Correlation function for the one-dimensional extended Hubbard model at quarter filling

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We examine the density-density correlation function in the Tomonaga-Luttinger liquid state for the one-dimensional extended Hubbard model with the on-site Coulomb repulsion $U$ and the intersite repulsion $V$ at quarter filling. By taking into account the effect of the marginally irrelevant umklapp scattering operator by utilizing the renormalization-group technique based on the bosonization method, we obtain the generalized analytical form of the correlation function. We show that, in the proximity to the gapped charge-ordered phase, the correlation function exhibits anomalous crossover between the pure power-law behavior and the power-law behavior with logarithmic corrections, depending on the length scale. Such a crossover is also confirmed by the highly-accurate numerical density-matrix renormalization group method.

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I. INTRODUCTION

One-dimensional (1D) electron and spin systems have been attracted much attention since they often exhibit nontrivial quasi-long-range-ordered behavior due to the large low-dimensional quantum fluctuation effects. The critical behavior in the 1D systems, which is called the Tomonaga-Luttinger liquid (TLL) state, has a long history of research and the low-lying modes are known to be described by collective gapless excitations and physical quantities show power-law behavior in the temperature and/or distance dependences. It has also been recognized that, in the systems with spin-rotational symmetry, logarithmic singularities appear in the magnetic-field-dependent corrections to the magnetization and the spin susceptibility and in the temperature-dependent corrections to the spin susceptibility, specific heat, and nuclear magnetic resonance etc. Motivated by such developments in the field, a number of numerical studies has been successfully performed to examine the logarithmic corrections in spin-chain systems. The spin-spin correlation function of the 1D $S = \frac{1}{2}$ Heisenberg model has been extensively studied as a most fundamental theoretical model to examine the presence of logarithmic corrections. At this moment, the correlation amplitudes in the asymptotic form of the correlation function can be exactly obtained. In contrast, only few efforts have been devoted to those of the Hubbard model due in part to the difficulty of analyzing. Therefore, the situation is much less satisfactory as far as the logarithmic corrections in the Hubbard model are concerned.

In the present paper, we focus on the logarithmic corrections in the equal-time density-density correlation function of the quarter-filled Hubbard model including the Coulomb repulsion between electrons on site $U$ and the nearest-neighbor sites $V$. So far this model has been analyzed as a minimal model to describe physical phenomena in organic solids. The Hamiltonian of the 1D extended Hubbard model at quarter-filling is given by

\[ H = -t \sum_{j,s} \left( c_{j,s}^\dagger c_{j+1,s} + H.c. \right) + U \sum_j n_{j,\uparrow} n_{j,\downarrow} + V \sum_j n_j n_{j+1}, \]

where $c_{j,s}$ is the annihilation operator on the $j$th site with spin $s(=\uparrow, \downarrow)$, and the density operators are $n_j = n_{j,\uparrow} + n_{j,\downarrow}$ and $n_{j,s} \equiv c_{j,s}^\dagger c_{j,s} = c_{j,s}^\dagger c_{j,s} - \frac{1}{2}$. The hopping energy between the nearest-neighbor sites is represented by $t$. It is known that, at zero temperature, the gapped charge-ordered (CO) state emerges in the large repulsive $U$ and $V$ region, where the phase boundary is determined numerically by using the exact diagonalization and the highly-accurate density-matrix renormalization group (DMRG) method. The mechanism of this quantum phase transition has also been addressed by the bosonization technique and the renormalization-group (RG) method. In this paper, we perform the detailed analysis on the equal-time correlation function $N(x) \equiv \langle n_j n_{j+x} \rangle$ in the TLL phase. The exponent of the correlation functions is characterized by so-called the TLL parameter $K_\rho$. Especially by focusing on the correlation function near the boundary to the CO insulating state, we show that it exhibits the nontrivial crossover, depending on the length scale, from the power-law behavior with logarithmic correction for short distance, to the pure power-law behavior for large distance.

The present paper is organized as follows. In Sec. II, the analytical form of the correlation function is obtained by utilizing the RG technique based on the bosonization method. In Sec. III, the analytical results are confirmed by using the highly-accurate DMRG method. The summary is given in Sec. IV. Detailed derivation of the analytical form of the correlation function is given in the Appendix.
II. BOSONIZATION APPROACH

In this section, we derive the generalized analytical form of the correlation function in the TLL state. We analyze the $U \to \infty$ limit case and the finite $U$ case separately, since the picture of the $U \to \infty$ can become transparent with the analogy of the spin-chain system which properties are well understood.

A. The $U \to \infty$ limit

In the $U \to \infty$ limit, since the double occupancy of electrons is excluded, the extended Hubbard model [Eq. (1)] reduces to the spinless half-filled model:

$$H_{U \to \infty} = -t \sum_j \left( d_j^d d_{j+1} + \text{H.c.} \right) + V \sum_j n_j^d n_{j+1}^d,$$

where $n_j^d = d_j^d d_j^\dagger$. It is well known that this model can be mapped onto the XXZ spin-chain model by using the Jordan-Wigner transformation and the physical properties have been extensively studied with both the exact treatment based on the Bethe ansatz and numerical approaches. Here we examine the analytical form of the correlation function by using the exact results obtained in the context of spin-chain problems.

The density operator is expressed in terms of the bosonic field operator $\varphi$ [16,31]

$$\rho(x) = \frac{n_j^d}{a} = \frac{1}{2\pi \eta} \frac{d\varphi}{dx} - \frac{(-1)^j}{\pi a} \sin \left( \frac{2\pi}{\eta} \varphi \right),$$

where $a$ is the lattice constant and we will set $a = 1$ in the following. The parameter $\eta$ can be related to the TLL parameter by $K_\rho = 1/(4\eta)$. The nonuniversal parameter $c$ will be shown later. The model Hamiltonian (2) can be expressed in terms of the bosonic field $\varphi$.

$$c(\eta) = 2 \left[ \frac{\Gamma(\eta/(2-2\eta))}{2\sqrt{\pi} \Gamma(1/(2-2\eta))} \right]^{1/2\eta} \exp \left[ \frac{1}{2} \int_0^\infty \frac{dt}{t} \left( \frac{\sinh(2\eta t - 1)}{\sinh(\eta t)} \cosh(1-\eta t) \right) - \frac{2\eta - 1}{\eta} e^{-2t} \right].$$

The numerical values of $A_2$ are shown in Table I. For $(U, V) = (\infty, 0)$, the quantity $c(\eta)$ becomes $c(\eta = 1/2) = 1$. We note here that the quantity $\alpha$ in Eq. (4) is the only unknown parameter, which is to be determined numerically.

Here we find that equation (4) has two different asymptotics: (i) In the short-range region, the power-law behavior with logarithmic correction is obtained, while (ii) the logarithmic correction disappears in the long-range region. By noting $(x/\alpha)^{-(8K_\rho - 2)} = \exp[-(8K_\rho - 2) \ln(x/\alpha)]$, the length scale $x_{\text{cross}}$ which characterizes crossover between these two regions is given by

$$x_{\text{cross}} = \alpha \exp[1/(8K_\rho - 2)].$$

We note that, for $V = V_c (= 2t)$, the logarithmic correction appears in the whole length scale. By noting $A_2 \to (2 - V/t)^{-1/4}/(\sqrt{2\pi})$ for $V \to V_c$, the explicit form of the correlation function (4) at $V = 2t$ is given by

$$N(x) = -\frac{1}{4\pi^2 x^2} + \frac{1}{(2\pi)^{3/2}} \frac{\cos 4k_F x}{x} \ln^{1/2}(x/\alpha)$$

for $(U, V) = (\infty, 2t).$
This formula was reported in Ref. [32] for the $S = \frac{1}{2}$ antiferromagnetic Heisenberg spin chain.

**B. For finite $U$**

Next we examine the generic $0 < U \neq \infty$ case. In this case, there appears the conventional $2k_F$ oscillation term in addition to the $4k_F$ one. We show that the additional logarithmic correction appears near the phase boundary to the CO phase, not only in the $4k_F$ oscillation term but in the $2k_F$ oscillation term.

Based on the conventional bosonization for electron systems, the density operator is given by

$$\rho(x) = \frac{1}{\pi} \frac{d\phi_\sigma}{dx} \sin(2k_Fx + \phi_\rho) \cos \phi_\sigma + \frac{2c_1}{\pi} \cos(4k_Fx + 2\phi_\rho), \quad (8)$$

where $\phi_\rho$ and $\phi_\sigma$ are the charge and spin phase fields. The $c_1$ and $c_2$ are nonuniversal numerical quantities satisfying $c_1 = 1$ and $c_2 = 0$ in the noninteracting case. In the similar way to the $U = \infty$ case, the most general form of the density-density correlation function is derived as (see Appendix)

$$N(x) = -\frac{1}{4\pi^2x^2} + \tilde{A}_1 \frac{\cos 2k_Fx}{x^{5/4}} \ln^{-3/2}(x/\alpha_\rho) \ln^{-1/8}(x/\alpha_\sigma) + \tilde{A}_2 \frac{\cos 4k_Fx}{x^{3/2}} \frac{1}{\ln(1 + (\alpha/x)^2 - 2k_F^2 \sigma/\alpha_\sigma)^{1/2}} \frac{1}{\ln(1 + (\alpha/x)^2 - 2k_F^2 \rho/\alpha_\rho)^{1/2}}, \quad (9)$$

where $\alpha_\rho$ and $\alpha_\sigma$ are the short-distance cutoff parameters for the charge and spin sectors, respectively. In the case of $U \neq \infty$, the coefficients $A_1$ and $A_2$, which are proportional to $c_1^2$ and $c_2^2$ respectively, are to be determined numerically. The logarithmic correction $\ln^{-3/2}(x/\alpha_\rho)$ in the $2k_F$ oscillating term appears due to the marginally irrelevant coupling of the spin channel. In the noninteracting limit $U = V = 0$, the quantity $A_2$ vanishes and the logarithmic correction $\ln^{-3/2}(x/\alpha_\rho)$ is replaced by a constant, and then the correlation function reproduces the trivial result $N(x) = -1/(\pi^2x^2) + \cos 2k_Fx/\alpha_\rho^2$.

From Eq. (9), we find that an anomalous logarithmic correction also appears in the $2k_F$ oscillating term near the boundary of the CO phase. On the phase boundary, the correlation function reads

$$N(x) = -\frac{1}{4\pi^2x^2} + \tilde{A}_1 \frac{\cos 2k_Fx}{x^{5/4}} \ln^{-3/2}(x/\alpha_\rho) \ln^{-1/8}(x/\alpha_\sigma) + \tilde{A}_2 \frac{\cos 4k_Fx}{(2\pi)^{3/2}} \ln^{-1/2}(x/\alpha_\rho)$$

for $(U, V) = (U_c, V_c)$ \quad (10)

where $\tilde{A}_1 \to 0$ and $\tilde{A}_2 \to 1$ for $(U_c, V_c) \to (\infty, 2)$.

### III. NUMERICAL RESULTS

For numerical confirmation of the logarithmic corrections, we employ the DMRG technique which provides very accurate data for the ground-state correlation functions of 1D correlated electron systems.\(^{33}\) We consider $L/2$ electrons on a chain with $L$ sites and calculate the equal-time density-density correlation function

$$N(x) = \langle n_j n_{j+x} \rangle - \langle n_j \rangle \langle n_{j+x} \rangle, \quad (11)$$

under the open-end boundary conditions (OBC). Here, the distance $x$ is centered at the middle of the system. The application of OBC enables us to obtain the correlation function \(^{(11)}\) quite accurately for very large finite-size systems up to $\sim O(1000)$ sites. However, the real-space DMRG method works with finite number of sites, so that we have to pay special attention to the finite-size effects for a precise comparison with the RG results. In the present calculations, the most problematic finite-size effect is the Friedel oscillation starting from the open edges. To eliminate it, we simply add on-site potential energy $V/2$ on both edge sites. It corresponds to a compensation of the “missing correlation” caused by the absence of their neighboring site. Hereby the Friedel oscillation is fairly suppressed.

On that basis, the remaining finite-size effects are investigated. We now choose some parameters in the vicinity of the CO phase where the finite-size effect is relatively large due to strong charge fluctuations. For these parameters, we calculate $N(x)$ for several chains with length up to $L = 1024$ sites and then obtain the extrapolated values to the thermodynamic limit ($L \to \infty$) using the finite-size-scaling analysis. By comparing the extrapolated values and the finite-size data, we find that $N(x \leq 200)$ in the thermodynamic limit can be
reproduced with extracted central 200 sites of a chain with $L = 512$ sites within a few percent error. The relative error in the ground-state energy, $\left| e(\infty) - e(512) \right| / e(\infty)$, is below 0.1%, where $e(L)$ is the ground-state energy per site for a chain with $L$ sites. Consequently, we will study the equal-time correlation function $N(x)$ for the central 200 sites of a chain with $L = 512$ sites without the finite-size-scaling analysis. We keep up to $m \approx 4000$ density-matrix eigenstates in the DMRG procedure and all the calculated quantities are extrapolated to the $m \to \infty$ limit. For your information, in this way we obtain $(A_1, A_2) = (0.991, -0.0003)$ [the exact are $(A_1, A_2) = (1, 0)$] for the coefficients of Eq. (9) in the non-interacting case $U = V = 0$ which poses a non-trivial problem to the DMRG method.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{(Color online) (a) DMRG results of the correlation function $N(x)$ for $(U, V) = (\infty, 1.95t)$. The solid line denotes a fitting with Eq. (4). Inset: $|N(x)|$ plotted on a log-log scale. (b) Estimated length scale of the logarithmic correction $x_{\text{cross}}$ as a function of $V/t$ for $U = \infty$.}
\end{figure}

A. The $U \to \infty$ limit

Let us first consider the correlation function $N(x)$ in the $U \to \infty$ limit. We now attempt to fit the DMRG results of $N(x)$ into the analytical form of Eq. (4). Since the exact solutions of $A_2$ and $K_\rho$ are available, the quantity $\alpha$ is the only fitting parameter in Eq. (4). Figure 1(a) shows the DMRG results of $N(x)$ for $(U, V) = (\infty, 1.95t)$. An excellent agreement of the DMRG data with the fitted line is found. We then obtain $\alpha = 0.0515$, which leads to $x_{\text{cross}} = 34.8$. It means that the logarithmic correction appears at $x \gtrsim 35$ for $V = 1.95t$. We note that the central 200 sites out of $L = 512$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{(Color online) DMRG results of the correlation function $N(x)$ for several sets of $(U, V)$. The solid lines denote fitting curves with Eq. (9). The estimated values of $x_{\text{cross}}$ and $K_\rho$ are also included.}
\end{figure}

B. For finite $U$

We next turn to the case of $U \neq \infty$. In this case, the numerical results of the correlation function $N(x)$ can be fitted with the analytical form of Eq. (9). Differently from the case of $U = \infty$, there are five fitting parameters; namely, $\alpha$, $\alpha_\sigma$, $A_1$, $A_2$, and $K_\rho$. Of them, $K_\rho$ may be obtained very accurately with the DMRG method via the derivative of charge structure factor at $q = 0$,

$$K_\rho = \frac{1}{2} \lim_{q \to 0} \langle n(q) n(-q) \rangle,$$

(12)
with \( q = 2\pi /L \) and \( n(q) = \sum_{\ell,s} e^{-iql} c_{\ell,s}^\dagger c_{\ell,s} \). Thus, we can reduce the fitting parameters from five to four. In Fig. 2, we show the fitting results of the correlation function \( \langle N(x) \rangle \) near the boundary of the CO phase for \( U = 5t \) and \( 10t \) [the critical boundary has been estimated as \( V_c \approx 3.70t \) (2.76\( t \)) for \( U = 5t \) (10\( t \))] in Ref. [28]. We can see that the DMRG data is in good agreement with the fitted line for all the parameter sets. From the obtained results of \( x_{\text{cross}} \), we find that the logarithmic correction appears for \( (U, V) = (5t, 3.5t) \) and \( (10t, 2.5t) \). Especially at \((U, V) = (5t, 3.5t)\), the length scale is extremely large \( x_{\text{cross}} \approx 1600\); it allows us to crossly notice that this point is very close to the boundary of the CO phase. Meanwhile, the logarithmic correction is hardly present for \( (U, V) = (5t, 3t) \) and \((10t, 2t)\). As a result, we confirm that the logarithmic correction is present also for \( U \neq \infty \) and its length scale grows rapidly near the CO phase boundary.

Finally, we discuss the correlation amplitudes, \( A_1 \) and \( A_2 \), of Eqs. (4) and (9). Figure 3 shows the DMRG results of the amplitude \( A_2 \) as a function of \( V/t \) for several values of \( U/t \). In the \( U = \infty \) limit, we can see an excellent agreement between the DMRG and exact results. We also find a very sharp increase near \( V = V_c = 2t \). For \( U = 5t \), the behavior of \( A_2 \) seems to be quite similar to that for \( U = \infty \); while, the amplitude \( A_1 \) is rapidly decreased near \( V = 3.70t \), e.g., \( A_1 \lesssim 10^{-2} \) at \( V \gtrsim 3 \). Thus, the \( 2k_F \) oscillating term would be negligible in the vicinity of the CO phase. When \( U = t \), the amplitude \( A_2 \) decreases with increasing \( V/t \) in reflecting that the \( 4k_F \) fluctuation is not enhanced by \( V \). We note that the two amplitudes \( A_1 \) and \( A_2 \) are rather small with the same order of magnitude for small \( U \) and larger \( V \) values.

IV. SUMMARY

We study the density-density correlation function in the TLL state for the 1D extended Hubbard model at quarter filling. Based on the bosonization and RG techniques, we obtain the generalized analytical form of the correlation function which exhibits anomalous power-law behavior with logarithmic corrections near the phase boundary to the CO insulating state. Using the DMRG method, we confirm the appearance of the logarithmic corrections not only in the \( U = \infty \) limit but also for finite \( U \). Moreover, we find that the length scale of the corrections grows rapidly near the CO phase boundary.

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APPENDIX A: DERIVATION OF THE ANALYTICAL FORM OF THE CORRELATION FUNCTION

In this appendix, we derive the generalized form of the correlation function [Eqs. (4) and (9)] based on the RG approach. In our derivation, we follow the formalism of the RG method developed in Ref. [30].

The RG equations for the TLL parameter \( K_\rho(l) \) and the 1/4-filled umklapp scattering \( G_u(l) \) are given by

\[
\frac{d}{dl} K_\rho(l) = -2G_u^2(l) K_\rho^2(l), \quad (A1a)
\]

\[
\frac{d}{dl} G_u(l) = [2 - 8K_\rho(l)]G_u(l), \quad (A1b)
\]

where the initial values are estimated based on the perturbative treatment in Ref. [30]. The TLL parameter in the low-energy effective theory can be evaluated from the fixed point value of \( K_\rho(l) \), i.e., \( K_\rho = K_\rho(\infty) \). The correlation functions for the \( 2k_F \) and \( 4k_F \) oscillation parts, defined as \( C_{2k_F}(x - x') \equiv 2(\sin(2k_F x + \phi_\rho(x)) \sin(2k_F x' + \phi_\rho(x'))) / \cos(2k_F(x-x')) \) and \( C_{4k_F}(x - x') \equiv 2(\cos(4k_F x + \phi_\rho(x)) \sin(2k_F x') + \phi_\rho(x')) / \cos(2k_F(x-x')) \), respectively, are given in the RG scheme by

\[
C_{2k_F}(x) = \exp \left[ - \int_0^{\ln(x/\alpha_0)} dlK_\rho(l) \right], \quad (A2a)
\]

\[
C_{4k_F}(x) = \exp \left[ - \int_0^{\ln(x/\alpha_0)} dl(4K_\rho(l) - 2G_u(l)) \right], \quad (A2b)
\]

where \( \alpha_0 \) is the short-distance cutoff. The couplings \( K_\rho(l) \) and \( G_u(l) \) are determined by solving Eq. (A1).

From Eq. (A1), we find that the fixed point values are given by \((K_\rho(\infty), G_u(\infty)) = (\frac{1}{2}, 0)\) on the phase boundary between the TLL and CO states. Near this phase boundary, the TLL parameter can be expanded as \( K_\rho(l) = \frac{1}{2} + \frac{1}{4}G_u(l) \), and we can treat \( G_u(l) \) perturbatively. Up to the second order in \( G_u(l) \) and \( G_u(l) \), the RG equations (A1) are rewritten as

\[
\frac{d}{dl} G_u(l) = -2G_u^2(l), \quad \frac{d}{dl} G_u(l) = -2G_u(l)G_u(l). \quad (A3)
\]

In the case of \( G_u(0) > |G_u(0)| \), the umklapp scattering \( G_u(l) \) flows to zero, i.e., is irrelevant, and \( G_u(l) \) has a finite fixed
point $G_\rho(\infty) \geq 0$. Thus the TLL parameter in the low-energy limit is given by $K_\rho = \frac{1}{4} + \frac{1}{4} G_\rho(\infty)$. The explicit solutions of Eq. (A3) are given by

$$G_\rho(l) = \frac{\theta}{2} \coth \left[ \theta l + \tanh^{-1}(\theta/2G_\rho(0)) \right], \quad (A4a)$$

$$G_u(l) = \frac{\theta}{2} \coth \left[ \theta l + \tanh^{-1}(\theta/2G_\rho(0)) \right], \quad (A4b)$$

where $\theta \equiv 2(G^2_u - G^2_\rho)^{1/2}$ is a scaling invariant quantity. Near the phase boundary, i.e., for small $\theta$, the umklapp scattering $G_u(l)$ approaches to zero very slowly as increasing $l$. By substituting Eq. (A4) into Eq. (A2), we obtain the analytical form of the correlation functions:

$$C_{2k_F}(x) = \left( \frac{\alpha_0}{x} \right)^{1/4 + \theta/8} \left( \frac{1 - d^{2\theta}}{1 - (d\alpha_0/x)^{2\theta}} \right)^{1/8}, \quad (A5)$$

$$C_{4k_F}(x) = \left( \frac{\alpha_0}{x} \right)^{1 + \theta/2} \left( \frac{1 + d^{\theta}}{1 + (d\alpha_0/x)^{\theta}} \right)^{3/2} \times \left( \frac{1 - (d\alpha_0/x)^{\theta}}{1 - d^{\theta}} \right)^{1/2}, \quad (A6)$$

where $d$ is the nonuniversal quantity depending on the initial values of RG equations, defined by $d \equiv \exp[-\theta^{-1} \tanh^{-1}(\theta/2G_\rho(0))]$. In terms of $K_\rho$, the parameter $\theta$ is given by $\theta = (8K_\rho - 2)$. By defining $\alpha \equiv d\alpha_0$ we can derive Eqs. (4) and (9).

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