Phase diagram of the one-dimensional half-filled extended Hubbard model

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We study the ground state of the one-dimensional half-filled Hubbard model with on-site (nearest-neighbor) repulsive interaction $U$ ($V$) and nearest-neighbor hopping $t$. In order to obtain an accurate phase diagram, we consider various physical quantities such as the charge gap, spin gap, Luttinger-liquid exponents, and bond-order-wave (BOW) order parameter using the density-matrix renormalization group technique. 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 do a cross-check to demonstrate the validity of our estimations. Thus, our results agree quantitatively with the renormalization group results in the weak-coupling regime ($U \lesssim 2t$), with the perturbation results in the strong-coupling regime ($U \gtrsim 6t$), and with the quantum Monte Carlo results in the intermediate-coupling regime. We also find that the BOW-CDW transition changes from continuous to first order at the tricritical point ($U_c, V_c$) ≈ (5.89$t$, 3.10$t$) and the BOW phase vanishes at the critical end point ($U_c, V_c$) ≈ (9.25$t$, 4.76$t$).

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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

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

(1)

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is creation (annihilation) operator of an electron with spin $\sigma$ at site $i$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is number operator. $t$ is 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 2$k_F$-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 non-perturbative 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, 8, 9, 10, 11, 12] and numerically [13, 14, 15, 16, 17]. Nevertheless, surprisingly their results are in few (quantitative) agreements with each other. The aim of this paper 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 $L \sim O(1000)$). In DMRG procedure we keep $m = 1200$ to 3000 density-matrix eigenstates, which are much larger than those in the previous DMRG studies [19, 20, 21], 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 $1 \times 10^{-11}$, 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

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

(2)

where $E(N_c, S_z)$ is the ground-state energy for a given number of electrons $N_c$ 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

$$\Delta_s = \lim_{L \to \infty} [E(N, 1) - E(N, 0)].$$  \hfill (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., $\Delta_s \lesssim 10^{-6}$. Therefore, for verifying the presence of the spin gap we consider the spin-spin correlation function

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

with $q = 2\pi / L$ and $s_i^z = n_{i\uparrow} - n_{i\downarrow}$. According to the Luttinger liquid theory [21], the long-range behavior of this function is governed by the LL spin exponents $K_\sigma (= \lim_{q \to 0} \pi S(q)/q)$. We find $K_\sigma = 0$ in the spin-gapped phase and $K_\sigma = 1$ everywhere else in the thermodynamic limit [22]. 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

$$B_i = \frac{1}{2} \sum_{\sigma} \langle c_{i\sigma}^+ c_{i+1\sigma} + c_{i+1\sigma}^+ c_{i\sigma} \rangle.$$  \hfill (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 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 order parameter near the phase boundaries at $U = 4t$. The charge (spin) gap is systematically extrapolated by performing a least-squares fit to the forth-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 $K_\sigma$ 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 $L^{-K_\rho}$ [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.

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
two orders of magnitude. In the CDW phase, it comes with this charge redistribution, the spin gap jumps by uniform, leads to the BOW-CDW transition. Associated between two kinds of charge configuration, i.e., CDW and value of $\Delta_c$ of $\Delta_c$ is discontinuous. However, the $\Delta_c$ 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 two orders of magnitude. In the CDW phase, it comes rapidly close to a line $\Delta_c = 3V - U$ 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 $K_\rho$ via the derivative of charge structure factor at $q = 0$

$$K_\rho = \lim_{K \to \infty} \frac{1}{2} \sum_{k,l} e^{iq(k-l)} (\langle nk_l \rangle - \langle n_k \rangle \langle n_l \rangle).$$  

Note that $K_\rho$ is finite only in the continuous Gaussian critical point [4, 11] for small $U$ and zero everywhere else. It was shown that the LL exponents can be obtained

FIG. 2: 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: 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., $\Delta_c = 3V - U$.

FIG. 4: 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 $U_t = 5.89t$. 

quite accurately with DMRG method [24]. In Fig. 4(a), we plot DMRG results of $K_p$ as a function of $U/t$ on the BOW-CDW boundary line. As $U/t$ increases, $K_p$ decreases from 1, reaches to $1/4$ at $(U_c, V_c) = (5.89t, 3.10t)$, and drops discontinuously to 0; namely, a metal-insulator transition occurs at $U = U_c$. Moreover, the $K_p$ curve is well-fitted by a function $K_p = 1 - 0.061 \sqrt{(U - U_c)/t}$ 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 $(B)$ on the BOW-CDW boundary as a function of $U/t$ in Fig. 4(b). $(B)$ 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.

![DMRG phase diagram of the 1D half-filled EHM. The BOW phase exists between the SDW and CDW phases.](image)

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 [22]. 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 agrees quantitatively with the RG results in the weak-coupling regime ($U < 2t$), with the perturbation results in the strong-coupling regime ($U > 6t$), 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 $(U_t, V_c) = (5.89t, 3.10t)$ 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.

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