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# Comment on “Ground State Phase Diagram of a Half-Filled One-Dimensional Extended Hubbard Model”

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In [1], Jeckelmann argued that the recently discovered bond-order-wave (BOW) phase [2, 3, 4] of the 1D extended Hubbard model does not have a finite extent in the  $(U, V)$  plane, but exists only on a segment of a first-order spin-density-wave–charge-density-wave (SDW-CDW) phase boundary. We here present quantum Monte Carlo results of higher precision and for larger system sizes than previously [3]. Using a direct finite-size scaling of the BOW correlations, we reconfirm that the BOW phase *does exist* a finite distance away from the phase boundary, which hence is a BOW-CDW transition curve. We only address the existence of the BOW phase and focus on a single value,  $U = 4$ , of the on-site interaction.

We first determine the critical value  $V_c$  of the nearest-neighbor interaction. Fig. 1(a) shows the  $V$ -dependence of the charge susceptibility  $\chi_c(q)$  at the smallest non-zero wave-number,  $q = 2\pi/N$ , for different system sizes  $N$  (for the definition of  $\chi_c$ , see [3]). The narrowing of the peak with increasing  $N$  and the convergence of the height indicate a charge gap for all  $V$  except at  $V_c$ , i.e., in disagreement with [1] we find a continuous phase transition at  $U = 4$ . The peak position gives  $V_c = 2.1602 \pm 0.0003$ , which improves considerably on the estimate  $V_c = 2.150 \pm 0.010$  reported in [1].

We next choose  $V = 2.10$ , where according to [1] there should be no long-range BOW. In Fig. 1(b) we show the corresponding correlation function  $C_B(r)$  at the longest distance,  $r = N/2$ , in periodic chains with up to  $N = 512$  sites. As a function of  $1/N$  for large  $N$ , the data scale linearly to a value which corresponds to dimerization  $\delta = \sqrt{C_B}/2 \approx 0.053$  (as defined in [1]). It is not clear why the density matrix renormalization group (DMRG) calculations of [1] failed to detect this rather strong BOW order. Dimerization was observed only on the transition curve to the CDW phase [1], where we instead find coexisting critical BOW and CDW fluctuations. The origin of this discrepancy at  $V_c$  could be that  $V_c$  was not determined to sufficient accuracy in [1].

In summary, our improved calculations do not agree with the phase diagram presented in [1] but reconfirm the finite extent of the BOW phase [3] as first suggested in [2]. The advantage of the Monte Carlo method we have used

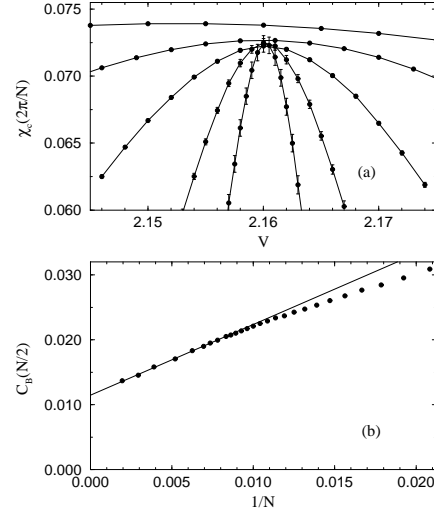


FIG. 1: (a) Charge susceptibility at  $q = 2\pi/N$  for  $N = 32, 64, 128, 256$ , and  $512$  (curvature increases with  $N$ ). (b) BOW correlation at distance  $r = N/2$  versus inverse system size ( $V = 2.10$ ), along with a linear fit to the large- $N$  data.

[3, 5] is that results can be obtained for large periodic systems, which are better suited for finite-size scaling than the open boundary conditions typically used in DMRG calculations on long chains. With the recently improved simulation algorithm [5] that we have used here, we hope to be able to determine the full extent of the BOW phase in the  $(U, V)$  plane.

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