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

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It has been well established that in both the weak- and strong-coupling limits, the phase transition from a spin-density wave (SDW) to a charge-density wave (CDW) in the half-filled extended-Hubbard model occurs precisely at the ratio $U/V_c=2$, where U and V are the on-site and intersite electron-electron interactions, respectively. However, a recent density-matrix renormalization group (DMRG) study and a previous Monte Carlo simulation jointly suggest a picture that challenges the well-established weak-coupling result. Here, a careful calculation shows such a picture is questionable. In particular, it clarifies the DMRG result, even with a moderate number of states kept in the density matrix, agrees with both the weak- and strong-coupling findings, and predicts a CDW/SDW phase boundary smoothly links those two coupling limits. Possible sources of these previous failures are discussed.

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Low-dimensionality and strong electron correlation introduce many intriguing properties. The phase transition from a spin-density wave (SDW) to a charge-density wave (CDW) in the one-dimensional extended Hubbard model at half filling is just one example. Although it has been investigated for more than two decades,[1] its real phase diagram is still controversial. The weak-coupling,[1] strong-coupling,[2] and Hartree-Fock theories[3] revealed that the SDW-to-CDW phase transition occurs at $U=2V$, but in the intermediate-coupling region, there is a clear deviation from the $U=2V$ line, as first noticed in small clusters.[4] A Monte Carlo (MC) simulation in a longer chain confirms this deviation,[5] but for many years there has been no alternative way to prove it. The advent of the density-matrix renormalization group[6] (DMRG) scheme changes the situation almost completely by allowing one to accurately compute the ground-state properties, in particular in one-dimensional systems. The first DMRG study[7] demonstrated that there is indeed a phase transition from the SDW to CDW, but the phase boundary was found to be much closer to $U=2V$ than that in the MC. In contrast to the DMRG results, the MC simulation failed to reproduce the weak-coupling limit results. Since in the first DMRG study the largest system size used is $N=24$ and the maximum number of states kept in the density matrix is $m=160$, it is very desirable to perform a computation with a larger system size N and higher truncation m.

A recent high-level DMRG calculation,[8] using the largest number of density-matrix eigenstates up to $m=1200$ and the largest system size $N=1024$, predicted a result, in excellent agreement with the MC results. Precisely such an excellent agreement worries us since a failure in the MC simulation at the weak-coupling limit calls the DMRG results into question. What is more troubling is that the same DMRG calculation[8] also contradicts both the very recent weak-coupling theory[9] and the new MC results[10] in predicting the bond-order wave phase. These contradictions cast doubts on the accuracy of the DMRG calculation and undermines the validity of the weak-coupling theory in such an important correlated system.

In order to clarify these apparent contradictions, we perform a sophisticated DMRG calculation by carefully examining the CDW/SDW phase boundary around the transition point. By systematically monitoring the convergence with both system size and the truncation, we show that in contrast to the previous DMRG study,[8] our DMRG results obtained even with a moderate truncation are consistent with both the weak- and strong-coupling limit results. We predict that a CDW/SDW phase border line smoothly connects the weak- and strong-coupling limits. A local minimum appears around $U/t=3-4$, which is missing in the previous MC[5] and DMRG[8] computations. The origin of those failures in the previous DMRG calculation is discussed.

The well-known extended Hubbard model is described by the following Hamiltonian:

$$\hat{H}=-t\sum_{i,\sigma}(\hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{i,\sigma}+\text{H.c.})+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}+V\sum_{i}\hat{n}_{i}\hat{n}_{i+1}, \tag{1}$$

where all the operators have their common meanings.[11–13] U and V are the on-site and intersite electron-electron interactions, respectively. Hereafter U and V are measured in units of t. The periodic boundary condition and half-filling case are considered. The system size N and the density-matrix truncation m will be given below. To determine the phase transition, we compute the correlation functions for CDW and SDW, which are defined as

$$C(\vec{q})=\frac{1}{N}\sum_{i,j}e^{i\vec{q}\cdot(\vec{R}_i-\vec{R}_j)}\langle\hat{n}_i\hat{n}_j\rangle \tag{2}$$

and

$$S(\vec{q})=\frac{1}{N}\sum_{i,j}e^{i\vec{q}\cdot(\vec{R}_i-\vec{R}_j)}\langle\hat{S}^z_i\hat{S}^z_j\rangle, \tag{3}$$

respectively. Here $\hat{n}_i=\Sigma_\sigma\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma}$, and $\hat{S}^z_i\equiv(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})$. $\langle\ \rangle$ denotes the expectation value in the ground state.

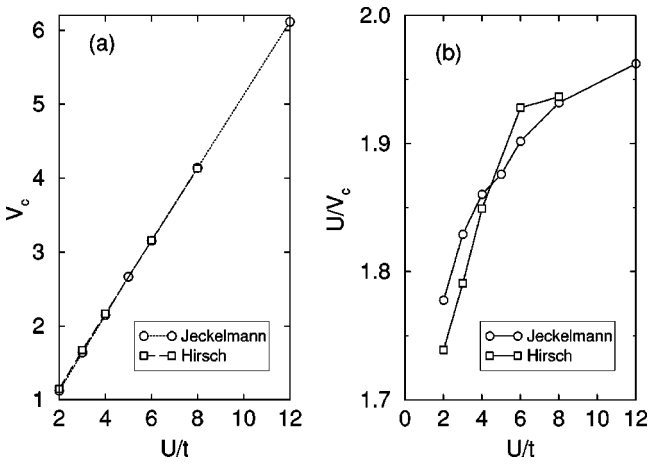

FIG. 1. (a) Phase diagram for the one-dimensional extended Hubbard model at half filling. The circles are from Ref. 8 and the squares are from Ref. 5. (b) The same data but plotted on the ratio U/V_c vs U diagram. The substantial deviation from 2 can be noted in the weak-coupling limit.

In order to have some sense how the phase transition develops, we start with a two-site model system with a periodic boundary condition.[14] At the half filling, there are four basis states: $\phi_1=|\uparrow\downarrow\rangle$, $\phi_2=|\downarrow\uparrow\rangle$, $\phi_3=|\uparrow\downarrow 0\rangle$, $\phi_4=|0\uparrow\downarrow\rangle$. It is easy to show that the ground state is

$$|\text{g.s.}\rangle=\frac{a}{\sqrt{2}}(|\phi_1\rangle-|\phi_2\rangle)+\frac{b}{\sqrt{2}}(|\phi_3\rangle+|\phi_4\rangle), \qquad (4)$$

where

$$a=4t/\sqrt{16t^2+(2V-\epsilon)^2}$$

and

$$b=(\epsilon-2V)/\sqrt{16t^2+(2V-\epsilon)^2}.$$

The eigenvalue $\epsilon=(U+2V-\sqrt{\Delta})/2$, where $\Delta=(U-2V)^2+64t^2$. From Eqs. (2) and (3), we find the correlation functions for CDW and SDW are $C(\pi)=2b^2$ and $S(\pi)=2a^2$, respectively. By equating $C(\pi)$ to $S(\pi)$, we obtain the phase boundary is at $U/V_c=2$. This simple example shows if $V>U/2$, the ground-state phase dominates with the CDW configurations ($|\uparrow\downarrow 0\rangle$ or $|0\uparrow\downarrow\rangle$), otherwise with the SDW configuration ($|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$). It is interesting to note that a sum rule appears $C(\pi)+S(\pi)=2$, but this rule is pertinent to the $N=2$ system only. As pointed out by Fourcade and Spronken a long time ago,[4] the phase boundary at $U=2V$ is specific to the two-site system, where the allowed momenta are only at $\pm\pi/2$ and the kinetic energy term vanishes identically. Consequently, the result does not differ from the atomic limit one ($t=0$) where the transition occurs at $U=2V$.[4]

In a system larger than $N=2$, the transition happens at $V_c>U/2$. Before we present our results, let us first look at the previous MC results by Hirsch[5] and the existing DMRG results by Jeckelmann[8] (adopted from Table I of Ref. 8). Figure 1(a) is a regular V_c versus U diagram and shows an excellent agreement between the MC and DMRG results, both of which predict that the phase transition boundary is slightly deviated from $U=2V_c$. The V_c-U plot is useful to show the phase diagram, but it is insensitive to the important difference between these two results because both data are so close to the $U=2V$ line. For the same sets of data, if we plot the ratio U/V_c versus U, then their differences become immediately clear. Figure 1(b) illustrates that in a large U limit, the DMRG results show a dip at $U=5$ and then approach to 2, while the MC results first show a linear dependence from $U=2$ to 4 and then a kink at $U=6$. The MC results saturate much faster than the DMRG results, but as U becomes larger, the difference between them becomes smaller, which is not surprising since normally the MC simulation works better for a larger U. In the small U limit, although the ratio U/V_c is smaller in the DMRG calculation than that in the MC simulation, both results show a similar trend and suggest a clear departure from the ratio $U/V_c=2$ which is a weak-coupling limit result.

Such a surprising departure is unexpected. In order to resolve this issue, we perform a careful DMRG calculation, and whenever possible we purposely avoid an extrapolation of our results since the extrapolation itself may introduce some uncertainty[4] and most importantly it makes a direct comparison almost impossible. Our DMRG computation starts with a careful sweep of V around the transition point with a very fine step. Depending on U, the steps used for V is normally between 0.01 to 0.005 in order to accurately determine the critical value V_c. Our smallest step is 0.001. Note that this small step does not mean that the smallest possible error for V_c is 0.001, but instead it means that for a fixed N, U, and m, the accuracy is within the 0.001 limit. With such a tiny step, the computational load is very heavy. The number of states kept in the density matrix is $m=400$ and the infinite system scheme is used. We locate the transition point by checking the correlation functions for SDW and CDW. In Fig. 2(a), we present two sets of data for $N=36$ (solid squares) and 40 (solid circles), together with those results by Hirsch[5] and Jeckelmann.[8] The result at $U=0$ is a weak-coupling result, not computed by the DMRG method. Our results show that as U decreases to zero or increases to the infinity, the ratio U/V_c asymptotically approaches 2, which fully agree with the weak- and strong-coupling limit theories. If we look at the trend more closely, we find that the ratio U/V_c reaches 2 much faster in the weak-coupling limit than that in the strong-coupling limit. A local minimum in the phase boundary line appears around $U=3$ and 4. This local minimum is expected since in both the weak- and strong-coupling limits U/V_c is equal to 2, one must have a borderline separating the CDW phase from SDW phase but linking these two extremes.[15]

We fit the boundary line to

$$U/V_c=2+\frac{a_0U}{a_1U^{a_3}+a_2}, \qquad (5)$$

where $a_0=-0.373$, $a_1=0.217$, $a_2=7.678$, and $a_3=2.512$. This function correctly shows that the ratio asymptotically approaches 2 as $U\to 0$ or $U\to\infty$. For a small U, (U/V_c-2) depends on U linearly, but for a larger U, (U/V_c-2)

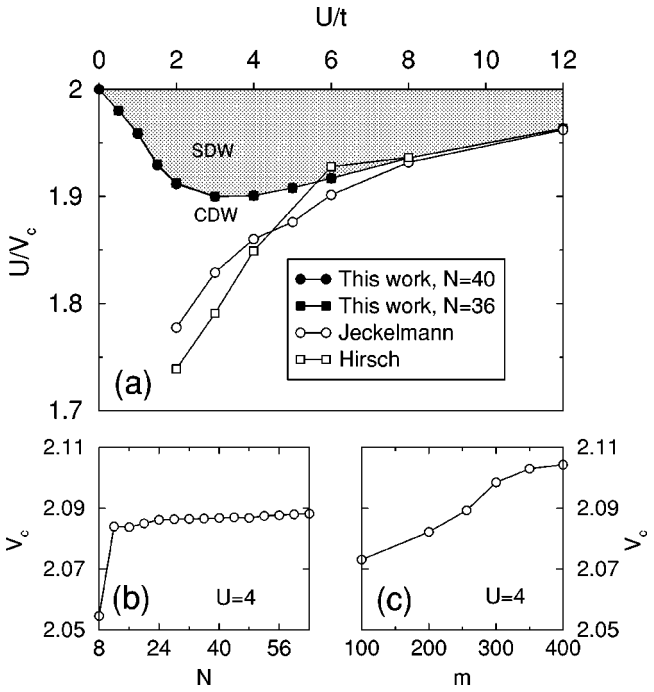

FIG. 2. (a) Comparison of the phase diagrams for the one-dimensional half-filled extended-Hubbard model. The DMRG data from this work are represented by the solid circles ($N=40$) and boxes ($N=36$) with $m=400$. No extrapolation has been made. The empty circles denote the DMRG results from Ref. 8 and the empty boxes represent the MC results from Ref. 5. (b) Dependence of V_c on the system size N with $m=256$. (c) Dependence of V_c on the number of states m kept in the density matrix for $N=40$.

$\approx a_0/a_1 U^{-3/2}$, which can be directly compared with the results by the g-ology and the strong-coupling theory.[15] We also check the finite-size effect of this borderline as a function of the system size. By comparing the results for two different system sizes, namely $N=36$ (solid boxes) and 40 (solid circles), we find that the overall finite-size effect is very small [see Fig. 2(a)] where the solid circles almost completely overlap the solid squares. The explicit size dependence of V_c for $U=4$ is shown in Fig. 2(b) where we keep 256 states in the density matrix. One notices that V_c quickly saturates after $N=24$. In addition, we find that the finite-size effect also depends on U: the effect is much smaller in the weak- and strong-coupling limits than that in the intermediate-coupling region.[15] We will come back to this point below.

If we compare our results [the filled boxes and circles in Fig. 2(a)] with the previous results [the empty circles and empty boxes in Fig. 2(a)], we find that in the strong-coupling limit our results agree with the previous DMRG results and in some sense the MC results, but there is a big difference in the intermediate and small U regions. Firstly, neither the previous MC[5] nor DMRG[8] calculations predict a local minimum. Secondly, these calculations predict a monotonic decrease of the ratio U/V_c with U, which directly contradicts the trend predicted by the weak-coupling theory.[1,9] To have a quantitative view, in Table I we list our results with system size $N=40$ and $m=400$ in the second column while the third, fourth, and fifth columns are the previous DMRG,[8] previous,[5] and recent[10] MC results, respectively. The last column shows the ratio U/V_c for the weak- and strong-coupling limits. One notices that the difference between our data and those previous results becomes larger for the intermediate and small U. Jeckelmann[8] claimed that his DMRG results agreed quantitatively with the recent quantum Monte Carlo simulations,[10] but we checked Ref. 10 and found that Ref. 10 only has a few points such as: one at $U=4$ and the other at $U=8$, while Ref. 8 has more than 7 points. It is entirely unclear to us how such a comparison could be done and how the quantitative agreement could be reached. We also noticed a similar problem in Ref. 8 about the bond-ordered wave phase.[16] Interestingly, we find that the DMRG results in Ref. 8 are in fact consistent with the previous MC results by Hirsch[5] (compare columns 3 and 4 in Table I).

Since the previous DMRG calculation[8] does not explicitly give information about the system size and the truncation m for all the results, it is not possible to make a quantitative comparison with his results on the equal footing. We decide

TABLE I. The second column shows our DMRG results computed at $m=400$ and $N=40$. The numbers in the parentheses are estimated. Note that no attempt has been made to extrapolate the results to the infinite-size and truncation limits (for the reason, see the text). The third column is the previous DMRG results (Ref. 8) while the previous (Ref. 5) and recent (Ref. 10) Monte Carlo results are in the fourth and fifth columns, respectively. The last column shows the weak- and strong-coupling limiting results.

U	V_c (this work)	V_c(Ref. 8)	V_c(Ref. 5)	V_c (Ref. 10)	U/V_c (limiting cases)
0					2
1	0.510(5)				
2	1.046(2)	1.125	1.15		
3	1.578(9)	1.640	1.675		
4	2.104(3)	2.150	2.163	2.16	
5	2.620(6)	2.665			
6	3.129(7)	3.155	3.158		
8	4.132(6)	4.141	4.131	4.14	
12	6.111(1)	6.115			
∞					2

to discuss several possible sources of errors. All the DMRG results have two related errors: (a) the finite-size effect and (b) the truncation error. For instance, for the same number of states kept in the density matrix, elongating the chain reduces the finite-size effect but increases the truncation error. This means that a large system size and a large truncation do not necessarily produce an accurate result. Our experience shows that it is always better to check the finite-size effect first at a moderate truncation m. After the convergence with system size is reached, one then converges the results with the truncation.

Another possible error comes from the fact that the convergence with m and N is U dependent. We find that it is better to use a most difficult U to check the convergence with N and m. In Fig. 2(c), we show such an example, where the system size is $N=40$ and $U=4$. One notices that due to the periodic boundary condition, the convergence of V_c with m is extremely slow.[17] From $m=100$ to 200, there is no indication of convergence. Only after $m=300$, then V_c begins to level off. The results converge smoothly when we increase m to 400. Notice that it is difficult to extrapolate those lower m results to higher m ones, which is why we avoid an extrapolation. Our detailed analyses and expensive calculations finally establish that the DMRG results are reliable and are fully consistent with both strong- and weak-coupling theories.

In conclusion, our careful study finally settles down the controversial issue raised by the recent DMRG and previous MC investigations. We clarify there is no discrepancy between the DMRG results and the weak-coupling theory, and predict that a CDW/SDW phase boundary smoothly connects the weak- and strong-coupling limits. Possible sources of previous failures are discussed. Our results may pave the way to accurately investigate other phase transitions which currently are under an intensive debate.[18]

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