Luttinger-liquid Parameter of Hubbard Chain and Hubbard Ladder

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(Received )

We study the Luttinger-liquid parameter $K_\rho$ of the Hubbard chain and the Hubbard ladder models by the ordinary perturbation method combined with the Luttinger-liquid relation. According to the Luttinger-liquid relation, the critical exponent $K_\rho$ is related to the charge susceptibility $\chi$ and the Drude weight $D$ by

$$ K_\rho = \frac{1}{2}(\pi \chi D)^{1/2}, $$

(1)

with

$$ \chi^{-1} = \frac{1}{N} \frac{\partial^2 E_g(n)}{\partial n^2}, \quad D = \frac{\pi}{N} \frac{\partial^2 E_g(\phi)}{\partial \phi^2}, $$

(2)

where $N$ is the number of lattice site, $n$ is electron density and $E_g$ is the total energy of the ground state as a function of $n$ and a magnetic flux $\phi$. If we calculate the ground state energy in some way, we can obtain $K_\rho$ through $\chi$ and $D$.

We apply the ordinary perturbation expansion in powers of $U$ to $E_g$,

$$ E_g = E_0 + e_1 + e_2 + \ldots, $$

where $E_0$ is the ground state energy of the non-interacting system and $e_i \ (i=1,2,\ldots)$ is the $i$-th order correction of $E_g$. According to the perturbation expansion of $E_g$, $\chi^{-1}$ and $D$ are given by

$$ \chi^{-1} = \chi_0^{-1} + x_1 U + x_2 U^2 + \ldots, \quad D = D_0 + d_1 U + d_2 U^2 + \ldots, $$

where $\chi_0^{-1}$ and $D_0 = 4\chi_0^{-1}/\pi$ are the inverse charge susceptibility and the Drude weight of the non-interacting system respectively. Coefficients $x_i$ and $d_i \ (i=1,2,\ldots)$ are the $i$-th order corrections of $\chi^{-1}$ and $D$, which are determined by the second differential coefficients of $e_i$ with respect to $n$ and $\phi$ respectively. In the Hubbard model, the first-order term $e_1$ is easily obtained as $e_1 = U \sum_i < n_i \uparrow > < n_i \downarrow > = UNn^2/4$. It leads

KEYWORDS: Luttinger-liquid, perturbation, Hubbard Ladder, superconductivity

§1. Introduction

Low-dimensional strongly correlated electron systems have been investigated extensively due to the possible relevance to high-temperature superconductivity. In particular, One-dimensional (1D) Hubbard-like models provide an important ground for understanding electron-correlation effects. It is well known that a single Hubbard chain has generic properties of Luttinger liquid state with gapless spin and charge modes for repulsive interaction. For attractive interaction, a superconducting state characterized by dominant paring correlations with a spin gap is realized.

Recently, weak coupling theory has been applied to the problem of ladder models, which are interesting as a first step towards 2D systems and may be relevant for some materials. The theory reveals that the systems remain typical non-Fermi-liquid properties as 1D electronic systems. At half-filling, they are Mott insulators, exhibiting gaps to all excitations. Upon doping, the gaps survive except one gapless charge mode and a superconducting (SC) paring characterized slowly power-low decay appears. According to the Luttinger-liquid theory, critical exponents of various types of correlation functions are determined by a single parameter $K_\rho$. It is predicted that the SC correlation function of ladder systems is dominant for $K_\rho > 0.5$ at lightly doping. It decays as $r^{-\rho (2\pi K_\rho)}$, whereas the “4kF” charge density wave (CDW) correlation function decays as $r^{-2K_\rho}$. The spin density wave (SDW) and “2kF” CDW correlation functions decay exponentially.

In spite of the good understanding of the single Hubbard chain which is exactly solved by the Bethe ansatz method, Hubbard ladder models are much less known. In fact, systematic treatment of $K_\rho$ as a function of interaction $U$ is not yet obtained. In this work we propose a simple method for calculating the Luttinger-liquid parameter $K_\rho$. It is the first and second-order perturbation expansion with respect to $U$ combined with the Luttinger-liquid relation. These results are compared with the Bethe ansatz and the numerical diagonalization results.

§2. Perturbation expansion of $K_\rho$

In the Luttinger liquid theory, some relations have been established as universal relations in one-dimensional models. The critical exponent $K_\rho$ is related to the charge susceptibility $\chi$ and the Drude weight $D$ by

$$ K_\rho = \frac{1}{2}(\pi \chi D)^{1/2}, $$

(1)

with

$$ \chi^{-1} = \frac{1}{N} \frac{\partial^2 E_g(n)}{\partial n^2}, \quad D = \frac{\pi}{N} \frac{\partial^2 E_g(\phi)}{\partial \phi^2}, $$

(2)

where $N$ is the number of lattice site, $n$ is electron density and $E_g$ is the total energy of the ground state as a function of $n$ and a magnetic flux $\phi$. If we calculate the ground state energy in some way, we can obtain $K_\rho$ through $\chi$ and $D$.

We apply the ordinary perturbation expansion in powers of $U$ to $E_g$,

$$ E_g = E_0 + e_1 + e_2 + \ldots, $$

where $E_0$ is the ground state energy of the non-interacting system and $e_i \ (i=1,2,\ldots)$ is the $i$-th order correction of $E_g$. According to the perturbation expansion of $E_g$, $\chi^{-1}$ and $D$ are given by

$$ \chi^{-1} = \chi_0^{-1} + x_1 U + x_2 U^2 + \ldots, \quad D = D_0 + d_1 U + d_2 U^2 + \ldots, $$

where $\chi_0^{-1}$ and $D_0 = 4\chi_0^{-1}/\pi$ are the inverse charge susceptibility and the Drude weight of the non-interacting system respectively. Coefficients $x_i$ and $d_i \ (i=1,2,\ldots)$ are the $i$-th order corrections of $\chi^{-1}$ and $D$, which are determined by the second differential coefficients of $e_i$ with respect to $n$ and $\phi$ respectively. In the Hubbard model, the first-order term $e_1$ is easily obtained as $e_1 = U \sum_i < n_i \uparrow > < n_i \downarrow > = UNn^2/4$. It leads
$x_1 = 1/2$ and $d_1 = 0$, where $e_1$ is independent of the flux $\phi$.

Substituting these values into eq. (1), we obtain $K_\rho$ within the first perturbation expansion:

$$1/K_\rho^2 \simeq 1 + \frac{\chi_0}{2} U.$$  \hspace{1cm} (3)

It shows that $K_\rho$ generally decreases with increasing the repulsive interaction $U$ in the weak coupling limit. It is noted that this approximation is equivalent to the Hartree-Fock (HF) approximation. The second-order term of the ground state energy $e_2$ is also easily obtained as

$$e_2 = \frac{U^2}{N} \sum_{k_1, k_2, q, \sigma} \frac{f(k_1) f(k_2) (1 - f(k_1 + q)) (1 - f(k_2 - q))}{\varepsilon(k_1) + \varepsilon(k_2) - \varepsilon(k_1 + q) + \varepsilon(k_2 - q)},$$

where $\varepsilon(k)$ is the non-interacting band and $f(k) = \theta(k_F - |k|)$. Using $e_2$, we can calculate $K_\rho$ up to order $U^2$ by

$$1/K_\rho^2 \simeq 1 + \frac{\chi_0}{2} U + (x_2 - \frac{\pi}{4} d_2) \chi_0 U^2,$$  \hspace{1cm} (4)

with

$$x_2 = \frac{1}{NU^2} \frac{\partial^2 e_2}{\partial n^2}, \quad d_2 = \frac{\pi}{NU^2} \frac{\partial^2 e_2}{\partial \phi^2}.$$  

In the following section, we will estimate the above integral and obtain $x_2$ and $d_2$ numerically.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\columnwidth]{fig1.png}
\caption{The coefficients of the second-order terms $x_2$ and $d_2$ as a function of $n$. The broken line represents $(x_2 - \frac{\pi}{4} d_2)$. The inset shows the ground state energy of the system as a function of $U$ by the first-order and the second-order perturbation calculation with the exact result at quarter-filling.}
\end{figure}

\section{Hubbard chain and Hubbard ladder}

At first, we examine the Hubbard chain model whose non-interacting band is given by $\varepsilon(k) = -2t \cos k$. In this case, we have $\chi_0^{-1} = \pi t \sin k_F$ and $K_\rho$ up to the first-order expansion of $U$

$$1/K_\rho^2 = 1 + U/2\pi t \sin k_F,$$  \hspace{1cm} (5)

where $k_F = \frac{2}{\pi} n$ is the Fermi wave number. This expression of $K_\rho$ is exactly equal to the result of bosonization method for the Hubbard chain.\(\blacksquare\)

To estimate $e_2$, we use $N = 200$ and 400 sites systems. We confirm that the size dependence of $x_2$ and $d_2$ are very small and negligible. In Fig.1, we show $x_2$ and $d_2$ as a function of $n$. These values seem to diverge at the limit $n \to 1$. It might reflect the insulator transition of the Hubbard chain at half-filling. We also show the ground state energy $E_g/N$ as a function of $U$ at quarter-filling. The result of $E_g/N$ is consistent with the exact result in the weak coupling region. In Figs.2(a) and (b), we show $K_\rho$ by the perturbation expansion with the ex-

\begin{figure}[h]
\centering
\includegraphics[width=0.4\columnwidth]{fig2.png}
\caption{$K_\rho$ as a function of $n$ by (a) the first-order and (b) the second-order perturbation expansion (b) with the exact result of the Bethe ansatz. The solid lines represent the results of the Bethe ansatz and the broken lines are that of the perturbation expansion.}
\end{figure}
act result of the Bethe ansatz. They show that the result of the perturbation expansion is consistent with the exact result in the weak coupling region. It also indicates that the second-order perturbation calculation agrees with the exact solution more than the first-order calculation in the weak coupling regime. In the strong coupling regime, \( K_\rho \) of the first-order calculation seems to be close to that of the exact solution at \( n \sim 0.4 \). However, it may be an accidental.

Next, we consider the Hubbard ladder Hamiltonian

\[
H = -t_l \sum_{i,\alpha,\sigma} \epsilon_{i,\alpha,\sigma} c_{i+1,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma} - t_r \sum_{i,\sigma} \epsilon_{i,\alpha,\sigma} c_{i+1,\alpha,\sigma} + h.c. + U \sum_{i,\sigma} n_{i,\alpha} \frac{\sigma}{2} n_{i,\alpha} \tag{6}
\]

where \( c_{i,\alpha,\sigma}^\dagger \) stands for a creation operator of an electron with spin \( \sigma \) at site \((i, \alpha)\) and \( U \) is the on-site interaction. Here, \( \alpha (= 1, 2) \) denotes legs and \( i \) is rung. In this case, non-interacting band is written as

\[ \epsilon^\pm(k) = -2t_l \cos k \pm t_r, \]

where \( \epsilon^+(k) (\epsilon^-(k)) \) represents the upper (lower) band and \( k \) is the wave vector. If we define \( k_{F-} (k_{F+}) \) as a Fermi point in the lower (upper) band, we find that \( \epsilon^-(k_{F-}) = \epsilon^+(k_{F+}) \) with \( k_{F-} + k_{F+} = k_F = n\pi \). The differential coefficient of \( \epsilon^-(k_{F-}) \) with respect to \( n \) leads the inverse charge susceptibility \( \chi^0 \). After a bit of calculation, we get

\[
\chi^0 = -t_l \pi \sin k_F \left\{ \frac{\cos k_F (1 - \cos k_F) + (t_r/t_l)^2 - \sin^2 k_F}{(1 - \cos k_F)^2} \right\} \times \left\{ (t_r/t_l)^2 - 2 \frac{\sin^2 k_F}{1 - \cos k_F} \right\}^{-1/2}.
\]

Substituting \( \chi^0 \) to eq.(3), we have \( K_\rho \) of the Hubbard ladder model analytically within the first-order perturbation methods.

When \( n \) is smaller than \( n_c \) which is determined by \( \epsilon^+(0) = \epsilon^-(\frac{\pi}{2n_c}) \), electrons are filled only in the lower band. The density of state of the lower band is a half of that of the chain model. Then, \( \chi_0 \) is given by \( 1/(2\pi \sin k_F) \) which is a half of that of the chain model. Within the first-order perturbation calculation, the upper band is irrelevant and the correction of \( K_\rho \) becomes a half of that of the chain model.

As well as the Hubbard chain model, we estimate the second-order terms \( \epsilon_2, x_2 \) and \( d_2 \) numerically. In Fig.3, we show \( x_2, d_2 \) and \( x_2 = \frac{1}{2} d_2 \) as a function of \( n \) at \( t_r/t_l = 1.0 \). For \( n > n_c = 0.5 \), the values of \( x_2 \) seem to be small, but the absolute values of \( d_2 \) are large. It shows that the values \( x_2 = \frac{1}{2} d_2 \) are positive and large. It indicates that the second-order term of the repulsion \( U \) reduces \( K_\rho \) as well as the first-order term. This result does not contradict the behavior of the SC correlation shown by the numerical diagonalization method. Figure 4 indicates \( K_\rho \) as a function of \( n \) at \( t_l/t_r = 1.0 \) by the first- and the second-order perturbation calculation.

On the other hand, for \( n < 0.5 \), the values \( x_2 = \frac{1}{2} d_2 \) are negative. In particular, the absolute values are very large near \( n = 0.5 \). It indicates that \( K_\rho \) is enhanced by the second-order term. In contrast to the case for \( n > 0.5 \), the existence of the upper band seems to produce an effective attraction in the second-order correction. This result may consist with an enhancement of the SC correlation shown by the numerical diagonalization method. Figure 4 indicates \( K_\rho \) as a function of \( n \) at \( t_l/t_r = 1.0 \) by the first- and the second-order perturbation calculation.

To clarify the validity of the perturbation expansion of \( K_\rho \), we examine a finite size system of the ladder model. We numerically diagonalize the Hamiltonian of 14 sites (7 unit cells) system by using the Lanczos algorithm.
We use the periodic boundary condition for $N_c = 8$, the Moebius boundary condition for $N_c = 10$ and the antiperiodic boundary condition for $N_c = 12$, where $N_c$ is the total electron number. This choice of the boundary condition gives either fully occupied or empty single particle orbitals (closed shell) and removes accidental degeneracy in the non-interacting case. The uniform charge susceptibility $\chi_c$ and the Drude weight $D$ is calculated from the ground state energy with the usual method.

In Fig.5, we show $K_\rho$ of the finite size system for the Hubbard ladder as a function of $U$. The solid circles represent the result of the numerical diagonalization for 7 rungs system at $t_e/t_l = 0.6$. The broken line represents the result of the first-order perturbation expansion and the dashed line is that of the second-order perturbation expansion. The inset shows the ground state energy of the system as a function of $U$ by the first-order and the second-order perturbation calculations with the result of the numerical diagonalization.

Fig. 5. $K_\rho$ of the finite size system for the Hubbard ladder as a function of $U$. The solid circles represent the result of the numerical diagonalization for 7 rungs system at $t_e/t_l = 0.6$. The broken line represents the result of the first-order perturbation expansion and the dashed line is that of the second-order perturbation expansion. The inset shows the ground state energy of the system as a function of $U$ by the first-order and the second-order perturbation calculations with the result of the numerical diagonalization.

§4 Summary and discussion

In this work we examine the Luttinger-liquid parameter $K_\rho$ of the Hubbard chain and the Hubbard ladder models by the ordinary perturbation method combined with the Luttinger-liquid relation. According to the Luttinger-liquid relation, we obtain $K_\rho$ at the first-order analytically and up to the second-order numerically. Comparing $K_\rho$ with the exact result of Bethe ansatz and that of the numerical diagonalization method, we show that the analysis of perturbation method is reliable in the weak coupling region.

Generally speaking, the validity of the perturbation expansion is not always obvious in 1D electron systems. However, it has been analytically shown that the ordinary perturbation expansion of the ground state energy of the Hubbard chain agrees with the expansion of the exact Bethe ansatz solution at half-filling. Although the convergence radius is zero, the perturbation is possible as an asymptotic expansion.

Away from half-filling, the integral equations of the Bethe ansatz solution are not analytically solved. However, we confirm that $e_2$ consists with the second-order term of $U$ in the Bethe ansatz solution numerically. It suggests that the perturbation expansion in powers of $U$ is also possible as an asymptotic expansion.

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