# Reply to "Comment on 'Accurate ground-state phase diagram of the one-dimensional extended Hubbard model at half filling' "

G. P. Zhang
*Department of Physics, Indiana State University, Terre Haute, Indiana 47809, USA*
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We respond to Jeckelman's Comment on our paper [G. P. Zhang, Phys. Rev. B **68**, 153101 (2003)], which discusses his previous work [E. Jeckelmann, Phys. Rev. Lett. **89**, 236401 (2002)]. We feel that it is important to point out that his previous results show a trend contradicting the weak-coupling limit, a conclusion that is independent of our calculation. Therefore, our comments on his previous results remain valid and our conclusion is unchanged.

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In his Comment,[1] Jeckelmann claims that our results[2] are inaccurate and our criticism of his previous work[3] is groundless, but unfortunately our conclusion is firmly grounded on a well-established fact, independent of our numerical calculation. The fact is that at the weak-coupling limit, $U/V_c$ must approach to 2. Jeckelmann's previous results deviate from 2, and therefore are questionable. Our conclusion is also supported by his own updated results. In the following, we will reply to his specific comments in detail. While his Comment[1] focuses on the discussion of his previous results in his paper,[3] we discuss both his old and updated results.

First, there exists an early density-matrix renormalization group (DMRG) calculation[4] on the phase transition in the extended Hubbard model. As shown in our previous papers,[2,4] since $V_c$ is so close to $U/2$, a $V_c$ vs $U$ plot or its variation is very insensitive to the phase-transition boundary. One sensitive method to accurately characterize the phase transition is to use the ratio $U/V_c$ representation. He plots the $U/V_c$ vs $U$ figure, but the problem in his previous results is still hidden behind other data (see his Figs. 1 and 2). To be clear, in Fig. 1 we show both his previous (circles) and current (boxes) data, which we will come back to below.

The Comment questions our calculation. All the numerical methods have their limitations. We are familiar with such references, including our own paper.[2] The results by Cannon *et al.* were obtained in small clusters.[5] Naturally, the finite-size effect is unavoidable. Hirsch's Monte Carlo (MC) results[6] were obtained at a fixed temperature $\tau$. Cannon *et al.* showed that the MC results depend on $\tau$. Thus, it is necessary to perform $\tau \to 0$ extrapolation in order to get accurate results. Nakamura[7] pointed out that the direct charge-density wave–spin-density wave (CDW-SDW) level crossing point has a large size effect for all regions. Our calculation, not different from all the other DMRG calculations, has several errors of different kinds: truncation error, finite-size effect, $U$-dependent error, numerical truncation error, and many others. That is why we were very careful when we presented our results.[2] Our results were obtained for a system of 40 sites, a truncation of 400 states, without any extrapolation and within the infinite-system algorithm. Our results are different from the above results since our calculations are done for longer chains, have smaller finite-size effects, do not have problems with temperature, and have a better control over state truncations. Therefore, the results tend to be more accurate. In particular, our results are fully consistent with both strong- and weak-coupling limit results. To be more convincing, we also have carefully investigated how the system size and the truncation affect our results (see Fig. 2 of our paper[2]).

Jeckelmann mentioned the infinite-system algorithm is known to give incorrect results for many systems, but this does not necessarily mean the results by the infinite-system algorithm are wrong. Without providing evidence, he asserts the failure of the standard infinite-system DMRG algorithm for the present problem. He goes on to provide one example in Ref. 13 of his Comment to justify his argument, but that paper is about a Bosonic Hubbard model, not about the extended Hubbard model.

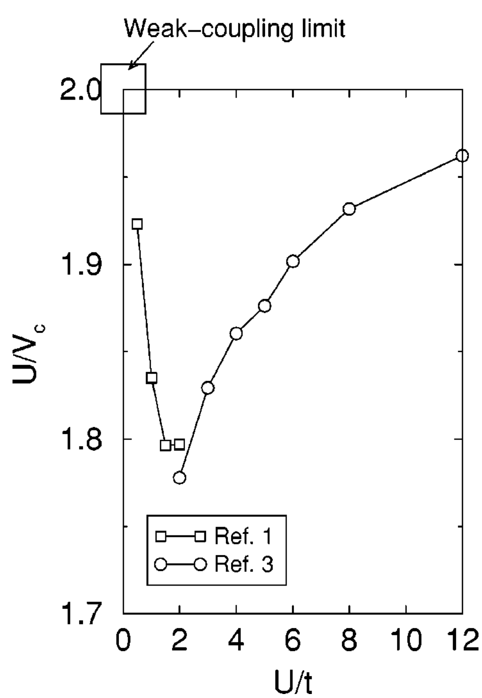


FIG. 1. The critical ratio $U/V_c$ vs $U$ obtained in Ref. 1 (boxes) and Ref. 3 (circles). A strong deviation from the weak-coupling limit is noticed in those circles. The weak-coupling limit is highlighted by a big box at the top left corner.

 

In his Comment, Jeckelmann tries to argue that his previous investigation focused on the intermediate and strong coupling regimes, but nowhere does his previous paper mention this. In addition, since the turning point of the phase transition occurs at about $U=2$, the trend is already clear from the results up to $U=2$, in contrast to his claim. A direct visual inspection of Fig. 1 already reveals that his old data are inconsistent with the weak-coupling limit (see the big box at the top left corner). This demonstrates that the high sensitivity of the ratio representation, which now has been extensively adopted by Jeckelmann's Comment[1] and other different groups,[8] can uncover an erroneous trend among those critical phase-transition points.

In conclusion, we emphasize that none of our comment on his previous paper nor our main conclusion has been changed.

[1] E. Jeckelmann, preceding Comment, Phys. Rev. B **71**, 197101 (2005).
[2] G. P. Zhang, Phys. Rev. B **68**, 153101 (2003).
[3] E. Jeckelmann, Phys. Rev. Lett. **89**, 236401 (2002).
[4] G. P. Zhang, Phys. Rev. B **56**, 9189 (1997).
[5] J. W. Cannon, R. T. Scalettar, and E. Fradkin, Phys. Rev. B **44**, 5995 (1991).
[6] J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984); Phys. Rev. B **31**, 6022 (1985).
[7] M. Nakamura, Phys. Rev. B **61**, 16 377 (2000).
[8] Y. Xie, R. Han, and X. Zhang, Phys. Rev. B **58**, 12 721 (1998); M. Vojta, R. E. Hetzel, and R. M. Noack, *ibid.* **60**, R8417 (1999); I. Baldea, H. Koppel, and L. S. Cederbaum, *ibid.* **63**, 155308 (2001).