# Ground-state phase diagram of the one-dimensional extended Hubbard model: A density-matrix renormalization-group approach

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We use the density-matrix renormalization group to calculate the phase diagram of the one-dimensional extended Hubbard chain at half filling. We find that for one specific $U$, the critical value of $V_c$ for the charge-density-wave versus spin-density-wave phase transition is smaller than that predicted from the Monte Carlo simulation. Our results are consistent with the strong- and weak-coupling limit results, whereas the previous results from the Monte Carlo simulations deviate from the weak-coupling limit result. As $U$ increases, we find that the first-order phase transition develops gradually. The tricritical point is estimated to occur at $U_c=4-6$, not $U_c=3$ as previously predicted from the Monte Carlo simulation. Due to the topological difference, we observe that with the periodic boundary condition, the phase transition is more abrupt for finite chains of length $N=4M$ than for chains of $N=4M+2$, where $M$ is an integer, for the same $U$ and $V$. The difference will diminish in the thermodynamic limit. [S0163-1829(97)08839-5]

Ground-state properties of the extended Hubbard model at half filling have been extensively studied. Both the weak-[1,2] and strong-coupling approximations[3] revealed that charge-density wave (CDW) to spin-density wave (SDW) phase transition occurs at $U=2V$ for all values of $U$. However, the exact results from small clusters show that the phase boundary is slightly deviated from the line $U=2V$, especially for larger $U$.[4] Monte Carlo (MC) calculation confirms this deviation.[5] In addition, the transition is found to be continuous for small $U$ and discontinuous for large $U$, with a crossover around $U\sim 3$. Cannon, Scalettar, and Fradkin[4] confirmed the presence of a tricritical point. But the tricritical point is found above $U_c=3.5$ and possibly as high as $U_c=5.0$, which is larger than the MC estimation. They also found that the tricritical point greatly depends on the $\Delta\tau$ and inverse temperature ($\beta$) of the MC simulation. Even for $\Delta\tau$ as low as 0.125, the indicated position of the tricritical point increases as $\Delta\tau$ decreases and lattice size increases at constant $\beta$. We noticed that $\Delta\tau=0.25$ was used in Ref. 5. Thus one should be careful in accepting their results. Up to now, there is no alternative scheme to evaluate the MC results. Especially around the phase transition, the transition point is very sensitive to numerical errors. Furthermore as the MC simulation becomes an important tool to many-body systems, one should have a clear idea about its performance.

In this paper, we employ a density-matrix renormalization-group (DMRG) approach to calculate the CDW-SDW phase transition.[6] DMRG is well suited for a one-dimensional system and its accuracy renders its wide application. Previous applications involve the Hubbard chain and Heisenberg model. It is expected that the DMRG calculation should give some definite results for the CDW-SDW transition. As far as we know, this is the first application of DMRG to the CDW-SDW transition. We find many interesting features and rectify several previous ambiguous or wrong results. (1) We have confirmed that the CDW-SDW transition occurs around $U=2V$. The deviation from $U=2V$ is found to be smaller than that from MC calculation. The MC calculation overestimated the deviation and predicted a wrong tendency for the weak-coupling limit. (2) With the periodic boundary condition and at the same $U$ and $V$, the phase transition is more abrupt for chains of length $N=4M$ than that for chains of $N=4M+2$. But the situation is just the reverse if one uses the antiperiodic boundary condition. It is expected that this difference will vanish in the thermodynamical limit. (3) The first-order phase transition develops gradually. The tricritical point $U_c$ is estimated to be around 4–6.

Our model Hamiltonian is

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

where all the operators have their common meanings. Hereafter we note that $U$ and $V$ are in units of $t$. The periodic boundary condition and the half-filling case are considered. We use the infinite-system DMRG algorithm and truncate the space by keeping $m=160$ states in each block. Although the periodic boundary condition is a less favorable case for DMRG, the discarded density matrix weight is typically below $10^{-8}$. We constantly choose a larger $m$ to check our results. Our numerical tests show that there is no significant change of our results even if we keep more states in each block.

After truncation, we found that the Hamiltonian matrix becomes dense, which becomes even denser with $V\neq 0$ and the periodic boundary condition. This strongly appeals for a powerful diagonalization algorithm while the convergence of the traditional Lanczos[7] and Davidson algorithms is very poor. We recently have developed a very efficient method to calculate eigenvalues and eigenvectors. The detailed algorithm will be reported elsewhere,[8] but the main idea is to find an optimized Lanczos chain length and collect all previous useful information along the chain just as one does in the

 

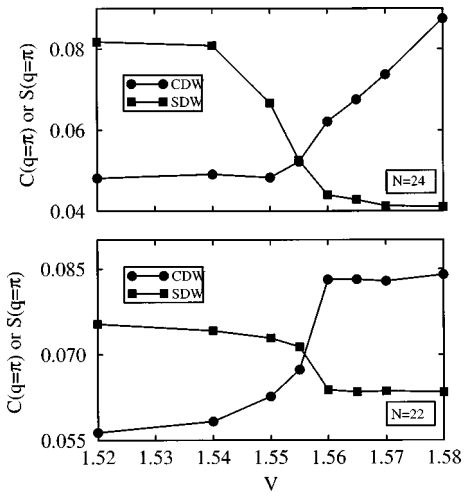


FIG. 1. At $U=3$ CDW and SDW structure factors vs $V$ for different chain lengths. Passing over the transition regime, the structure factors change more abrupt for the chain of $N=24$.

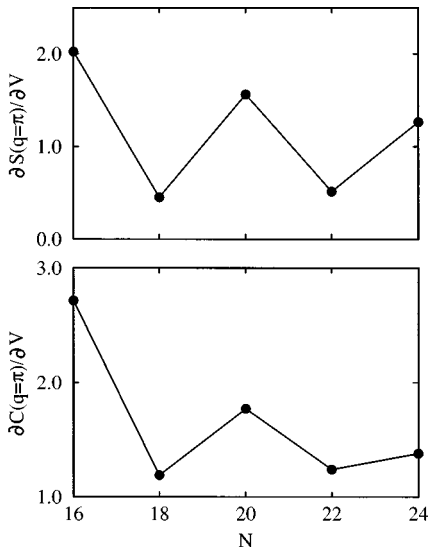


FIG. 2. The derivatives of the SDW and CDW structure factors with respect to $V$ at $V_c$ and $U=3$ are staggering for chains of lengths $N=4M$ and $4M+2$.

conjugate gradient algorithm. This new algorithm accelerates the convergent rate, as we found, at least six times compared to traditional algorithms. The improvement becomes more significant for hardly converged states.

To determine the transition point, we first study the behavior of correlation functions for CDW and SDW. The CDW structure factor is defined as

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

where $\hat{n}_i=\Sigma_\sigma \hat{c}^\dagger_{i,\sigma}\hat{c}_{i,\sigma}$. The SDW structure factor is defined as

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

where $S^z_i\equiv(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})$ and $\langle\ \rangle$ denotes the expectation value in the ground state.

In order to obtain a critical value $V_c$ at a fixed $U$ for the CDW-SDW transition precisely, we choose steps for $V$ as small as 0.01 or even 0.005 while Hirsch chose the step 0.1. Such small steps help us to visualize the details around the transition point, but the total cpu time needed is expensive. It is worth noting that due to this tiny step, it is not easy to observe the sharp transition even for a discontinuous transition. Surely on a broader region, one must see such discontinuity more clearly.

For the finite chains, there is a topological difference between chains with lengths $N=4M$ and $4M+2$. Previously Kivelson *et al.*[9] have found that this difference leads to an absolute instability of $4M$ rings with respect to dimerization, while rings with $4M+2$ members will only dimerize if $\alpha^2/Kt_0$ exceeds an $N$-dependent critical value. The difference between $N=4M$ and $4M+2$ vanishes as $N\to\infty$. We found that actually this very difference also results in a different phase transition behavior. For the periodic boundary condition, the CDW-SDW phase transition appears more abrupt for chains of $N=4M$ than that for chains of $N=4M+2$ (see Fig. 1). This conclusion holds true for both periodic and antiperiodic boundary conditions. But for the antiperiodic boundary condition, the conclusion is just the reverse. To illustrate this, in Fig. 1 we plot the correlation functions at $q=\pi$ for $N=22$ and $N=24$ size systems with $U=3$ and periodic boundary condition. Away from the transition point the main features of the phase diagrams for these two chains are roughly similar, but around the transition point, compared with the chain with length $N=22$, the phase transition is more abrupt for the chain of length $N=24$.

To have a clear vision of the above difference, we calculate the derivatives $C'=\partial C(q=\pi)/\partial V|_{V=V_c}$, and $S'=\partial S(q=\pi)/\partial V|_{V=V_c}$ at the transition point $V_c$. In Fig. 2, we show these derivatives for $U=3$ as the function of the chain length. A staggering behavior for both $S'$ and $C'$ is observed. For chains of length $N=4M$, the corresponding derivatives are smaller than that for chains of $N=4M+2$, for example, for $N=16$, $S'=2.0$ and $N=18$, $S'=0.45$, which reflects that the phase transition is more abrupt for chains of $N=4M$. This difference is more obvious from $\partial S(q=\pi)/\partial V|_{V=V_c}$. We also use antiperiodic boundary condition to check the results. Now the phase change for chains with length $4M+2$ becomes more sharp. Exact diagonalization for $N=6$ system shows that a typical SDW configuration dominates up to the transition point, and after the transition point CDW configuration appears almost suddenly. For chains with $N=4$ or 8, the CDW configuration gradually competes with the SDW configuration as $V$ approaches the transition point. In order to explain this, Meinders *et al.*[10] discussed that near the phase transition, states that have a three-site unit cell, such as, for instance, the state $|0\underline{\uparrow\uparrow\downarrow}0\underline{\uparrow\uparrow\downarrow}\rangle$, become important. These states are frustrated in four and eight sites while for six sites they are not frustrated. But we think that this difference is a finite-size effect. In the thermodynamic limit, this difference will vanish as one may see that, in Figs. 2(a) and 2(b), the difference of the derivatives between chains with lengths $4M$ and $4M+2$ becomes smaller as the chain length increases. For example, the difference of $S'$ between chains $N=18$ and 20 is 1.1, while the difference between $N=22$ and 24 is 0.7. A finite-

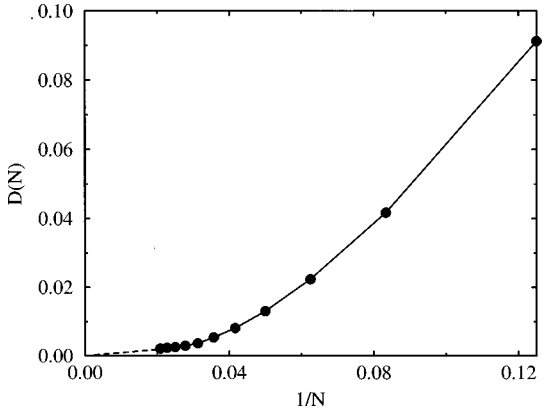


FIG. 3. The difference $D(N)$ between $S(N)$ and $S(N+2)(N=4M)$ diminishes as the chain length increases. Here $U=4$ and $V=2$.

size scaling analysis shows that the difference vanishes as $N\rightarrow\infty$ (see Fig. 3). In Fig. 3, we show $D(N)=|S(q=\pi,N)-S(q=\pi,N+2)|$ as the function of $1/N$ $(N=4M)$ for $U=4$ and $V=2$. A polynomial fit reveals that $D(N)$ scales like $4.7N^{-1.84}-0.04N^{-0.71}$.

The tiny step for $V$ enables us to determine the transition point precisely and we obtained the critical values $V_c$ of the infinite chain limit by extrapolation. We estimate that the critical value $V_c$ for $U=3$ is 1.555. This value is smaller than the MC prediction. The MC result is $V_c^{\mathrm{MC}}=1.675$. Hereafter $V_c^{\mathrm{MC}}$ refers to the critical value from the Monte Carlo simulation. Actually we find that the MC results are always larger than our DMRG results. For $U=2$, our result is $V_c=1.028$, while the MC simulation predicted $V_c^{\mathrm{MC}}=1.15$; $U=4$, $V_c=2.082$ $(V_c^{\mathrm{MC}}=2.163)$; $U=6$, $V_c=3.112$ $(V_c^{\mathrm{MC}}=3.158)$. It is known that both weak- and strong-coupling theories predict the CDW-SDW transition to occur at $U=2V$, i.e., $U/V=2$. It should be pointed out that Hirsch's results are only consistent with the strong-coupling limit, not the weak-coupling one.

In Fig. 4, both our results and Hirsch's data are shown.

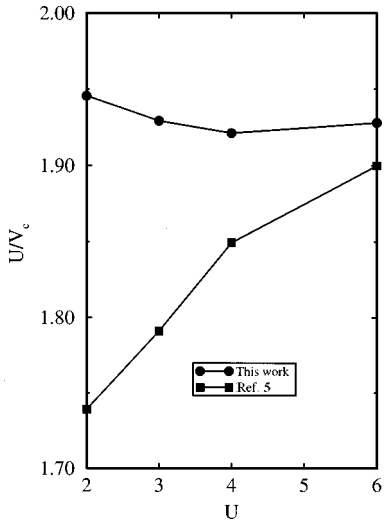


FIG. 4. Our data (dots) have a correct asymptotic behavior as they approach 2 in both weak- and strong-coupling limits, but the MC results (boxes) failed to reproduce the weak-coupling tendency.

Our data are well consistent with both the weak- and strong-coupling theoretical predictions, namely, at both large and small $U$ limits, $U/V_c$ approaches 2. But for large $U$, the convergence to 2 with $U$ is much slower than that for small $U$. A minimum point appears around $U=4$, which we ascribe to a typical intermediate strength regime. The MC results predict a roughly correct tendency for large $U$, but the asymptotic behavior of $U/V_c$ to 2 is faster than our results. For small $U$, a great deviation of $U/V_c$ from 2 is noted. We suspect that such a strong deviation may become even worse in higher-dimensional systems. It is suggested that one should be careful in accepting some MC results.

One of the main reasons for the above difference between our results and the MC data is largely due to the fact that MC simulation results are hardly converged to the low temperature (small $\Delta\tau$) limit. In Ref. 5, Hirsch did not provide an extrapolation study by choosing different $\Delta\tau$, thus one has no idea about how good his approach is. But from Ref. 4, one may notice that the tricritical point, which will be discussed in the next paragraph, is really dependent on $\Delta\tau$. Thus it is believable that this is one of the major reasons for the big error above. To evaluate our results, we have carefully checked our scheme by keeping more states in the superblocks. But no significant qualitative difference has been observed.

As mentioned in the Introduction, the MC results revealed that the tricritical transition appears at $U_c=3$. But the exact Lanczos results for small clusters suggested a larger $U_c$. Before we go further, we should go back to the definitions of the first- and second-order phase transitions. Theoretically the first-order transition requires that the first derivative of physical quantity with respect to its variable is divergent while the second-order transition means a finite value of the first derivative. Thus it is expected that for the first-order transition, $C'=\partial C(q)/\partial V|_{V=V_c}\rightarrow\infty$, or $S'=\partial S(q)/\partial V|_{V=V_c}\rightarrow\infty$. Numerically, however, one mostly observes a large number instead of a real divergence. The reason is that (a) numerically one cannot change $V$ by an infinitely small number, and (b) the difference between two $C(q)$'s or $S(q)$'s is always finite. Eventually the derivatives are finite. Thus one has difficulty with the above definition. In order to circumvent this difficulty, we try a moderate definition. For two different $U_1$ and $U_2$, one can get two derivatives, $S_1'$ and $S_2'$ or $C_1'$ and $C_2'$. If the ratio between $S_2'$ and $S_1'$ or between $C_2'$ and $C_1'$ exceeds an amount, for instance, 4, the first-order phase transition is defined for that with the larger derivative.

In Fig. 5, we plot the derivatives $\partial S(q=\pi)/\partial V|_{V=V_c}$ for different $U$ and different chain lengths. For $U=2$, a staggering behavior versus $N$ is observed, which reflects again the difference between chains of lengths $N=4M$ and $N=4M+2$. But for chains of $N=4M$, as chain length increases, the amplitude decreases, while for chains of $N=4M+2$ it slightly increases. In the infinite chain limit both amplitudes should settle down to a finite value. It is estimated that for $U=2$ in the infinite length limit, $\partial S(q=\pi)/\partial V|_{V=V_c}$ is less than 1.0. Such a small value indicates that for $U=2$, the CDW-SDW phase transition is of second order. For $U=3$, if the MC results are reliable, we are in the first-order transition regime. Comparing the derivative of the structure factor for

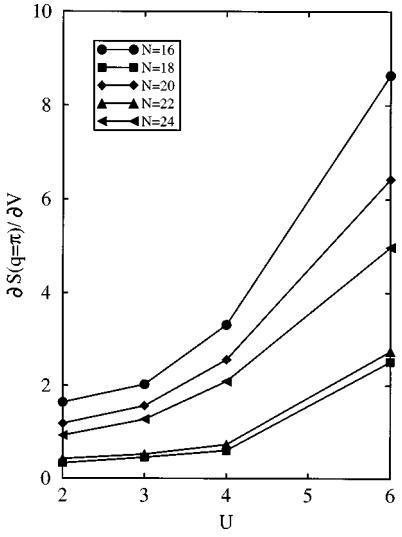


FIG. 5. The derivative of $S(q=\pi)$ vs $U$ changes smoothly, but a rapid increase comes after $U=4$, which may indicate that the first-order transition develops.

$U=3$ with that for $U=2$, one cannot see an obvious difference between them, although a slightly large derivative is observed for $U=3$, which reveals that the phase transition is still second order.

After $U=4$, the derivative increases sharply, which may signify that the first-order transition is established. One may notice for shorter chains and the $N=4M$ system that the increase is more significant; i.e., the phase transition is more likely to be in a first-order transition regime. This is consistent with the conclusion of Ref. 4. They discovered that as lattice size increases, the tricritical point increases and would approach an asymptotic value. Since the largest size they used is 12 sites, it is not possible for them to determine this from their data. But here we are able to address this problem more clearly. Since finite chains with lengths $N=4M$ and $4M+2$ have different asymptotic behaviors, the asymptotic value of $\partial S(q=\pi)/\partial V|_{V=V_c}$ for each $U$ at the infinite chain length limit should lie in the area that is bounded by their corresponding derivatives for finite chains of $N=4M$ and $4M+2$. Based on this, we estimate that at $U=6$ and in the infinite chain limit, the derivative $\partial S(q=\pi)/\partial V|_{V=V_c}$ is about 4 times larger than that of $U=2$, which may suggest that the phase transition at $U=6$ is already in the first-order regime. From Fig. 5, one may notice that the first-order phase transition develops continuously, and there is no such clear cut as one may expect initially; thus it is very difficult to determine $U_c$ precisely. We suggest that $U_c$ lie in the range, 4–6, but never below 3. Our results support Cannon *et al.*'s earlier speculation.[4]

In conclusion, we exploit a density-matrix renormalization-group approach to study the phase diagram of the one-dimensional extended Hubbard model. It is found that the critical values $V_c$ are smaller than the previous MC results. For $U=2$, the critical value $V_c$ is 1.028; $V_c=1.555$, 2.082, 3.112 for $U=3,4,6$, respectively. Our data have a correct asymptotic behavior that coincides with both the weak- and strong-coupling predictions, while the MC results are not consistent with the results of the weak-coupling limit. The tricritical point $U_c$ is estimated to lie between 4 and 6, but never as small as 3.

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[1] V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. Devreese, R. Evrand, and V. van Doren (Plenum, New York, 1979).
[2] D. Cabib and E. Callen, Phys. Rev. B **12**, 5249 (1971).
[3] R. A. Bari, Phys. Rev. B **3**, 2662 (1971).
[4] J. W. Cannon, R. T. Scalettar, and E. Fradkin, Phys. Rev. B **44**, 5995 (1991).
[5] J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984); also see J. E. Hirsch, Phys. Rev. B **31**, 6022 (1985).
[6] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[7] C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255 (1950).
[8] G. P. Zhang (unpublished).
[9] S. Kivelson, Ting-Kuo Lee, Y. R. Lin-Liu, Ingo Peschel, and Lu Yu, Phys. Rev. B **25**, 4173 (1982).
[10] M. B. J. Meinders, J. Brink, J. Lorenzana, and G. A. Sawatzky, Phys. Rev. B **52**, 2484 (1995).