Dimerization in a Half-Filled One-Dimensional Extended Hubbard Model

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We use a density-matrix renormalization group method to study quantitatively the phase diagram of a one-dimensional extended Hubbard model at half filling by investigating the correlation functions and structure factors. We confirmed the existence of a novel narrow region with long-range bond-order-wave order that was highly controversial recently between the charge-density-wave phase and Mott insulator phase. We determined accurately the position of the bicritical point $U_b \simeq 7.2t$, $V_b \simeq 3.746t$, which is quite different from previous studies.

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Much effort has been devoted to understanding the effects of strong electronic correlations on quasi-one-dimensional systems. These materials including conjugated polymers, Cu oxides, and Ni halides exhibit rich phase diagrams and display huge ultrafast optical nonlinearity which point to promising optoelectronic applications [1–4]. The one-dimensional (1D) extended Hubbard model (EHM) with the nearest-neighbor repulsion V in addition to the on-site repulsion U is a standard minimal model that can describe these rich physical properties. Although this model has been investigated for more than two decades [5], its ground-state phase diagram is still controversial [6–16]. In the limit $V = 0$ [17], the ground state is in the Mott insulating state where the spin sector shows quasi-long-range order of a spin density wave. With use of weak-coupling renormalization group analysis [5], a continuous phase transition is obtained at $U = 2V$ from charge-density-wave (CDW) to spin-density-wave (SDW) phases. Strong-coupling calculations using second-order perturbation theory [5] gave a first-order phase transition also at $U = 2V$. This means that there exists a crossover between these two phase transitions at a bicritical point in the intermediate-coupling regime. This picture was supported by both numerical [6,7,10] and analytical [7–9] studies and had been regarded for a long time as the complete phase diagram of the 1D EHM at half filling. However, the precise location of the bicritical point where the nature of the transition changes has been a subject of many investigations and remains uncertain [6–16].

Recently, by using level crossings in the excitation spectra obtained by exact diagonalization, Nakamura [11] pointed out that a novel spontaneously dimerized phase which is also called the bond-order-wave (BOW) phase exists for small to intermediate values of U and V in a narrow strip between CDW and SDW phases. This remarkable proposal was confirmed by stochastic series-expansion Monte Carlo calculations [13,15] and reformulated weak-coupling field theory [12] where higher-order terms were included but was questioned by a high-level density-matrix renormalization group (DMRG) investigation [14] that shows the existence of a BOW phase only on a segment of a first-order SDW-CDW phase boundary. On the other hand, Zhang [16] cast doubts on the accuracy of the DMRG calculation and predict that an SDW-CDW phase boundary smoothly connects the weak- and strong-coupling limits.

In order to clarify these apparent contradictions, we perform an extensive numerical study of 1D EHM at half filling in the vicinity of $U = 2V$ using the DMRG [18] technique. In contrast to the previous DMRG studies [10,14,16], we mainly calculate the BOW correlation functions and structure factors that are the most direct evidence for the long-range BOW phase. Carefully using various finite-size scaling skills for different physical quantities defined below, we confirm that the recently discovered BOW phase [11] of the 1D EHM does have a finite extent in the (U, V) plane, but its width is much smaller, as has been predicted by the Monte Carlo method [13]. The position of the bicritical point where the BOW phase vanishes is determined accurately. The value is much higher than any previous results [6–8,10,12–14], while surprisingly it is consistent with the point given in Ref. [14] where Jeckelmann argued that the BOW phase exists up to an upper limit which is smaller than $8t$. However, the point is not identical to the bicritical point. This can be understood as the result of increasing frustration in the spin degrees of freedom [9,14]. Furthermore, we find that the first-order phase transition takes place for $U \lesssim 2V$ rather than $U \gtrsim 2V$ obtained from reformulated weak-coupling field theory [12]. Using the same methods described below for U up to $16t$ with the interval of $\Delta U = 0.2t$, we quantitatively determine the phase diagram of the 1D EHM at half filling for the first time.

The Hamiltonian of the 1D EHM is defined as follows

$$H = -t\sum_l B_{l,l+1} + U\sum_l n_{l\uparrow}n_{l\downarrow} + V\sum_l n_l n_{l+1}, \qquad (1)$$

where $n_{l\sigma} \equiv c^+_{l,\sigma}c_{l,\sigma} - \frac{1}{2}$, $n_l \equiv n_{l\uparrow} + n_{l\downarrow}$, $c^+_{l,\sigma}$ denotes the creation operator of an electron at the lth site with spin σ, and the bond-charge density operator $B_{l,l+1}$ is

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$$B_{l,l+1} \equiv \sum_{\sigma} (c^{+}_{l,\sigma} c_{l+1,\sigma} + c^{+}_{l+1,\sigma} c_{l,\sigma}). \quad (2)$$

As is well known, DMRG is a very accurate numerical method for the ground-state properties of a 1D quantum system with short-range interactions [18]. Here we applied the finite-size DMRG algorithm with open boundary conditions to study the Hamiltonian (1) at half filling. This method allows us to probe directly correlation functions and structure factors associated with SDW, CDW, and BOW in the ground state. Lattices up to 512 sites were used in our studies. The largest number of states kept in the calculation was $m = 512$ per block. The hopping integral t is set to 1 as the energy unit. The weight of the discarded states was typically about 10^{-7}–10^{-14} depending on whether the system is in its critical state or not in the final sweep. The convergence tests as functions of number of states kept and system size were carefully performed. We checked our DMRG calculations against exact numerical results for noninteracting ($U = V = 0$) chains (up to 512 sites) and results from exact diagonalization for interacting ($U \neq 0$, $V \neq 0$) chains (up to 14 sites). Excellent agreement was found in both cases. Furthermore, for a given chain length, we extrapolate our DMRG results to the limit of vanishing discarded weight. When interactions are turned on, there exist finite excitation gaps on finite chains, so the accuracies of all quantities we calculated are not worse than those of the noninteracting case. Thus, numerical errors in our work could be safely estimated to be smaller than 10^{-4}.

First, we will introduce a method that can be simply used to determine the phase boundaries of the BOW phase directly. The BOW structure factor is given by

$$S_{\mathrm{BOW}}(q) = \frac{1}{L} \sum_{lr} e^{iqr} (\langle B_{l,l+1} B_{l+r,l+r+1} \rangle - \langle B_{l,l+1} \rangle \langle B_{l+r,l+r+1} \rangle). \quad (3)$$

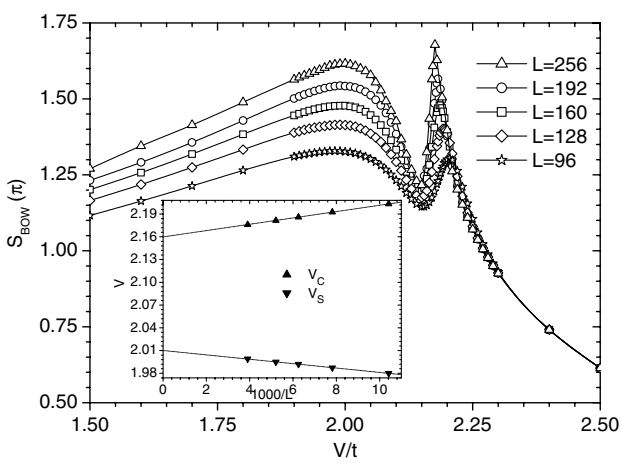

FIG. 1. Behavior of $S_{\mathrm{BOW}}(\pi)$ across the phase boundary for $U/t = 4.0$. The inset shows a linear extrapolation of the critical values V_c and V_s with the inverse of chain length $1/L$.

As pointed out by Nakamura [11], phase transitions on the CDW-BOW and BOW-MI phase boundary are of Gaussian type and Kosterlitz-Thouless (KT) type, respectively; the real space staggered bond fluctuation correlation function falls off algebraically as

$$(-1)^r (\langle B_{l,l+1} B_{l+r,l+r+1} \rangle - \langle B_{l,l+1} \rangle \langle B_{l+r,l+r+1} \rangle) \sim r^{-\eta}. \quad (4)$$

Away from phase boundaries, this quantity falls off exponentially. Thus, for a finite-size system, the $S_{\mathrm{BOW}}(\pi)$ is expected to reach a maximum at the critical points. Figure 1 shows the results of the $S_{\mathrm{BOW}}(\pi)$ for different system sizes with $U/t = 4.0$ and $1.5 \leq V/t \leq 2.5$. As expected, the $S_{\mathrm{BOW}}(\pi)$ peaks twice for all the different system sizes we calculated, clearly indicating that there exist two phase transitions. The inset of Fig. 1 shows a linear extrapolation of these two critical values with the inverse of the chain length $1/L$. We find that the larger the system is, the smaller the BOW phase becomes. Nevertheless, the BOW phase remains finite at the thermodynamic limit. Compared with other recent numerical methods [11,13,14], we find this to be the most accurate way to locate the BOW phase boundaries.

Then we will further prove the existence of a finite-width BOW phase established by our method. The most direct evidence is the BOW correlation function

$$C_{\mathrm{BOW}}(r) = (-1)^r \left(\frac{1}{L} \sum_{l} \langle B_{l,l+1} B_{l+r,l+r+1} \rangle - \overline{B}^2 \right), \quad (5)$$

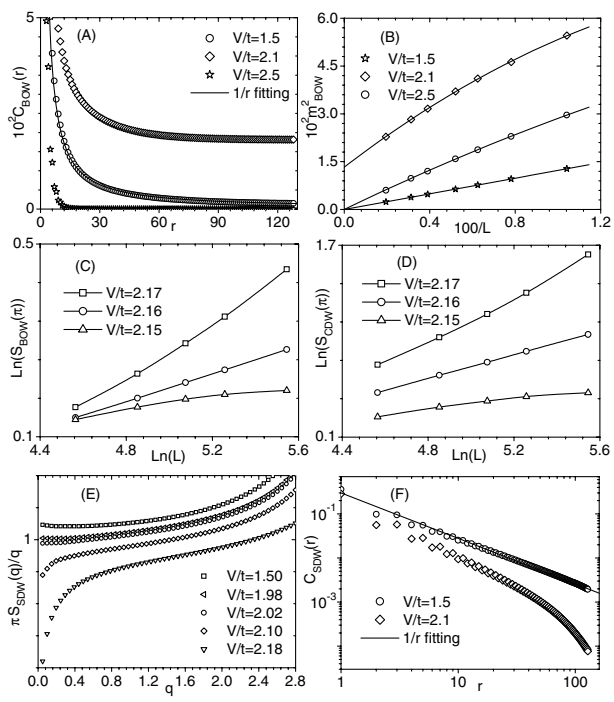

FIG. 2. Finite-size analyses for BOW, CDW, and SDW correlation functions and structure factors in the vicinity of the two phase transitions at V_c and V_c for $U/t = 4.0$.

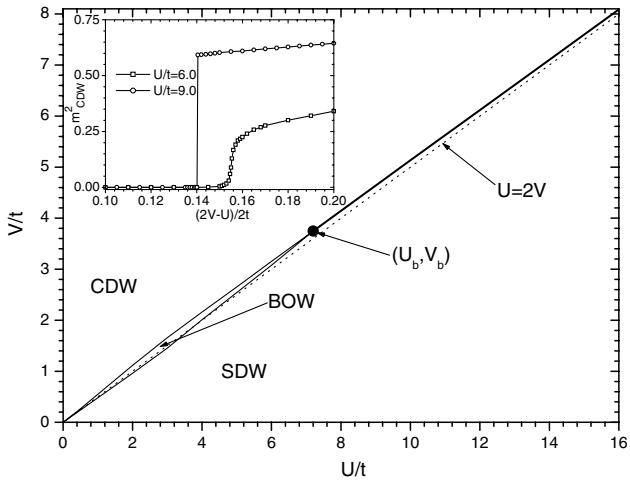

FIG. 3. Phase diagram of the half-filled extended Hubbard model. The bicritical point is at $(U_t, V_t) \simeq (7.2t, 3.746t)$. The inset shows V dependence of the CDW order parameters m_{CDW} across the phase boundary for $U = 6t$ and $U = 9t$ in the thermodynamic limit.

where $\overline{B} = \frac{1}{L}\sum_l \langle B_{l,l+1}\rangle$. In Fig. 2(a), we show the staggered BOW correlation functions with increasing nearest-neighbor repulsion V at $U/t = 4.0$. To avoid boundary effects, we perform only the average in (5) over 256 sites in the middle of the 512-site system. The results indicate that there exist three different phases in model (1) since the staggered BOW correlation functions show three distinct types of behavior as r increases: (i) It decays exponentially at $V/t = 1.5$, indicating that the system has no BOW order; (ii) it converges to a nonzero constant, indicating that the system is in the long-range BOW phase at $V/t = 2.1$; (iii) it decays as $1/r$ at $V/t = 2.5$, indicating that the system is in the Mott insulating phase. Besides the data we show in Fig. 2(a), we also compare our DMRG results with quantum Monte Carlo calculation [13] at $U/t = 4.0$, $V/t = 2.14$ for $L = 128$ and 256. The amplitudes of the oscillations at large distances are the same. The BOW order parameter in the thermodynamic limit,

$$\Delta_{\mathrm{BOW}} = \lim_{L\to\infty} \frac{1}{L}\sum_l (-1)^l \langle B_{l,l+1}\rangle, \tag{6}$$

can be obtained by fitting $m_{\mathrm{BOW}}(L)(=\sqrt{\sum_r C_{\mathrm{BOW}}(r)/L})$ with a second-order polynomial in $1/L$ since $m_{\mathrm{BOW}}(L) \to \Delta_{\mathrm{BOW}}$ for $L \to \infty$. Figure 2(b) shows such extrapolations. We find that $m^2_{\mathrm{BOW}}(L)$ approaches zero when $V/t = 1.5$ and 2.5 but remains finite when $V/t = 2.1$. The strength of dimerization is consistent with quantum Monte Carlo calculation [15] while another recent DMRG investigation [14] has not detected this rather strong BOW order.

In order to give more convincing evidence, we did another finite-size analysis in the vicinity of these two phase transitions. Let us start from the first phase transition at $U = U_c$. Figure 2(c) presents plots of $\ln[S_{\mathrm{BOW}}(\pi)]$ versus $\ln[L]$ for $U/t = 4.0$ and three different values of V/t around the first critical point. Data points for $V/t = 2.16$ indeed fall on a straight line, indicating critical scaling for the BOW fluctuations. At the other two points $V/t = 2.15$ and 2.17, data points behave nonlinearly due to the exponential decay term. Applying the same finite-size analysis to the CDW structure factor

$$S_{\mathrm{CDW}}(q) = \frac{1}{L}\sum_{lr} e^{iqr}(\langle n_l n_{l+r}\rangle - \langle n_l\rangle\langle n_{l+r}\rangle), \tag{7}$$

we can also explore the nature of the first phase transition. The linear behavior of $\ln[S_{\mathrm{CDW}}(\pi)]$ around $V/t = 2.16$, shown in Fig. 2(d), confirms the vanishing of the charge gap at the first phase-transition point.

Next, we determine the location of the phase transition of KT type. As argued by Nakamura [11], it is a quantum phase transition of the KT type. This makes it difficult to determine the phase boundary directly from the behavior of $S_{\mathrm{SDW}}(\pi)$

$$S_{\mathrm{SDW}}(q) = \frac{1}{L}\sum_{lr} e^{iqr}\langle s^z_l s^z_{l+r}\rangle \tag{8}$$

due to the finite-size effects. Instead, we apply an indirect method, used by Sengupta *et al.* [13,19], to confirm the second phase transition. It is well known [8] that, if the ground state of a 1D system is spin gapless, the spin-spin correlation falls algebraically with exponent equal to 1. It has been further shown [20] that in the spin-gapless phase $S_{\mathrm{SDW}}(q)/q \to 1/\pi$ as $q \to 0$ whereas in the spin-gapped phase $S_{\mathrm{SDW}}(q)/q \to 0$. Even a very small spin gap can be detected in this way, since it is in practice sufficient to see the $\pi S_{\mathrm{SDW}}(q)/q$ decay below 1 for small q to conclude that a spin gap must be present. From Fig. 2(e), we can see the behavior of $\pi S_{\mathrm{SDW}}(q)/q$ for $U/t = 4.0$ and different values of V/t. In the gapless region, logarithmic corrections [21] make it difficult to observe the approach to 1 as $q \to 0$. In analogy with spin systems [22], we expect the leading logarithmic corrections to vanish at the point where spin gap opens, and therefore exactly at the critical point there should be a clear scaling to 1. Based on results shown in Fig. 2(e), we estimate the BOW-MI boundary to be at $V/t = 2.0 \pm 0.01$ at $U/t = 4.0$ which is consistent with the results shown in Fig. 1. Figure 2(f) further provides evidence for the transition from the spin-gapped state, as identified by the exponential decay of the staggered SDW correlation function, to the spin-gapless state, as characterized by the $1/r$ decay of the SDW correlation function,

$$C_{\mathrm{SDW}}(r) = \frac{1}{L}(-1)^r \sum_l \langle s^z_l s^z_{l+r}\rangle. \tag{9}$$

Now let us determine the bicritical point. As we mentioned above, Nakamura [11] first argued that there exists

an extended BOW phase for couplings weaker than a bicritical point, which is supported by numerical [13] and analytical [12] studies where the bicritical point is given as $U_b \approx 4.76t$ and $U_b \approx 5t$, respectively. However, a recent DMRG calculation [14] disagreed with this picture and pointed out that the BOW phase exists only on the first-order SDW-CDW phase-transition line for intermediate-coupling U starting from the bicritical point $U_b \approx 3.7t$ to an upper limit which is smaller than $8t$. In order to give a more convincing result, we have studied the phase transitions in a wide range of coupling U starting from $2t$ to $9t$ with the interval of $\Delta U = 0.2t$ as carefully as we displayed above. We find that the width of the BOW phase will shrink to 0 at $U \approx 7.2t$ in the thermodynamic limit, and the extrapolation of the BOW order parameter will go to 0 for all the couplings V at $U > 7.2t$ which indicate the vanishing of long-range BOW phase and the merging of these two continuous phase transitions into one. Furthermore, we also calculate the V dependence of the CDW order parameters $m^2_{\mathrm{CDW}}(L)(= (1/L)\sum_r(-1)^r \times (1/L)\sum_l \langle n_l n_{l+r}\rangle)$ across the phase boundary for U up to 16. From the inset of Fig. 3, we can see that the characteristics of a second-order transition for $U = 6t$ and a first-order transition for $U = 9t$ are indeed quite apparent. The points are obtained from calculating the CDW order parameters for the chain length $L = 192$, 256, 320, 512, and then extrapolating to the thermodynamic limit $L \to \infty$. The transition point $V_c \approx 4.143$ for $U = 8t$ and $V_c \approx 6.116$ for $U = 12t$ are consistent with previous results [13,14].

The phase diagram obtained from DMRG calculations described above is shown in Fig. 3. The BOW phase exists from weak coupling up to a bicritical point where the two continuous transition lines meet. With the increasing of U and V along the line $U = 2V$, the BOW phase first expands and then shrinks up to the bicritical point. Beyond this point, the BOW phase disappears and the first-order transition from the CDW to SDW phase can be obtained. This phase diagram is similar to the schematic one in Ref. [13] except that the width of the BOW phase becomes much smaller and extends to much larger coupling. The first-order phase transition takes place for $U \lesssim 2V$ rather than $U \gtrsim 2V$ reported in Ref. [12]. Our result does not agree with the location and the width of the BOW phase given in Ref. [14] while the upper limit of the BOW phase is consistent with each other.

In conclusion, we have studied 1D half-filled EHM using the DMRG method. The quantitative phase diagram is obtained by investigating correlation functions and structure factors for the first time. The novel spontaneously dimerized phase does have finite width in the (U, V) plane. Our estimate for the bicritical point where the BOW phase vanishes and the nature of the transition changes is $U_b/t \approx 7.2$, $V_b/t \approx 3.746$. The extension of dimerization to rather strong coupling can be understood as the results of increasing frustration in the spin degrees of freedom [9,14].

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