectrum is therefore gapless and the spin-spin correlations decay with distance r as $(-1)^r/r$ [2]. Hence, the ground state is a quantum critical staggered spin-density wave (SDW). In the simplest *extended Hubbard model*, a nearest-neighbor repulsion V is also included. The Hamiltonian is, in standard notation and with $t = 1$ hereafter,

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

The low-energy properties for $V \lesssim U/2$ are similar to those at $V = 0$. For higher V, the ground state is a staggered charge-density-wave (CDW), where both the charge and spin excitations are gapped. The transition between the critical SDW and the long-range-ordered CDW has been the subject of numerous studies [3–14]. Until recently, it was believed that the SDW-CDW transition occurs for all $U > 0$ at $V \gtrsim U/2$ and that it is continuous for small U ($\lesssim 5$) and first order for larger U. However, based on a study of excitation spectra of small chains, Nakamura argued that there is also a bond-order-wave (BOW) phase [10], where the ground state has a staggered modulation of the kinetic energy density (dimerization), in a narrow region between the SDW and CDW phases for U smaller than the value at which the transition changes to first order. Previous studies [6–9] had indicated an SDW state in this region. Nakamura's BOW-CDW boundary coincides with the previously determined SDW-CDW boundary. The presence of dimerization and the accompanying spin gap were subsequently confirmed using quantum Monte Carlo (QMC) simulations [11,12]. The BOW phase now also has a weak-coupling theory [13].

The existence of an extended BOW phase has recently been disputed. Jeckelmann argued, on the basis of density-matrix-renormalization-group calculations, that the BOW exists only on a short segment of the first-order part of the SDW-CDW boundary [14], i.e., that the transition always is SDW-CDW and that BOW order is induced only on part of the coexistence curve. However, QMC calculations demonstrate the existence of BOW order well away from the phase boundary [12].

Although several studies agree on the *existence* of an extended BOW phase [10–13], the shape of this phase in the (U, V) plane has not yet been reliably determined. The system sizes used in the exact diagonalization study [10] were too small for converging the SDW-BOW boundary (i.e., the spin-gap transition) for $U \gtrsim 4$. In the previous QMC studies [11,12], the emphasis was on verifying the presence of BOW order and the phase transitions for $U \approx 4$. In this Letter, we present the complete phase diagram. Taking advantage of recent QMC algorithm developments—stochastic series expansion with directed-loop updates [15] in combination with the quantum generalization [11] of the parallel tempering method [16]—we have carried out high-precision, large-chain (up to $L = 1024$) calculations for sufficiently high U (≤ 12) to locate the point at which the BOW order vanishes. In agreement with Ref. [14], we find that the BOW exists also above the U at which the transition to the CDW state becomes first order. However, long-range BOW order exists also below this point, and, hence, *the point at which the nature of the transition changes from continuous to first order is on the BOW-CDW boundary.*

The phase diagram we find here is qualitatively similar to that obtained in a fourth-order strong-coupling expansion, where the transition to the CDW state is determined

by comparing the energies of the large-V CDW state and the effective spin model including nearest- and next-nearest-neighbor interactions J and J' [8]. The BOW phase corresponds to the spontaneously dimerized phase of the spin chain, i.e., $J'/J > 0.241$ [17]. In Fig. 1, we compare our QMC phase boundaries with the strong-coupling result; the procedures giving the QMC boundaries will be discussed below. We will show that the system is a Luther-Emery liquid on the continuous BOW-CDW boundary, i.e., the charge gap vanishes and the spin gap remains open. Evidence supporting this type of transition was also presented in Ref. [11]. Here we will further argue that the change to a first-order transition corresponds to the Luttinger charge exponent K_ρ reaching the value $1/4$.

We extract the SDW-BOW and BOW-CDW boundaries using the charge and spin exponents K_ρ and K_σ. If there is a spin or charge gap, the corresponding exponent vanishes. Otherwise the equal-time correlation function $C_\rho(r) \sim r^{-(K_\sigma+K_\rho)}$, $C_\sigma(r) \sim r^{-(K_\sigma^{-1}+K_\rho)}$. If nonzero, the spin exponent $K_\sigma = 1$ as a consequence of spin-rotation invariance [18]. On periodic chains the exponents can be conveniently extracted from the static structure factors $S_{\rho,\sigma}(q)$ [19],

$$S_{\rho,\sigma}(q) = \frac{1}{L}\sum_{j,k} e^{iq(j-k)}\langle (n_{\uparrow j} \pm n_{\downarrow j})(n_{\uparrow k} \pm n_{\downarrow k})\rangle, \quad (2)$$

in the limit $q \to 0^+$:

$$K_{\rho,\sigma} = \pi S_{\rho,\sigma}(q_1)/q_1, \qquad q_1 = 2\pi/L, \qquad L \to \infty. \quad (3)$$

If there indeed are three successive phases, SDW-BOW-CDW, as V is increased at a fixed value of U, then the spin exponent $K_\sigma = 1$ in the SDW phase and $K_\sigma = 0$ everywhere else. The charge exponent $K_\rho = 0$ everywhere, except exactly at the BOW-CDW transition point if this is a continuous quantum phase transition (i.e., if the charge gap vanishes). In contrast, if the transition is first order, then $K_\rho = 0$ also on the phase boundary. Using the relation (3) for a finite system, any discontinuities will naturally be smoothed, and one can only expect to observe $\pi S_{\rho,\sigma}(q_1)/q_1$ developing sharp features as L is increased. In Fig. 2, we show results demonstrating this for several different system sizes at $U = 4$, 6, and 8.

Looking first at the charge exponent, if $K_\rho > 0$ on the BOW-CDW boundary and $K_\rho = 0$ elsewhere, then one can expect a peak developing in $\pi S_\rho(q_1)/q_1$ versus V. The peak position corresponds to the critical V, and the peak height should converge to K_ρ. If the transition is first order, $\pi S_\rho(q_1)/q_1$ should converge to zero for all V, but one can still expect some structure at the phase boundary for finite L as the nature of the ground state changes. In Fig. 2, for $U = 4$ and 6 the development of sharp peaks is apparent. For $U = 4$, the peak height converges to a nonzero value, implying a continuous transition at $V \approx 2.160$ with $K_\rho \approx 0.43$. For $U = 6$, the convergence to a value > 0 is not clear, but the transition point is given accurately by the peak position, which shows very little size dependence. It has been shown previously that the transition is first order for $U = 6$ [6,11], and the peak should therefore in fact converge to zero. The rather slow decay reflects the proximity to the point at which the transition becomes continuous. For $U = 8$, the peak does not sharpen, but instead a step develops at the critical V.

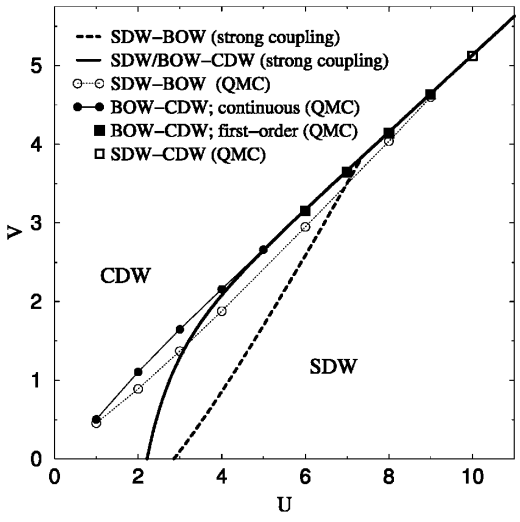

FIG. 1. QMC and strong-coupling phase diagram. The BOW is located between the SDW-BOW and BOW-CDW curves.

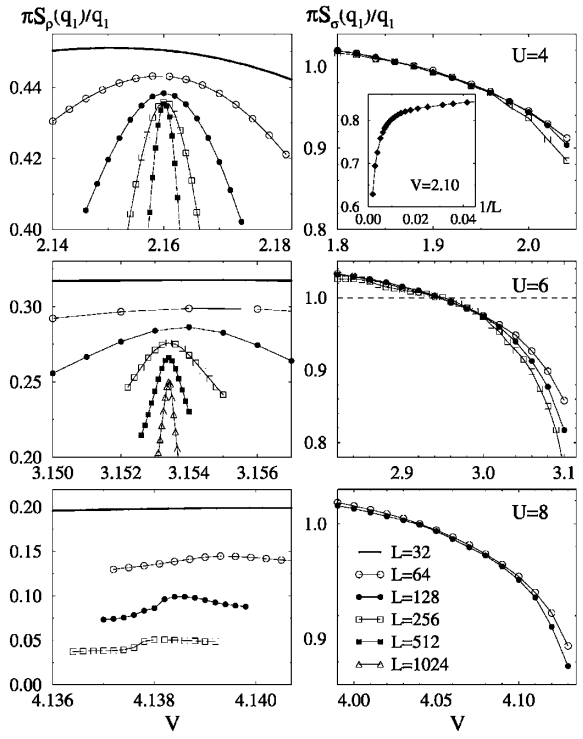

FIG. 2. Long-wavelength charge (left panels) and spin (right panels) structure factors vs V for $U = 4$ (top), 6 (middle), and 8 (bottom). The system sizes are indicated in the lower-right panel. The $U = 4$ inset shows the dependence on the inverse lattice size at $V = 2.10$.

The whole curve converges to 0 as $L \to \infty$. The transition is, hence, strongly first order in this case, in agreement with previous calculations. As seen in Fig. 1, and as observed already by Hirsch [6], the locations of the $U = 6$ and 8 critical points agree very well with the strong-coupling expansion [20].

In the SDW phase, one cannot expect to easily find $\pi S_\sigma(q_1)/q_1 \to 1$ exactly, due to logarithmic corrections that affect various quantities strongly even for very long chains [21,22]. However, the log corrections are known to vanish in the frustrated $J - J'$ spin chain at its dimerization transition [23], and, hence, since the SDW-BOW transition should be of the same nature, the log corrections should vanish here as well. The transition at fixed U should therefore be signaled by $\pi S_\sigma(q_1)/q_1$ crossing 1 from above as V is increased. Because of the vanishing log corrections at the transition, the crossing point with 1 should not move significantly as L is increased, but the drop below 1 should become increasingly sharp, and eventually $\pi S_\sigma(q_1)/q_1$ should approach 0 inside the BOW phase. This method was used in Ref. [11] and gave a slightly higher critical V for the SDW-BOW transition at $U = 4$ than the exact diagonalization [10]. We now have results for a wider range of couplings. The results shown in Fig. 2 are in accord with the above discussion for all three U values; $\pi S_\sigma(q_1)/q_1$ crosses 1 at a V point which does not move visibly between $L = 64$ and $L = 256$. For larger V, one can see a sharper drop for the larger system sizes. The size dependence at $U = 4$, $V = 2.1$ is shown in an inset. Here the convergence to 0, i.e., the presence of a spin gap, is apparent. If the spin gap is small, as it is close to the phase boundary, the convergence to 0 will obviously occur only for very large systems.

Results such as those shown in Fig. 2 were used to determine the phase boundaries in Fig. 1. As already noted, the BOW aspect of the phase diagram differs from previous proposals [10,11,13,14] in that the BOW-CDW transition can be either continuous or first order, i.e., *the change of order occurs on the BOW-CDW boundary*. The existence of two special points, one where the transition order changes and one at higher U where the BOW vanishes, was also suggested by Jeckelmann [14], who, however, insists that the BOW does not exist for small U where the transition to the CDW state is continuous (i.e., his phase diagram has no continuous BOW-CDW transition). We have carried out calculations for U down to 1, and, as shown in Fig. 1, we still find a BOW phase there. Most likely, in view also of weak-coupling arguments [13], the BOW extends down to $U = 0^+$. We find no BOW for $U \gtrsim 9$. In the strong-coupling expansion, using the couplings J and J' derived by van Dongen [8], the effective spin model is gapped, i.e., $J' > 0.241J$ [17], above the dashed curve in Fig. 1. The $J - J'$ mapping is not applicable beyond the transition into the CDW state, which (the solid curve in Fig. 1) was previously calculated by comparing the fourth-order CDW and $J - J'$ energies [8]. The fourth-order BOW region ends at $U \approx 7$, where the spin-gap curve crosses the CDW-transition curve. This is slightly lower than what we find based on QMC. The strong-coupling BOW extends down to smaller U, V, but clearly the fourth-order result cannot be expected to be quantitatively accurate in this region. Nevertheless, the spin-frustration mechanism consistently explains the presence of an SDW-BOW transition and an extended BOW phase. Spin frustration was previously cited by Jeckelmann [14], but, surprisingly, he used it in support of a BOW of vanishing extent.

Next, we consider the nature of the BOW-CDW transition. As discussed in Refs. [10,13], the continuous critical point for small U is described by a Gaussian free (charge) boson theory, characterized by the parameter K_ρ. At generic values of (repulsive) U, V, the leading "$4k_F$" umklapp process is present, and has scaling dimension $\Delta_{4k_F} = 2K_\rho$ and is, hence, relevant ($\Delta_{4k_F} < 2$) for $K_\rho < 1$. At the BOW-CDW transition, this operator vanishes, leading to a vanishing of the charge gap. For consistency, no other relevant operators should be present, which would otherwise require fine-tuning to zero, making the Gaussian theory a multicritical point. The most dangerous candidate is the "$8k_F$" umklapp process, with $\Delta_{8k_F} = 4\Delta_{4k_F} = 8K_\rho$, so a continuous Gaussian critical point is possible only for $1 > K_\rho > 1/4$. Even in this range, the Gaussian theory is an unusual critical point with *nonuniversal* behavior, e.g., the correlation length exponent $\nu = 1/(2 - 2K_\rho)$.

Extrapolated QMC results for K_ρ on the BOW-CDW boundary are shown in Fig. 3. The finite-size corrections appear to be of the form $1/L^\alpha$, with a U dependent exponent α. At $U = 4$, $\alpha \approx 1$, as shown in the inset of Fig. 3. For larger U, α decreases rapidly and is difficult to determine accurately for $U \gtrsim 5$. The extrapolated K_ρ value at $U = 5$ in Fig. 3 should be regarded as an upper bound. At $U = 6$, the extrapolated $K_\rho < 1/4$, and, hence, we expect an eventual drop to 0. This is consistent with clear signals of a first-order transition [11]. Also at $U = 5.5$ there are signs of first-order behavior, e.g., in order

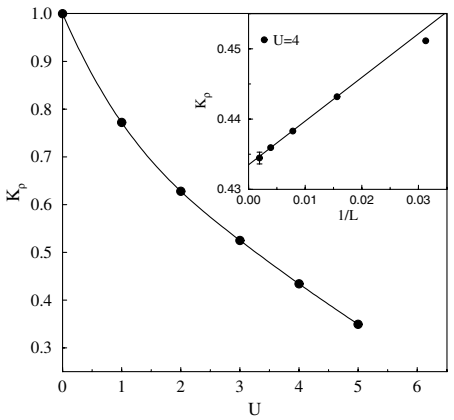

FIG. 3. QMC results for Luttinger charge exponent on the BOW-CDW boundary (solid circles). The inset shows the finite-size scaling for $U = 4$.

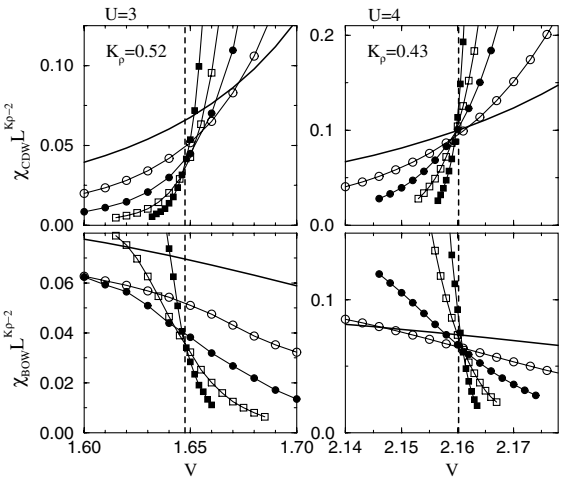

FIG. 4. Finite-size scaling of the BOW and CDW susceptibilities for $U = 3$ (left) and 4 (right). The symbols correspond to different system sizes as in Fig. 2. The dashed lines indicate the independently determined critical points.

parameter histograms such as those considered in Ref. [11]. We believe that the change from a continuous to a first-order transition occurs between $U = 5$ and 5.5.

What is the nature of the tricritical point at which the transition becomes first order? The simplest scenario is that this is the last (marginally) stable point of the Gaussian fixed line, i.e., with $K_\rho = 1/4$. This hypothesis predicts that the critical K_ρ continuously approaches $1/4$ as the tricritical point $U = U_t$ is approached from below, as $K_\rho - 1/4 \sim \sqrt{(U_t - U)/U_t}$. We do not have sufficient data to verify this form, but it is consistent with a sharp drop to 0 between $U = 5$ and 5.5 (Fig. 3), required since at $U = 5.5$ the transition should be first order. Hence, we favor this behavior over the *a priori* consistent (but less simple) possibility of a nontrivial "strong coupling" tricritical fixed point far from the Gaussian line.

To further demonstrate the Luther-Emery state on the continuous BOW-CDW curve, we study the finite-size scaling of the CDW and BOW susceptibilities, $\chi_{\mathrm{CDW}}(\pi)$ and $\chi_{\mathrm{BOW}}(\pi)$ (with their standard Kubo-integral definitions [11]). Both the charge and bond correlations should decay as $(-1)^r r^{-K_\rho}$ [18], implying that the susceptibilities scale with system size as L^{2-K_ρ}. Thus, $\chi(\pi)L^{K_\rho-2}$ curves for different L should intersect at the critical BOW-CDW point. Figure 4 shows results for $U = 3$ and 4, using the K_ρ values determined above. For $U = 4$, the expected scaling can be observed even for small systems. For $U = 3$, the corrections are larger, and the asymptotic scaling sets in only for $L \gtrsim 128$. This is clearly due to the smaller spin gap at $U = 3$, which implies a longer length scale below which remaining spin correlations affect the charge and bond fluctuations.

In summary, we have determined the ground state phase diagram of the extended Hubbard model at half filling. The dimerized BOW phase can be explained by spin frustration. The BOW-CDW transition changes from continuous to first order between $U = 5$ and 5.5. On the critical (U, V) curve, the system is a Luther-Emery liquid, with a charge exponent K_ρ decreasing from 1 as U is increased from 0. We have argued that the minimum $K_\rho = 1/4$ and that the BOW-CDW transition becomes first order when this value is reached.

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