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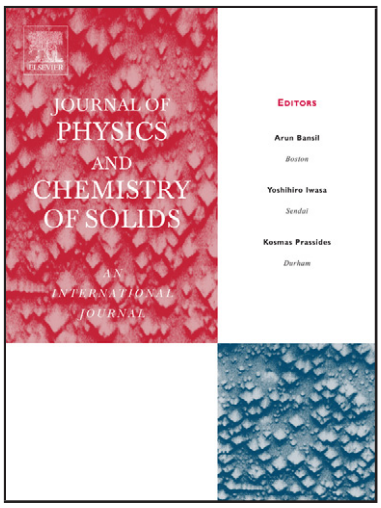

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Ground-state properties of the one-dimensional extended Hubbard model at half filling

S. Ejima [a] and S. Nishimoto [b]

[a] *Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany*

[b] *Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany*

Abstract

The density-matrix renormalization group (DMRG) technique is used to study the ground-state properties of the one-dimensional half-filled Hubbard model with on-site (nearest-neighbor) repulsive interaction U (V) and nearest-neighbor hopping t. We calculate the static spin structure factor to consider the spin degrees of freedom. We notice a striking difference of the static spin structure factor among the spin-density-wave, charge-density-wave (CDW), and bond-order-wave (BOW) phases. Based on the results, we identify the BOW-CDW transition at small (large) U value as continuous (of first order). We also calculate the double occupancy to consider the charge degrees of freedom. For large U, the double occupancy show a discontinuous jump at the BOW-CDW critical point and it implies first order transition. With decreasing U, the jump becomes smaller and vanishes at the tricritical point $U_{\rm t} \approx 5.961t$. This value is close to our previous estimation $U_{\rm t} = 5.89t$ obtained with other quantities. Consequently, the results of static spin structure factor and double occupancy support the accuracy of our ground-state phase diagram.

Key words: extended Hubbard model, quantum phase transition, bond order wave
PACS: 71.10.Fd, 71.10.Pm, 71.30.+h

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In recent years, the research of quasi-one-dimensional (1D) materials has come once again to the fore in the field of condensed matter physics [1]. From the theoretical point of view, one of the simplest models for the materials is the 1D Hubbard model. The ground-state properties of the 1D Hubbard model is well-understood using the exact Bethe-ansatz solution: for any finite on-site repulsion $U > 0$ at half band-filling, the charge sector is gapped because of the Mott-Hubbard transition and the spin sector is gapless with the dominant $2k_{\rm F}$-spin-density-wave (SDW) correlation. It is known, however, that the Coulomb interaction is not sufficiently screened in the 1D materials [2,3]. And, we also

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add the nearest-neighbor Coulomb interaction $V(>0)$. Then a rich phase diagram may be expected due to the competition between the effects of U and V: within the g-ology scheme, the system is (basically) insulating with the $2k_{\rm F}$-SDW correlation for $V \lesssim U/2$ and with the $2k_{\rm F}$-charge-density-wave (CDW) correlation for $V \gtrsim U/2$; furthermore, the existence of a bond-order-wave (BOW) phase between the SDW and CDW phases has been proposed on the basis of non-perturbative numerical results [4]. The system is called as the 1D half-filled extended Hubbard model (EHM), of which Hamiltonian is given by

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

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is creation (annihilation) operator of an electron with spin σ at site i, and $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is number operator. t is nearest-neighbor hopping integral and U (V) is on-site (nearest-neighbor) Coulomb interaction.

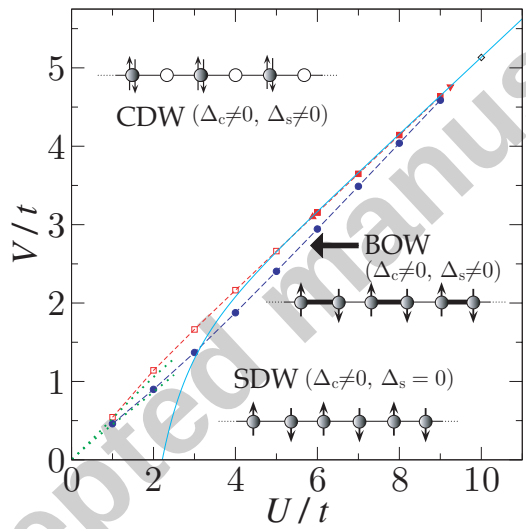

Fig. 1. Ground-state phase diagram of the 1D half-filled EHM. The symbols represent the DMRG results as follows: the SDW-BOW phase boundary (filled circles), the continuous BOW-CDW phase boundary (empty squares), the first-order BOW-CDW phase boundary (filled squares), the tricritical point (filled triangle), and the critical end point (empty triangle). The solid and dotted lines correspond to the strong-coupling [7] and the weak-coupling [9] results, respectively.

The ground-state phase diagram of the 1D half-filled EHM is still controversial, though there are a number of analytical [5–10] and numerical [11–15] studies. Quite recently, in order to put an end to the controversy, we have re-examined the phase diagram using the density-matrix renormalization group (DMRG) method with considerable accuracy [16]; we determined the SDW-BOW and BOW-CDW phase boundaries based on the results of various physical quantities such as the charge gap, spin gap, Luttinger exponents, and

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BOW order parameter (see Fig. 1). As for the phase boundaries, our results agree quantitatively with the renormalization-group results [9] in the weak-coupling regime ($U \lesssim 2t$), with the perturbation results [7] in the strong-coupling regime ($U \gtrsim 6t$), and with the quantum Monte Carlo results [13] in the intermediate-coupling regime. In addition, we obtained the tricritical point $(U_{\rm t}, V_{\rm t}) = (5.89t, 3.10t)$ where the BOW-CDW transition changed from continuous to first order, and the critical end point $(U_{\rm c}, V_{\rm c}) = (9.25t, 4.76t)$ where the BOW phase disappears. In this paper, we calculate the static spin structure factor as well as the double occupancy of the 1D half-filled EHM and show that these results support our previous study [16].

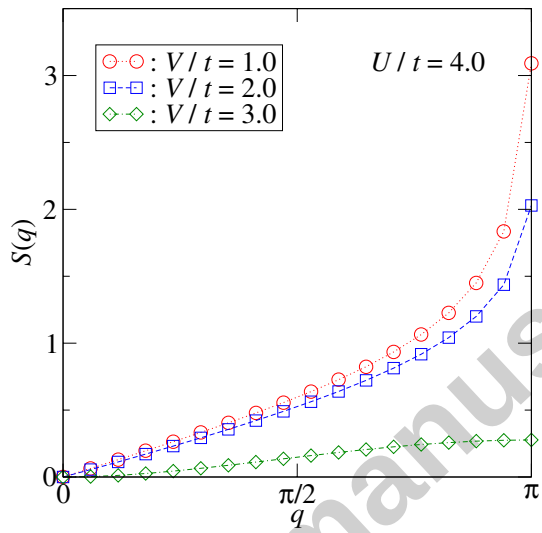

Fig. 2. Static spin structure factor $S(q)$ for $U = 4t$ and $L = 34$. The dotted lines are guides to the eye.

First, we calculate the static spin structure factor $S(q)$ to evaluate the spin degrees of freedom. A drastic change of $S(q)$ could be driven by the phase transitions because the spin structures are quite different among the three phases (see Fig. 1). The static spin structure factor is defined as

$$S(q) = \frac{1}{L}\sum_{j,k} e^{iq(j-k)}\langle (S_j^z - \langle S_j^z\rangle)(S_k^z - \langle S_k^z\rangle)\rangle, \tag{2}$$

where the sum runs over all sites of the system and $\langle\cdots\rangle$ denotes the ground-state expectation value. We apply the periodic boundary conditions which are preferred for calculations of the momentum-dependent quantities [17] and study systems up to chain length $L = 34$. The number of density-matrix eigenstates kept is $m = 3000$ and the maximum truncation error is 1.0×10^{-6}. In Fig. 2, we show the calculated results of the static spin structure factor $S(q)$ for $U = 4t$ and $L = 34$. At $U = 4t$, the SDW-BOW (BOW-CDW) transition occurs at $V \approx 1.877t$ ($2.164t$) [16]. Thus, the three curves in the figure represent results for three different phases; namely, the results for $V = t$,

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$2t$, and $3t$ correspond to the SDW, BOW, and CDW phases, respectively. In the SDW phase, $S(q)$ is basically the same as that of the 1D Heisenberg model [18] and it can be approximately fitted by the 'gross' curve $S(q) \approx -\ln(1-\frac{q}{\pi})$. In the BOW phase, one might expect much reduction of $S(q)$ in association with the exponential decay of $\langle(S_j^z - \langle S_j^z\rangle)(S_k^z - \langle S_k^z\rangle)\rangle$ with $|j-k|$ driven by the appearance of the spin gap. Indeed, $S(q)$ is just slightly reduced around $q=\pi$ relative to that in the SDW phase. Since the spin gap is still very small ($\Delta_s \sim 10^{-3}t$), the short-range spin-spin correlations must be hardly affected. In the CDW phase, the antiferromagnetic spin-spin correlation seems to be fairly suppressed due to the formation of on-site spin-singlet bound state, though $S(q)$ has still the maximum at $q=\pi$. Each the spin-singlet pair is increasingly isolated with increasing V/t and $S(q)$ approaches to zero for all q in the limit of $V/U \to \infty$. Note that the zero derivative of $S(q)$ at $q=0$ indicates the existence of the spin gap. It is also interesting that the shape of $S(q)$ is similar to that of a gas of bound state, i.e., $S(q) \propto 1-\cos(q)$ [19].

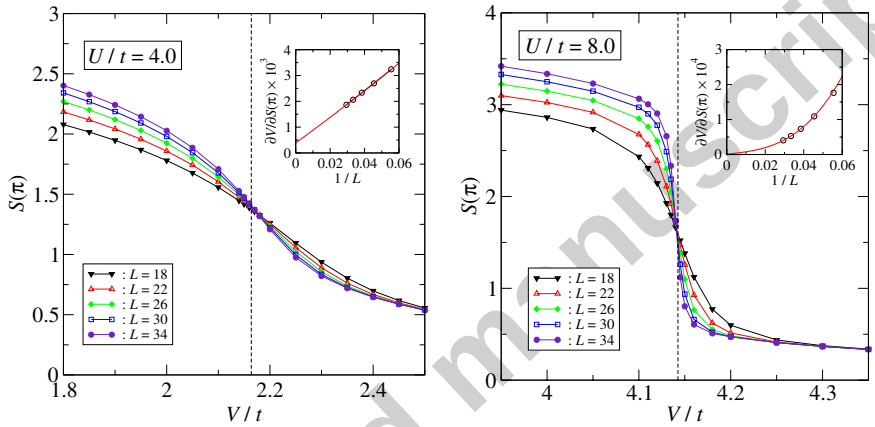

Fig. 3. $S(\pi)$ as a function of V/t at $U=4t$ (left) and $U=8t$ (right) for several kinds of chain lengths. The dotted line denotes the BOW-CDW transition point for each U/t values.

Next, we focus on the behavior of $S(\pi)$ with V to investigate how the antiferromagnetic spin-spin correlation is suppressed. In Fig. 3, we show the system-size dependence of $S(\pi)$ in the vicinity of the BOW-CDW transition, as a function of V/t with fixed $U=4t$ and $8t$. When $U=4t$, we can see gradual decreases of $S(\pi)$ for all system sizes with increasing V/t, reflecting the rapid development of the spin gap. Although the shape of $S(\pi)$ becomes steeper as L increases, the transition seems to be continuous in the thermodynamic limit. To confirm it, we scale the inverse slope of $S(\pi)$ at the critical point with the inverse system size, as shown in the inset of Fig. 3. The extrapolated value to $1/L \to 0$ is 0.00039. It means that the slope of $S(\pi)$ at the BOW-CDW transition remains finite in the thermodynamic limit and the transition is continuous. Let us then turn to the case of $U=8t$. Differently from the case of $U=4t$, $S(\pi)$ decreases rapidly around the BOW-CDW transition and changes slowly otherwise. The slope of $S(\pi)$ at the critical point becomes sharper quickly with increasing L and the inverse slope is extrapolated to zero in $L \to \infty$, i.e., the slope diverges

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in the thermodynamic limit. Thus, the BOW-CDW transition for $U = 8t$ must be of first order. The discontinuous transition is concerned with the abrupt charge redistribution from the BOW to CDW phases. We also note that the slow decrease of $S(\pi)$ below (above) the transition point is associated with very small spin gap (strong charge disproportionation) in the BOW (CDW) phase.

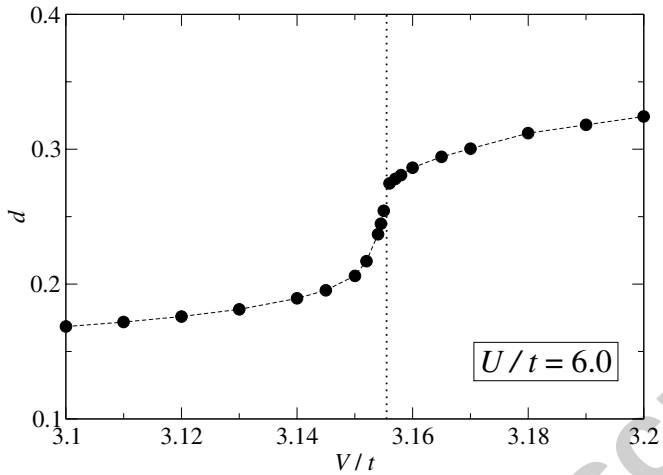

Fig. 4. Extrapolated data for the double occupancy d as a function of V/t for $U = 6t$. The dotted line denotes the BOW-CDW critical point. The dashed line is a guide to the eye.

Finally, we consider the double occupancy d to confirm that the BOW-CDW transition changes continuous to first order between $U = 4t$ and $8t$. We apply the open boundary conditions which allows us to calculate physical quantities quite accurately for very large systems with the DMRG method. We study systems with $L \leq 256$ and carry out the finite-size scaling analysis. The number of density-matrix eigenstates kept is $m = 2000$ and the maximum truncation error is 1.0×10^{-9}. With the open boundary conditions, the CDW is a state with a broken translational symmetry and one of two degenerate ground states is picked out by initial conditions of the calculation. Thus, the double occupancy is defined as the average value for central two sites,

$$d = \frac{1}{2} \lim_{L \to \infty} \left| \langle d_{L/2} + d_{L/2+1} \rangle \right|, \tag{3}$$

where $d_i = n_{i\uparrow} n_{i\downarrow}$. In the strong-coupling limit $U, V \gg t$, we find $d = 0$ in the SDW state and $d = 1/2$ in the CDW state; in the weak-coupling limit $U, V \ll t$, we find $d = 1/4$. If U and V completely cancel each other out, we also find $d = 1/4$. In Fig. 4, we show the $L \to \infty$ extrapolated results of the double occupancy d as a function of V/t for $U = 6t$. We can see an increase of d with increasing V/t and a discontinuous jump at the BOW-CDW critical point. The discontinuity clearly indicates that the transition is of first order. We also note that d crosses $1/4$ at the critical point. It is consistent

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with the fact that the BOW-CDW transition is derived by the competition between the effects of U and V. Recently, it has been suggested that the double occupancy has no discontinuity for $U = 6t$ using the DMRG algorithm applied to transfer matrices (TMRG) [15]. In the TMRG study, the interval between the calculated points around the critical point is still wider than our estimation of the jump, so that it may possibly include the discontinuity.

Let us now investigate the U-dependence of the discontinuous jump Δ_d. In Fig. 5, we plot the $L \to \infty$ extrapolated values of the discontinuous jump Δ_d at the BOW-CDW critical point as a function of U/t. For $U/t \to \infty$, doubly occupied sites are alternated with empty sites with no charge fluctuation and, thus, Δ_d is exactly 1/2. With decreasing U/t from $U/t \to \infty$, the charge fluctuation is increasingly allowed and Δ_d decreases. We find Δ_d vanishes just below $U/t = 6$. Near the vanishing point, the data is well-fitted by a function $\Delta_d = \alpha(U - \beta)^\gamma$ with $\alpha = 0.139$, $\beta = 5.961$, and $\gamma = 0.594$. It leads to the tricritical point $U_\mathrm{t} \approx 5.961t$ and it is consistent with our another estimation [16].

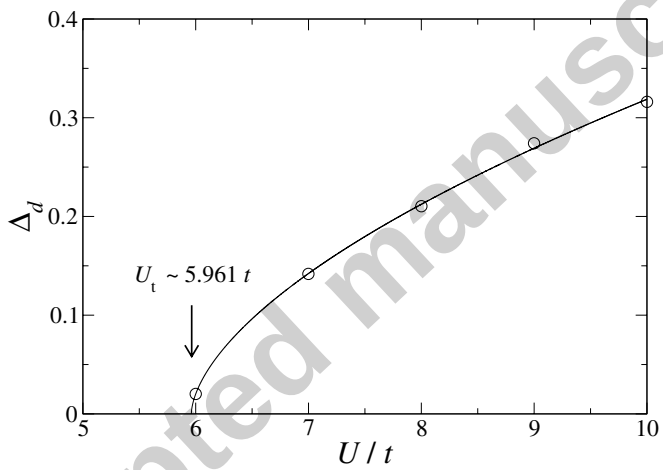

Fig. 5. Extrapolated data for the jump Δ_d in the double occupancy at the phase transition. The line is a fit $\Delta_d = 0.139(U - 5.961)^{0.594}$.

In summary, the ground-state properties of the 1D half-filled EHM are studied using the DMRG method. First, we calculate the static spin structure factor to consider the spin degrees of freedom. We notice a striking difference of the static spin structure factor among the three phases with distinct spin structures. Next, we identify the BOW-CDW transition at $U = 4t$ ($8t$) as continuous (of first order) from the behavior of $S(\pi)$ near the critical point. Finally, the double occupancy is calculated to consider the charge degrees of freedom. For $U = 6t$, a discontinuous jump of the double occupancy at the BOW-CDW critical point is found and it implies first order transition. We estimate the tricritical point $U_\mathrm{t} \approx 5.961t$ as a point where the discontinuous jump shrinks to zero. This value is quite close to our previous estimation $U_\mathrm{t} = 5.89t$ obtained with other quantities. Consequently, all the results shown

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in this paper support the accuracy of our ground-state phase diagram.

References

[1] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford University Press, 2004).

[2] R. Egger and H. Grabert, Phys. Rev. Lett. **79**, 3463 (1997).

[3] S. Bellucci and J. González, Eur. Phys. J. B **18**, 3 (2000).

[4] M. Nakamura, J. Phys. Soc. Jpn. **68**, 3123 (1999); Phys. Rev. B **61**, 16377 (2000).

[5] J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984).

[6] J. W. Cannon and E. Fradkin, Phys. Rev. B **41**, 9435 (1990); J. W. Cannon, R. T. Scalettar, and E. Fradkin, Phys. Rev. B **44**, 5995 (1991).

[7] P. G. J. van Dongen, Phys. Rev. B **49**, 7904 (1994).

[8] J. Voit, Rep. Prog. Phys. **58**, 977 (1995).

[9] M. Tsuchiizu and A. Furusaki, Phys. Rev. Lett. **88**, 056402 (2002).

[10] K-M. Tam, S-W. Tsai, and D. K. Campbell, Phys. Rev. Lett. **96** 036408 (2006).

[11] E. Jeckelmann, Phys. Rev. Lett. **89** 236401 (2002).

[12] P. Sengupta, A. W. Sandvik, and D. K. Campbell, Phys. Rev. B **65**, 155113 (2002).

[13] A. W. Sandvik, L. Balantz, and D. K. Campbell, Phys. Rev. Lett. **92**, 236401 (2004).

[14] Y. Z. Zhang, Phys. Rev. Lett. **92**, 246404 (2004).

[15] S. Glocke, A. Klümper, and J. Sirker, Phys. Rev. B **76**, 155121 (2007).

[16] S. Ejima and S. Nishimoto, Phys. Rev. Lett. **99**, 216403 (2007).

[17] S. Nishimoto and M. Arikawa, Int. J. Mod. Phys. B **21**, 2262 (2007).

[18] M. Karbach and K. -H. Mütter, Z. Phys. B **90** 83 (1993).

[19] F. F. Assaad and D. Würtz, Phys. Rev. B **44**, 2681 (1991).

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