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

In [1], Jeckelmann argued that the recently discovered bond-order-wave (BOW) phase [2–4] 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 address only 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. Figure 1(a) shows the V dependence of the charge susceptibility $\chi_c(q)$ at the smallest nonzero wave number, $q = 2\pi/N$, for different system sizes N (for the definition of χ_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 [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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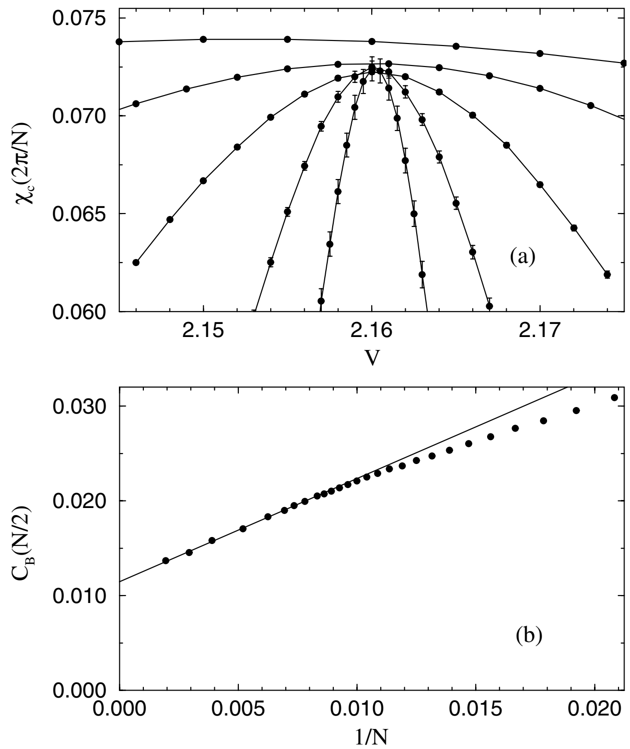

FIG. 1. (a) Charge susceptibility at $q = 2\pi/N$ for $N = 32, 64, 128, 256$, and 512 (curvature increases with N). (b) BOW correlation at distance $r = N/2$ versus inverse system size ($V = 2.10$), along with a linear fit to the large-N data.

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