Phase Diagram of the One-Dimensional Half-Filled Extended Hubbard Model

Satoshi Ejima[1] and Satoshi Nishimoto[2]

[1]*Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany*
[2]*Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany*

(Received 26 July 2007; published 20 November 2007)

We determine the ground-state phase diagram of the one-dimensional half-filled Hubbard model with on-site (nearest-neighbor) repulsive interaction U (V) and nearest-neighbor hopping t using the density-matrix renormalization group technique. Based on the results of the excitation gaps, Luttinger-liquid exponents, and bond-order-wave (BOW) order parameter, we confirm that the BOW phase appears in a substantial region between the charge-density-wave (CDW) and spin-density-wave phases. Each phase boundary is determined by multiple means and it allows us to make a cross-check on the validity of our estimations. We also find that the BOW-CDW transition changes from continuous to first order at the tricritical point $(U_t, V_t) \approx (5.89t, 3.10t)$ and the BOW phase shrinks to zero at the critical end point $(U_c, V_c) \approx (9.25t, 4.76t)$.

DOI: 10.1103/PhysRevLett.99.216403 PACS numbers: 71.10.Fd, 71.10.Pm, 71.30.+h

For several decades quasi-one-dimensional (1D) materials, e.g., organic conductors [1], conjugated polymers [2], and carbon nanotubes [3], have been a main subject of research in the field of condensed matter physics. A minimal electronic model which can describe their basic properties is the 1D extended Hubbard model (EHM) [4]. The Hamiltonian is given by

$$H = -t\sum_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1\sigma} + \text{H.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i\sigma\sigma'} n_{i\sigma}n_{i+1\sigma'}, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is creation (annihilation) operator of an electron with spin σ at site i, and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is number operator. t is the nearest-neighbor hopping term and U (V) is on-site (nearest-neighbor) Coulomb interaction. Despite the geometric simplicity, this model at half filling is believed to exhibit a variety of phases due to strong quantum fluctuations.

Within the g-ology scheme [5], the system has merely two insulating phases when the interaction strengths are positive: for $U < 2V$ the ground state is $2k_F$-charge-density wave (CDW), where both the charge and spin excitations are gapped; for $U > 2V$ a Mott insulator with $2k_F$-spin-density wave (SDW), where the spin excitation has no gap. However, based on nonperturbative numerical results, Nakamura argued that there is also a bond-order-wave (BOW) phase, where the ground state has a long-range staggered bond order, between the CDW and SDW phases [6]. So far much effort has been devoted to fix the ground-state phase diagram both analytically [7–12] and numerically [13–17]. Nevertheless, surprisingly their results are in few (quantitative) agreements with each other. The aim of this Letter is to produce a highly accurate phase diagram of the 1D half-filled EHM and to resolve the apparent contradictions.

We employ the density-matrix renormalization group (DMRG) method, which is one of the most powerful numerical techniques for studying 1D many-body systems [18]. With open-end boundary conditions, ground-state and low-lying excited-states energies as well as expectation values of physical quantities can be obtained quite accurately for very large finite-size systems [up to sites $L \sim \mathcal{O}(1000)$]. In DMRG procedure we keep $m = 1200$ to 3000 density-matrix eigenstates, which are much larger than those in the previous DMRG studies [13,16,17], and all the calculated quantities are extrapolated to the $m \to \infty$ limit. In this way, the maximum truncation error, i.e., the discarded weight, is less than 1×10^{-11}, while the maximum error in the ground-state energy is $\Delta E/t \sim 10^{-8}$–10^{-7}. We strongly argue that such large m values and the m extrapolation are essential for required accuracy of the measurements.

In order to determine the phase diagram including two phase boundaries, we calculate several physical quantities. Each boundary is determined by multiple means from the quantities and it allows us to do a cross-check on the estimates. First, to obtain the BOW-CDW boundary we calculate the charge gap

$$\Delta_c = \lim_{L\to\infty}[E(N+2,0) + E(N-2,0) - 2E(N,0)]/2, \tag{2}$$

where $E(N_e, S_z)$ is the ground-state energy for a given number of electrons N_e and z component of total spin S_z. We take $N = L$ for half-filled case. In the atomic limit $t = 0$, the phase boundary becomes a line $U = 2V$ with $\Delta_c = U(= 2V)$. If finite t is introduced, the system can gain some kinetic energy of the order of t near the BOW-CDW instability due to the competition between the on-site and nearest-neighbor Coulomb interactions. Thus, the charge gap is minimized at the BOW-CDW boundary. Next, to evaluate the SDW-BOW boundary we calculate the spin gap

$$\Delta_s = \lim_{L\to\infty}[E(N,1) - E(N,0)]. \tag{3}$$

If $V \ll U/2$, the system is a Mott insulator with $2k_F$ SDW. The electrons are uniformly distributed over the system, so that there is no spin gap. As V increases, the charge fluctuations are enhanced, and then a transition from the SDW phase to the BOW phase occurs. In the BOW phase, the electrons polarize alternatively and spin-singlet bound states are formed on dimers. Consequently, we can make an estimate of the SDW-BOW boundary as a point where the spin gap begins to develop. However, for some parameters the spin gap is too small to figure out if it remains finite, i.e., $\Delta_s \lesssim 10^{-6}t$. Therefore, for verifying the presence of the spin gap we consider the spin-spin correlation function

$$S(q) = \frac{1}{L}\sum_{kl} e^{iq(k-l)}(\langle s_k^z s_l^z\rangle - \langle s_k^z\rangle\langle s_l^z\rangle) \tag{4}$$

with $q = 2\pi/L$ and $s_i^z = n_{i\uparrow} - n_{i\downarrow}$. According to the Luttinger liquid theory [19], the long-range behavior of this function is governed by the LL spin exponents K_σ [$= \lim_{q\to 0}\pi S(q)/q$]. We find $K_\sigma = 0$ in the spin-gapped phase and $K_\sigma = 1$ everywhere else in the thermodynamic limit [20]. This criterion enables us to estimate the SDW-BOW critical point precisely. Although we can obtain all the phase boundaries with the quantities mentioned above, the BOW order parameter is also studied for making extra sure. The order parameter simply gives the boundaries between the BOW phase and the other phases. The BOW operator is given as

$$B_i = \tfrac{1}{2}\sum_\sigma (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}), \tag{5}$$

and we define the BOW order parameter $\langle B\rangle$ as an amplitude of the BOW oscillation in the center of the system, i.e., $\langle B\rangle = \lim_{L\to\infty}|\langle B_{L/2} - B_{L/2+1}\rangle|$. For $\langle B\rangle \neq 0$, a long-range order of the BOW state appears.

A careful extrapolation of these quantities is necessary to extract the correct value in the thermodynamic limit $L \to \infty$. We thus study various lengths of chains with $L = 32$ to 512 and perform finite-size-scaling analysis based on the L dependence of the quantities. Figure 1 shows the finite-size-scaling analyses for (a) the charge gap, (b) spin gap, (c) spin-spin correlation function, and (d) BOW parameter near the phase transitions at $U = 4$. The charge (spin) gap is systematically extrapolated by performing a least-squares fit to the fourth-order polynomial in $1/L$, reflecting the holon (spinon) band structure around the band edge. Then, an estimation of the LL spin exponent in the thermodynamic limit is not so simple for finite-size calculations. In the spin-gapless phase, one cannot expect easily find $K_\sigma \to 1$ exactly due to logarithmic corrections. However, the logarithmic corrections are known to vanish at which the spin gap opens, in analogy with the dimerization transition in the $J_1 - J_2$ model [21]. In the spin-gapped phase, there is a similar difficulty as follows: if the spin gap is small, the convergence of K_σ to 0 will obviously occur only for very large systems. As a result, we will estimate the critical point where the spin gap opens by $\pi S(q)/q$ crossing 1 at $q \to 0$. This method was primarily used in Ref. [14]. Let us now turn to the BOW order parameter. Since the order parameter in the thermodynamic limit is very small compared to the finite-size results, a well-controlled finite-size extrapolation is mandatory. In our calculations, the most problematic finite-size effects are the Friedel oscillation due to the open edges. Assuming that the amplitude of the Friedel oscillation in the center of a finite chain scales as L^{-K_ρ} [22], the BOW order parameter would be well extrapolated as a function of $1/L^{K_\rho}$. For example, we may expect $K_\rho \approx 0.5$ in the vicinity of the SDW phase, so that $\langle B\rangle$ is scaled better by $1/\sqrt{L}$ than by $1/L$ near the SDW phase.

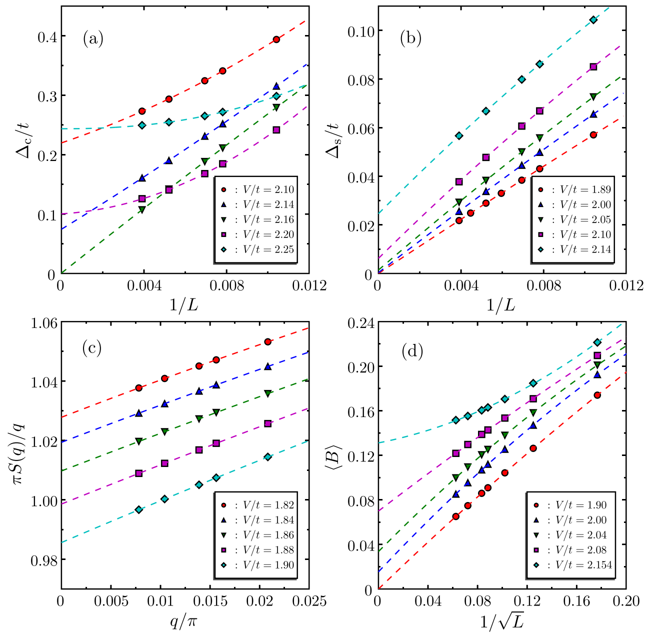

FIG. 1 (color online). Finite-size-scaling analyses for (a) the charge gap, (b) spin gap, (c) spin-spin correlation function, and (d) BOW order parameter near the phase boundaries at $U = 4t$.

Figure 2 shows the extrapolated results of (a) the charge gap, (b) spin gap, (c) spin correlation function, and (d) BOW order parameter around the phase transitions ($U \sim 2V$) as a function of V/t for $U = 4t$. Let us look at the charge gap to estimate the BOW-CDW phase boundary. The charge gap decreases with approaching to a point $V \approx 2.164t$ and vanishes smoothly at the point. In other words, both the BOW and CDW insulating gaps start to develop gradually at the point. It means that a continuous transition between the BOW and CDW phases occurs at the critical point $V \approx 2.164t$. Note that the BOW insulating gap is of the nature of the Mott type. We now turn to the SDW-BOW phase boundary. We find that the spin gap is finite for $V \gtrsim U/2$ and decreases with decreasing V. The critical point appears to lie around $V = 1.9t$ from the dis-

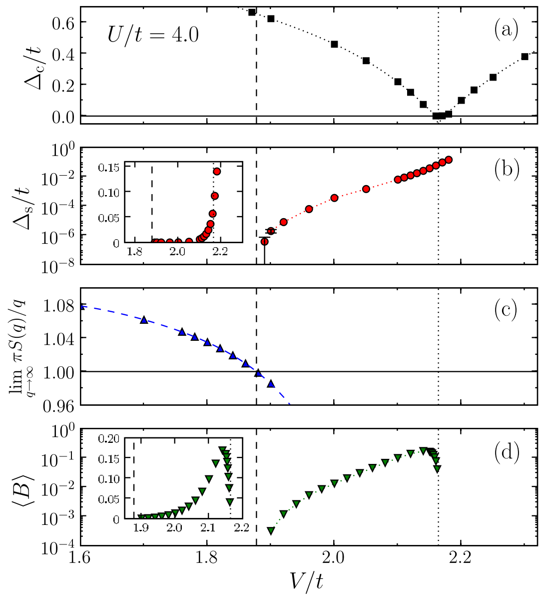

FIG. 2 (color online). Extrapolated results of (a) the charge gap, (b) spin gap, (c) spin-spin correlation function, and (d) BOW order parameter near the phase transition for $U = 4t$. The dashed and dotted lines denote the SDW-BOW and BOW-CDW critical points, respectively. Insets: same quantities plotted with another scale.

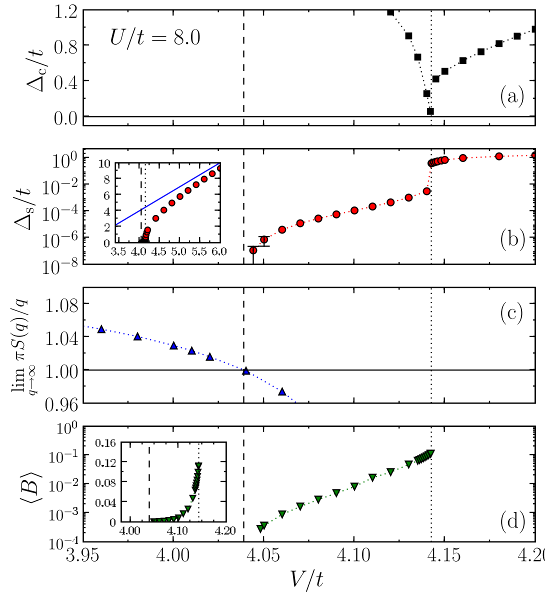

FIG. 3 (color online). The same quantities as in Fig. 2 but for $U = 8t$. Solid line in the inset of (b) denotes the spin gap in the $V/U \to \infty$ limit, i.e., $\Delta_s = 3V - U$.

appearance point of the spin gap. The crossing point with $\pi\lim_{q\to 0} S(q)/q = 1$ gives a more precise estimation of the critical point $V \approx 1.877t$. Correspondingly, the BOW order parameter has finite values only in the region $1.877t \leq V \leq 2.164t$. With increasing V, $\langle B\rangle$ rises exponentially from the SDW-BOW critical point, reaches the maximum value ~ 0.18 around $V = 2.14t$, and goes down to zero at the BOW-CDW critical point. Note that both values of the critical points are in good agreement with those of the previous quantum Monte Carlo (QMC) study [15].

Figure 3 shows the same quantities as in Fig. 2 but for $U = 8t$. Near the SDW-BOW phase boundary $V \approx 4.039t$, the behavior of all the quantities is qualitatively similar to those in the case of $U = 4t$. On the other hand, the physical properties seem to be discontinuous at the BOW-CDW phase boundary $V \approx 4.142t$, which indicates that the transition is of first order. At the boundary, the charge gap remains finite and the slope of Δ_c with respect to V is discontinuous. However, the value of Δ_c must be continuous since a competition between two kinds of charge configuration, i.e., CDW and uniform, leads to the BOW-CDW transition. Associated with this charge redistribution, the spin gap jumps by 2 orders of magnitude. In the CDW phase, it comes rapidly close to a line $\Delta_s = 3V - U$ which becomes exact in the $V/U \to \infty$ limit. Also, the BOW order parameter develops with approaching the BOW-CDW boundary and disappears at the transition point.

Whereas the BOW-CDW transition is continuous for $U = 4t$, it is of first order for $U = 8t$. Hence, a tricritical point (U_t, V_t) at which the transition changes from continuous to first order, must exist on the BOW-CDW boundary, as suggested in Refs. [13,15]. To evaluate the tricritical point, we examine the LL charge exponent K_ρ via the derivative of charge structure factor at $q = 0$ [23]

$$K_\rho = \lim_{L\to\infty} \frac{1}{2} \sum_{kl} e^{i(2\pi/L)(k-l)} (\langle n_k n_l\rangle - \langle n_k\rangle\langle n_l\rangle). \qquad (6)$$

Note that K_ρ is finite only in the continuous Gaussian critical point [6,11] for small U and zero everywhere else. It was shown that the LL exponents can be obtained quite accurately with DMRG method [24]. In Fig. 4(a), we plot DMRG results of K_ρ as a function of U/t on the BOW-CDW boundary line. As U/t increases, K_ρ decreases from 1, reaches 1/4 at $(U_t, V_t) = (5.89t, 3.10t)$, and drops discontinuously to 0; namely, a metal-insulator transition occurs at $U = U_t$. Moreover, the K_ρ curve is well fitted

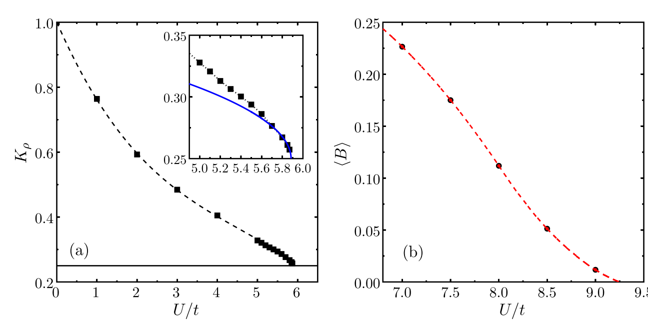

FIG. 4 (color online). Extrapolated results of the LL charge exponent (a) and the BOW order parameter (b) on the BOW-CDW boundary line. Inset: expanded view around the tricritical point $U_t = 5.89t$.

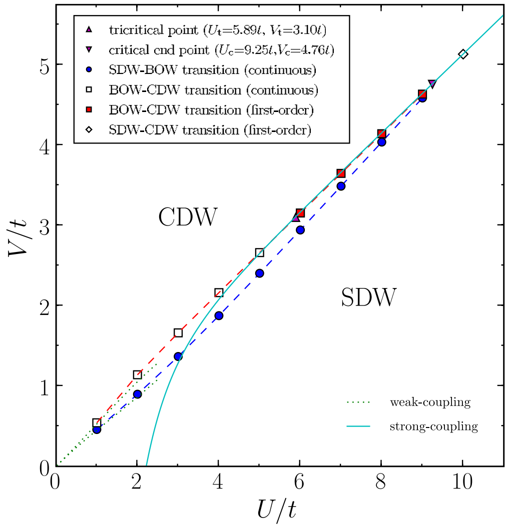

FIG. 5 (color online). DMRG phase diagram of the 1D half-filled EHM. The BOW phase exists between the SDW and CDW phases.

by a function $K_\rho - 1/4 = 0.061\sqrt{(U_t - U)/t}$ near the tricritical point [see inset of Fig. 4(a)]. It implies that the transition is of the Kosterlitz-Thouless type. Let us now consider a point at which the BOW phase shrinks to 0, which is called a "critical end point". The BOW state is still stable around the tricritical point and therefore the critical end point (U_c, V_c) would exist for $U_c > U_t$. For a fixed U $(>U_t)$, the BOW order parameter has a maximum around the BOW-CDW boundary. To find the critical end point, we plot $\langle B\rangle$ on the BOW-CDW boundary as a function of U/t in Fig. 4(b). $\langle B\rangle$ decreases with increasing U/t and reaches to 0 at $(U_c, V_c) = (9.25t, 4.76t)$. For $U \geq U_c$, the transition is always first-order SDW-CDW one.

In Fig. 5 we sum up our results as the ground-state phase diagram. One can see good agreement with the weak-coupling renormalization group (RG) results [11] as well as the strong-coupling perturbation results [9]. The BOW phase has a maximum width at $U \sim 4t$, which is concerned with the fact that the effective nearest-neighbor exchange interaction is the largest at the intermediate couplings of U in the half-filled Hubbard model [25]. It is so because the large exchange interaction promotes the formation of spin-singlet pair if the charge fluctuation is introduced by V. Accordingly, we confirm that the magnitude of the spin gap is maximized around $U \sim 4t$ in the BOW phase.

In summary, we study the ground-state phase diagram of the 1D half-filled EHM using DMRG method. We calculate several quantities with considerable accuracy to determine the SDW-BOW and BOW-CDW boundaries. As for the phase boundaries, our data agree quantitatively with the RG results in the weak-coupling regime ($U \lesssim 2t$), with the perturbation results in the strong-coupling regime ($U \gtrsim 6t$), and with the QMC results in the intermediate-coupling regime. We also find that the BOW-CDW transition changes from continuous to first order at the tricritical point $(U_t, V_t) = (5.89t, 3.10t)$ and it locates far from the critical end point $(U_c, V_c) = (9.25t, 4.76t)$. Since the previous DMRG results could be insufficient in accuracy, our results are not in agreement with them. We thus believe that our DMRG results bring a sound conclusion and put an end to the controversy on the phase diagram of the 1D half-filled EHM.

We would like to thank R. M. Noack, E. Jeckelmann, F. Gebhard, S. Glocke, and J. Sirker for useful discussions. We are grateful to M. Tsuchiizu for his RG results and helpful discussions.

[1] T. Ishiguro and K. Yamaji, *Organic Superconductors* (Springer-Verlag, Berlin, 1990).
[2] *Conjugated Conducting Polymers*, edited by H. Kiess (Springer-Verlag, Berlin, 1992).
[3] H. Ishii *et al.*, Nature (London) **426**, 540 (2003).
[4] D. Baeriswyl, in *Theoretical Aspects of Band Structures and Electronic Properties of Pseudo-One-Dimensional Solids*, edited by R. H. Kamimura (Reidel, Dordrecht, 1985), pp. 1–48.
[5] V. J. Emery, in *High Conducting One-Dimensional Solids*, edited by J. T. Devreese, R. Evrand, and V. van Doren (Plenum, New York, 1979).
[6] M. Nakamura, J. Phys. Soc. Jpn. **68**, 3123 (1999); Phys. Rev. B **61**, 16 377 (2000).
[7] J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984).
[8] J. W. Cannon and E. Fradkin, Phys. Rev. B **41**, 9435 (1990); J. W. Cannon *et al.*, Phys. Rev. B **44**, 5995 (1991).
[9] P. G. J. van Dongen, Phys. Rev. B **49**, 7904 (1994).
[10] J. Voit, Rep. Prog. Phys. **58**, 977 (1995).
[11] M. Tsuchiizu and A. Furusaki, Phys. Rev. Lett. **88**, 056402 (2002).
[12] K-M. Tam *et al.*, Phys. Rev. Lett. **96**, 036408 (2006).
[13] E. Jeckelmann, Phys. Rev. Lett. **89**, 236401 (2002).
[14] P. Sengupta *et al.*, Phys. Rev. B **65**, 155113 (2002).
[15] A. W. Sandvik *et al.*, Phys. Rev. Lett. **92**, 236401 (2004).
[16] Y. Z. Zhang, Phys. Rev. Lett. **92**, 246404 (2004).
[17] S. Glocke *et al.*, Phys. Rev. B **76**, 155121 (2007).
[18] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).
[19] J. Sólyom, Adv. Phys. **28**, 201 (1979).
[20] J. Voit, Phys. Rev. B **45**, 4027 (1992).
[21] S. Eggert, Phys. Rev. B **54**, R9612 (1996).
[22] S. R. White *et al.*, Phys. Rev. B **65**, 165122 (2002).
[23] M. Dzierzawa, in *The Hubbard Model*, edited by D. Baeriswyl *et al.*, NATO Advanced Study Institutes, Ser. B Vol. 343 (Plenum, New York, 1995), pp. 327.
[24] S. Ejima *et al.*, Europhys. Lett. **70**, 492 (2005).
[25] Y. H. Szczech *et al.*, Phys. Rev. Lett. **74**, 2804 (1995).