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

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It is shown that Guoping Zhang's results [G. P. Zhang, Phys. Rev. B **68**, 153101 (2003)] for the charge-density wave-phase boundary in the half-filled one-dimensional extended Hubbard model are incorrect and that his criticism of my work [E. Jeckelmann, Phys. Rev. Lett. **89**, 236401 (2002)] is groundless.

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In Ref. 1, Guoping Zhang presented density-matrix renormalization group (DMRG) results that contradict my DMRG calculations[2] and Hirsch's quantum Monte Carlo (QMC) simulations[3] for the charge-density-wave (CDW) phase boundary in the one-dimensional extended Hubbard model at half filling. In this Comment I show that Guoping Zhang's results are inaccurate and that his criticism of my work is groundless.

Although the phase diagram of the extended Hubbard model is still partially controversial (see Refs. 2, 4, 5 and references therein), the CDW phase boundary $V_c(U)$ in the parameter space (U,V) was determined years ago[3,6] and has not been disputed in recent studies.[2,4,5,7,8] In Fig. 1, I show the results of various numerical investigations for $V_c(U)-U/2$ in the weak to intermediate coupling regime. There is an excellent overall agreement between Hirsch's QMC simulations,[3] the exact diagonalizations of Cannon *et al.*,[6] Nakamura's level crossing analysis,[7] the stochastic series expansion QMC (SSE-QMC) simulations of Sandvik *et al.*,[4,8] Yuzhong Zhang's DMRG calculations,[5] and my DMRG calculations.[2] In particular, my results agree quantitatively[10] with the most recent and accurate numerical simulations.[4,5,7,8] Only Guoping Zhang's DMRG data[1,9] deviate systematically from the other results. Therefore, there is clearly a problem with his calculations.

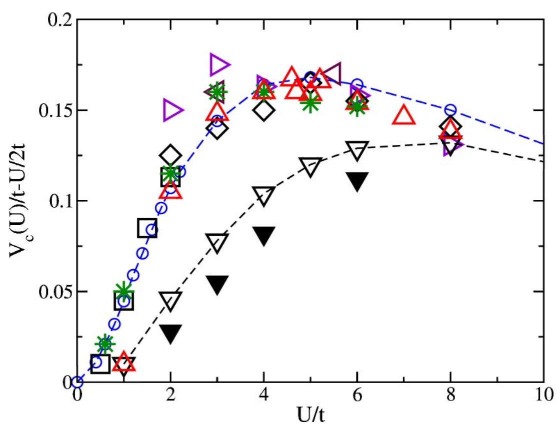

FIG. 1. (Color online) Results for the CDW phase boundary $V_c(U)$: QMC simulations (Ref. 3) (right triangle); exact diagonalizations (Ref. 6) (left triangle); level crossing analysis (Ref. 7) (circle); SSE-QMC simulations (Refs. 8 and 4) (up triangle); author's DMRG calculations [from Ref. 2 (diamond) and new results (square)]; Yuzhong Zhang's DMRG calculations (Ref. 5) (star); and Guoping Zhang's DMRG calculations (infinite-system algorithm) in Ref. 1 (open down triangle) and in a previous work (Ref. 9) (solid triangle). The dashed lines are guides for the eye.

The discrepancy between the various DMRG calculations[1,2,5,9] is not surprising. Guoping Zhang uses the *infinite-system* DMRG algorithm while Yuzhong Zhang and I use the more accurate *finite-system* DMRG algorithm.[11] It is well known[12] that for many problems the infinite-system algorithm yields incorrect results while the finite-system algorithm gives essentially exact (numerical) results. In particular, it is essential to use the more reliable finite-system DMRG algorithm for inhomogeneous systems such as a CDW ground state. Therefore, the discrepancy between Guoping Zhang's results and all other works just demonstrates the failure of the standard infinite-system DMRG algorithm for the present problem. (See Ref. 13 for another example of the infinite-system algorithm failure and Ref. 14 for the successful investigation of the same problem with the finite-system algorithm.)

In his paper, Guoping Zhang wrongly claimed that my DMRG calculations (and the QMC simulations of Ref. 3) failed to reproduce the weak-coupling limit result $V_c(U)=U/2$. In Refs. 2 and 3, the investigation of the phase diagram was focused on the intermediate- and strong-coupling regimes (i.e., $U \geqslant 2t$) and no analysis of the weak-coupling limit $U \ll t$ was performed. Here I present additional results for $V_c(U)$ calculated with DMRG for weaker cou-

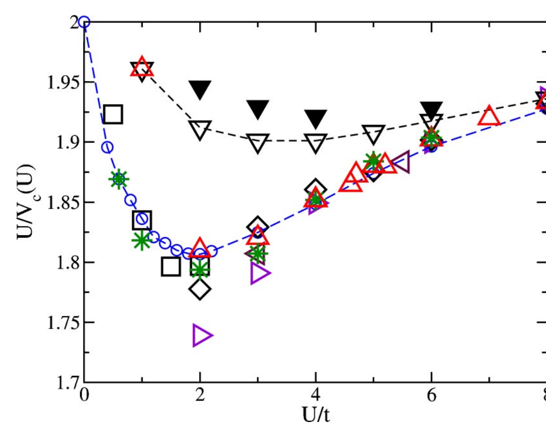

FIG. 2. (Color online) Same results as in Fig. 1 but displayed using Zhang's representation (U/V_c vs U).

plings: $V_c/t=0.260\pm 0.003$ for $U/t=0.5$, $V_c/t=0.545\pm 0.005$ for $U/t=1$, and $V_c/t=0.835\pm 0.005$ for $U=1.5t$. Moreover, I have calculated $V_c(U=2t)/t$ more accurately and found 1.113 ± 0.005 (in agreement within the error bars with the value given in Ref. 2). These results are shown in Fig. 1 as squares. They agree perfectly with other works[4,5,7] and, clearly, they approach the weak-coupling result $V_c(U)=U/2$ in the limit $U\rightarrow 0$. In Figs. 1 and 2 of Ref. 1, Guoping Zhang used a different representation of the data, $U/V_c(U)$ vs U, to analyze the weak-coupling limit. In Fig. 2, I show again all data of Fig. 1 using this representation. Clearly, the minimum of the ratio $U/V_c(U)$ occurs for U slightly smaller than $2t$ and the weak-coupling limit is recovered only for U smaller than $2t$. Therefore, the $U\rightarrow 0$ limit of $U/V_c(U)$ cannot be determined using numerical data for $U\geqslant 2t$ and the Figs. 1 and 2 of Ref. 1 are misleading. The DMRG and QMC data for $U\geqslant 2t$ presented in Refs. 2 and 3 are fully compatible with the weak-coupling limit $V_c(U)=U/2$, contrary to Guoping Zhang's assertion in Ref. 1.

In summary, comparisons with the results available in the literature confirm the accuracy and reliability of the DMRG calculations presented in Ref. 2. Guoping Zhang's results and conclusion are faulty due to the inappropriate use of the infinite-system DMRG algorithm.

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