

Jeckelmann Replies: In their Comment [1], Sandvik, Sengupta, and Campbell present some numerical evidence to support the existence of an extended bond-order-wave (BOW) phase at couplings (U, V) weaker than a tricritical point (U_t, V_t) [2,3] in the ground state phase diagram of the one-dimensional half-filled U - V Hubbard model. They claim that their results do not agree with the phase diagram proposed in my Letter [4], which shows a BOW phase for couplings stronger than the critical point only. However, I argue here that their results are not conclusive and do not refute the phase diagram described in the Letter.

First, while the parameter $U = 4t$ used in the Comment is smaller than the tricritical coupling U_t found in Ref. [3], it is larger than other estimations of U_t (see references in the Letter). Therefore, results for $U = 4t$ only are not sufficient to determine the position of the BOW phase with respect to the tricritical point, which is the most important qualitative difference between the phase diagram in the Letter and those described in Refs. [2,3]. To prove the existence of a BOW phase at couplings weaker than the tricritical point, one should use parameters U smaller than any estimation of U_t .

Second, the finite-size-scaling analysis of the charge susceptibility $\chi_c(q)$ in Fig. 1(a) of the Comment is misleading. A correct analysis is to take the limit $N \rightarrow \infty$ first and then look at the $q \rightarrow 0$ limit. Sandvik, Sengupta, and Campbell take both limits simultaneously ($q = 2\pi/N$), which can lead to incorrect results. For instance, the function $F_N(q) = 1/(qN)$ vanishes if the limit $N \rightarrow \infty$ is taken first, but tends to a constant $1/2\pi$ if both limits are taken simultaneously. Thus, the results shown in the Comment are no proof of a continuous phase transition as a function of V for $U = 4t$.

Third, although I cannot rigorously exclude the existence of an extended BOW region in the phase diagram, my results show that its width would certainly be much smaller than predicted in Ref. [2]. The main features of the BOW phase (as compared to the competing Mott insulator phase) are (i) a long-range-ordered BOW (dimerization) and (ii) a spin gap. I have found a vanishing spin gap in the thermodynamic limit for the example presented in Fig. 1(b) of the Comment. In their previous work [3], Sengupta, Sandvik, and Campbell did not present any conclusive evidence for the opening of a spin gap in an extended region outside the charge-density-wave regime. It is possible that the spin gap is too small to be detected in the finite systems investigated ($N \leq 1024$ sites), but it is as likely that finite-size effects and an arbitrary extrapolation to the infinite system limit

are responsible for the rather small dimerization reported in the Comment. I consider that the existence of the BOW phase is demonstrated only in those cases for which numerical results are consistent. In particular, both the extrapolated spin gap and the extrapolated dimerization should be clearly larger than zero.

Fourth, the discrepancies between the Sandvik, Sengupta, and Campbell results and my results are certainly not a failure of the density matrix renormalization group (DMRG) method nor an effect of open boundary conditions. In the ground state, the staggered bond order of an open finite chain is always larger than in a corresponding periodic system because of the Friedel oscillations induced by the chain edges. For both types of boundary conditions the staggered bond order obtained with DMRG decreases with increasing numerical accuracy (i.e., an increasing number m of density-matrix eigenstates kept). Thus, DMRG results for an open finite system systematically *overestimate* the dimerization of the infinite system. The likely cause of the discrepancies is the difficulty in extrapolating numerical results to the thermodynamic limit in the critical region $U \approx 2V$.

Finally, the most significant finding in my Letter is the presence of the BOW phase at couplings clearly stronger than the tricritical point. This fundamentally contradicts the theory [2] predicting an extended BOW phase only at couplings weaker than (U_t, V_t) . Nevertheless, Sandvik, Sengupta, and Campbell do not dispute this finding nor provide any explanation for this failure of the theory that they claim to confirm in their Comment.

In conclusion, none of the numerical results presented in the Comment refute the conclusions of my Letter. While the phase diagram presented in the Letter is partially based on some hypotheses, it is supported by reliable numerical results and a consistent theory.

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