Weak-Coupling Approach to Hole-Doped \( S = 1 \) Haldane Systems

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As a weak-coupling analogue of hole-doped \( S = 1 \) Haldane systems, we study two models for coupled chains via Hund coupling; coupled Hubbard chains, and a Hubbard chain coupled with an \( S = 1/2 \) Heisenberg chain. The fixed point properties of these models are investigated by using bosonization and renormalization group methods. The effect of randomness on these fixed points is also studied. It is found that the presence of the disorder parameter inherent in the Haldane state in the former model suppresses the Anderson localization for weak randomness, and stabilizes the Tomonaga-Luttinger liquid state with the spin gap.

The Heisenberg spin chain with integer spin shows a remarkable feature, so-called the Haldane gap. Recently, hole-doping into \( S = 1 \) Haldane gap systems was realized in \( \text{Y}_2\text{BaNiO}_4 \). It inspires theoretical interest in the effects of carrier-doping into Haldane systems, which have not been studied well so far. In this paper we consider weak-coupling models for hole-doped Haldane systems (HDHS); coupled Hubbard chains via Hund coupling (referred to as model I) and a Hubbard chain coupled with an \( S = 1/2 \) Heisenberg chain (model II). The model I corresponds to the case where the energy levels of electrons which compose the \( S = 1 \) state are almost degenerate, whereas the model II to the case where these levels are largely separated, and the lower level can be considered to be localized. Coupled chain problems have been studied extensively in several contexts. The model I is somehow related to the models studied in \( \text{Y}_2\text{BaNiO}_4 \), and the model II is the Kondo lattice model considered in with ferromagnetic coupling. Applying Abelian and non-Abelian bosonization methods, we investigate low-energy properties of these models, and find that they show quite different behaviors at the fixed points. We also study the effects of randomness on these fixed points, which may play a crucial role for HDHS because the hole-doping inevitably induces randomness to the system. By using replica trick and renormalization group analysis, we find that the quantum disordered state inherent in Haldane systems suppresses the Anderson localization for weak randomness.

We first consider the model I without randomness. The Hamiltonian is given by

\[
H = -t \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c. + U \sum_{i} c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \\
- \sum_{i} d_{i\sigma}^\dagger d_{i+1\sigma} + h.c. + U \sum_{i} d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} \\
+ J \sum_{i} \mathbf{S}_{c,i} \cdot \mathbf{S}_{d,i},
\]  

(1)

where \( c_{i,\sigma} \) and \( c_{i,\sigma}^\dagger \) etc., are the annihilation and creation operators of electrons, \( U \) is on-site coulomb interaction in each chain, and \( \mathbf{S}_{c,i} = c_{i,\alpha}^\dagger \sigma_{\alpha,\beta} c_{i,\beta} / 2 \) with the Pauli matrix \( \sigma \), etc. Here the last term is the Hund coupling interaction with \( J < 0 \). At half-filling, in the strong coupling limit \( J \to -\infty \), the model reduces to the \( S = 1 \) Heisenberg chain which possesses the Haldane gap. Even for small \( |J| \), the system has a finite gap, and belongs to the universality class of the Haldane state. We study low-energy properties of this model away from half-filling by applying standard Abelian bosonization methods. We first linearize the dispersion of electrons and express the electron operators in terms of boson fields \( \phi_{\sigma\alpha} \) and \( \theta_{\sigma\alpha} \), etc. which satisfy the commutation relation \( [\phi_{\sigma\alpha}(x), \theta_{\sigma\alpha}(x') \] = i\Theta(x - x') \)\(^4\). Introducing the boson fields, \( \phi_\pm = (\phi_\uparrow \pm \phi_\downarrow) / \sqrt{2} \) for the spin sector and \( \phi_\pm^{(c)} = (\phi_\uparrow^{(c)} \pm \phi_\downarrow^{(c)}) / \sqrt{2} \) for the charge sector where \( \phi_\alpha = (\phi_\uparrow^{(c)} - \phi_\downarrow^{(c)}) / \sqrt{2} \) and \( \phi_\uparrow^{(c)} = (\phi_\uparrow + \phi_\downarrow) / 2 \) with \( a = c, d \), and their canonical conjugate momenta \( \Pi_\pm \) and \( \Pi_\pm^{(c)} \), we can write down the bosonized Hamiltonian as

\[
H = H_c + H_s
\]

\[
H_c = \sum_{\nu = \pm, c} \int dx \left[ \frac{v_\nu^{(c)}}{2K_\nu} (\partial_x \phi_\nu^{(c)})^2 + \frac{v_\nu^{(c)} K_\nu^{(c)}}{2} \Pi_\nu^{(c)} \right]
\]

\[
H_s = \sum_{\nu = \pm, c} \int dx \left[ \frac{v_\nu}{2K_\nu} (\partial_x \phi_\nu)^2 + \frac{v_\nu K_\nu}{2} \Pi_\nu \right]
+ \frac{\text{const.}}{\alpha^2} \int dx |J_1 \cos \sqrt{4\pi} \phi_- \cos \sqrt{4\pi} \theta_- |
+ \frac{\text{const.}}{\alpha^2} \int dx |J_2 \cos \sqrt{4\pi} \phi_+ \cos \sqrt{4\pi} \theta_- |
+ \frac{\text{const.}}{\alpha^2} \int dx (J_3 \cos \sqrt{4\pi} \phi_+ + 2J_4 \cos \sqrt{4\pi} \theta_- )
+ \frac{\text{const.}}{\alpha^2} \int dx (J_5 \cos \sqrt{4\pi} \phi_+ \cos \sqrt{4\pi} \phi_- ),
\]  

(2)

where \( v_\nu^{(c)} \), \( v_\nu \), \( K_\nu^{(c)} \) and \( K_\nu \) are Luttinger liquid parameters in each sector. Here we dropped irrelevant terms with oscillating factors and irrelevant intra-chain backward scattering terms. We also omit Umklapp terms because we are concerned with the case away from half-filling. The charge mode, \( \phi_\uparrow^{(c)} \), is completely decoupled and hence it is described by \( U(1) \) Gaussian the-
ory with central charge $c = 1$ (Tomonaga-Luttinger liquid \[4\]). Initially in the renormalization procedure, $J_1 = J_2 = J_3 = J_4 = J_5 = J$. These coupling constants are renormalized in different ways. From simple dimensional analysis, it is easily seen that $J_1$-term is always irrelevant. In the case of strong correlation limit, $U \rightarrow \infty$, the scaling dimension of the field, $\cos \sqrt{4 \pi \phi_{\pm}^{(c)}}$ is close to $1/2$. For small $J$, the dimension of $J_2$-term is thus smaller than $2$ and generates spin gap in $\phi_+$ mode and charge gap in $\phi_-^{(c)}$ mode. In this case the mass gap is also open either in $\phi_-$ mode or $\theta_-$ mode. The state with the mass gap in $\phi_-$ mode corresponds to the Ising Neel ordered state with the non-vanishing order parameter $\lim_{i-j-\infty}(-1)^{i-j} \langle S_i^x S_j^x \rangle = (\cos \sqrt{2 \pi \phi_+}) (\cos \sqrt{2 \pi \phi_-})$, whereas that with the mass gap in $\theta_-$ mode to the quantum disordered state which is a weak-coupling analogue of the Haldane state characterized by the hidden string order $\lim_{i-j-\infty} \langle S_i^z \exp(\pi \sum_{k=i}^{j-1} S_k^z S_k^z) \rangle = (\cos \sqrt{2 \pi \phi_+}) (\cos \sqrt{2 \pi \phi_-})$. The mechanism for the spin gap formation is similar to that for the coupled spin chains \[4\]. In the present case, the spin-gap state with massive $\theta_-$ mode realizes at half-filling \[4\] and hence it remains massive away from half-filling, because $\phi_-^{(c)}$ mode is already massive in this parameter region. Then the fixed point is the metallic state with the spin gap $d$ in Haldane. A similar spin-gap state was obtained \[11\] for $J$ or Hubbard chains coupled via transverse hopping \[11\]. At this fixed point, dominant correlations develop in the inter-chain singlet pairing and “$4 \hbar \Omega$” CDW. The order parameters are, respectively, given by $O_{SS}(x) = \langle c_{L\sigma}(x) d_{R-\sigma}(x) + c_{R\sigma}(x) d_{L-\sigma}(x) \rangle$, $O_{CDW}(x) = \langle c_{L\sigma} d_{R\sigma}^{\dagger} d_{R\sigma} c_{R\sigma} \rangle$. The correlation functions of these order parameters show algebraic decay; $\langle O_{SS}(x)O_{SS}(0) \rangle \sim x^{-1/2K_+^{(c)}}$ and $\langle O_{CDW}(x)O_{CDW}(0) \rangle \sim x^{-K_{-}^{(c)}/2}$. In our case $K_{-}^{(c)} < 1$ and hence the fluctuation for “$4 \hbar \Omega$” CDW is more dominant than that for singlet superconductivity.

We now discuss the effects of random impurities on this fixed point. The effects of randomness on Tomonaga-Luttinger liquid were investigated by several authors \[12\] \[13\]. Here we apply renormalization group methods used by Giamarchi and Schulz \[12\]. We introduce the random impurity potential,\[13\]

\[ H_{imp} = \sum_\sigma \int dx [\xi(x) (c_{\sigma R}^{\dagger} c_{\sigma R} + d_{\sigma R}^{\dagger} d_{\sigma R}) + h.c.], \]

with the Gaussian distribution,

\[ P_\xi = \exp(-D_\xi^{-1} \int \xi^*(x) \xi(x) dx). \]

Here we omit forward scatterings because they can be incorporated into the shift of the chemical potential and do not affect the fixed point properties. In order to deal with the quenched disorder we use a replica trick. We consider the case for weak randomness and incorporate only the first order contribution in $D_\xi$. Then there is no coupling between different replica indices, which will be omitted below. Applying a standard renormalization group analysis \[12\], we obtain the scaling equations up to the lowest order in $J$ and $D_\xi$,

\[ \frac{dD_\xi}{dl} = \left( \frac{3 - K_+}{2} - \frac{K_-^{(c)}}{2} - \frac{K_{-}^{(c)}}{2} \right) D_\xi - J_3 D_\xi - J_5 D_\xi, \]

\[ \frac{dJ_1}{dl} = (2 - K_- - K_{-}^{(c)}) J_3 - D_\xi, \]

\[ \frac{dJ_4}{dl} = (2 - 1) J_4 - \frac{K_-}{2} - K_{-}^{(c)}, \]

\[ \frac{dJ_5}{dl} = (2 - K_- - K_{-}^{(c)}) J_5 - D_\xi, \]

\[ \frac{dK_+}{dl} = \frac{v_+}{2 v_+^{(c)}} D_\xi K_+^2 - \frac{v_+}{2 v_+^{(c)}} J_3^2 K_+^2, \]

\[ \frac{dK_-}{dl} = \frac{v_-}{2v_-^{(c)}} D_\xi K_-^2 - \frac{v_-}{2v_-^{(c)}} J_3^2 K_-^2 + \frac{2v_-}{2v_-^{(c)}} J_4^2, \]

\[ \frac{dD_\xi}{dl} = \frac{v_+}{2v_+^{(c)}} (J_3^2 + 4J_4^2 + J_5^2) K_+^2, \]

where we did not display the equations irrelevant to the following discussions, and omitted the renormalization effects due to $J_2$ term, because they do not change the intrinsic results. Since the quantum disordered spin-gap state realizes in the pure system, we initially have $2 - K_+ - K_-^{(c)} > 0$, $2 - K_- - K_{-}^{(c)} < 0$, and $2 - 1/K_- - K_{-}^{(c)} > 0$. We can see from eqs.\[11\] and \[13\] that the values of $K_+$ and $K_{-}^{(c)}$ are reduced by the randomness, and hence $2 - K_- - K_{-}^{(c)} > 0$ holds in the process of the renormalization. Then from eq.\[11\], $J_5$ scales to the strong-coupling regime and gaps open in $\phi_+$ and $\phi_-^{(c)}$, resulting in $K_+ + K_{-}^{(c)} \rightarrow 0$. Moreover eq.\[11\] indicates the fixed point value of $J_3$ is $D_\xi/(2 - K_- - K_{-}^{(c)})$, and hence the terms including $J_3$ in eqs.\[13\] and \[14\] are negligible to the lowest order in $D_\xi$. As a result, eqs.\[13\], \[14\], and \[15\] become

\[ \frac{dD_\xi}{dl} = \left( \frac{3 - K_+}{2} - \frac{K_-^{(c)}}{2} \right) D_\xi, \]

\[ \frac{dJ_4}{dl} = (2 - 1) J_4, \]

\[ \frac{dK_+}{dl} = \frac{v_+}{2v_+^{(c)}} D_\xi K_+^2 + \frac{v_+}{2v_+^{(c)}} J_4^2. \]
Fig. 1. Plots of $1/K_-(l)$ vs $D_\xi(l)$ for some initial values of $J_4$. The initial values of $1/K_-$, $D_\xi$, and $K_+(c)$ are taken as 0.7, 0.01, and 0.6.

Solving these equations, we have $K_- \to \infty$, because the spin gap in $\theta_-$ mode opens in the absence of randomness. Thus from eq. (12), $D_\xi$ scales to 0 and the randomness becomes irrelevant. These arguments are confirmed by the numerical results for renormalization flows calculated by eqs. (13) $\sim$ (14) (Fig. 1). Note that the suppression of $D_\xi$ is due to the spin gap formation by $J_4$-term, that is, the presence of the non-vanishing disorder parameter, $\langle \cos \sqrt{\pi\theta_-} \rangle$. Therefore we can say that the Tomonaga-Luttinger liquid state in the charge sector is protected from the transition to the Anderson localization by the quantum spin disorder. The physical reason of the suppression of the Anderson localization may be understood from the transition to the Anderson localization by the quantum spin disorder. The suppression of the disorder parameter, $\langle \cos \sqrt{\pi\theta_-} \rangle$, becomes irrelevant. These arguments are confirmed by Fig. 1. Plots of $1/K_-(l)$ vs $D_\xi(l)$ for some initial values of $J_4$. The initial values of $1/K_-$, $D_\xi$, and $K_+(c)$ are taken as 0.7, 0.01, and 0.6.

We have checked that for sufficiently large initial values of $D_\xi$ and small initial values of $J_4$, $D_\xi$ scales to a value larger than unity before $J_4$ scales to the strong-coupling regime, and our weak-coupling treatment for randomness breaks down (see also Fig. 1). Although in this case we do not know the fixed point properties, it seems plausible to expect that sufficiently strong randomness may destroy the Tomonaga-Luttinger liquid state and bring about the transition into the Anderson localization state. It may also lead to the destruction of the quantum spin disorder. Although our discussions here for localization-delocalization transition rely on weak-coupling renormalization group methods, we think that the qualitative features should not be changed even if we take into account higher-order corrections in $J$.

We wish to note that the suppression of the Anderson localization for weak randomness is not due to the development of superconducting fluctuation as found before [3, 4] because in the present case the fluctuation of the “$4k_F$” CDW is more dominant than that of superconductivity. The presence of the quantum spin disorder in the Haldane state indeed prevents impurity potential from pinning the CDW. It may be a new type of depinning effect of the CDW. Hence, if a doped-Haldane system belongs to the class of model I, we can observe the power-law behavior in correlation functions more easily, owing to the stability of Tomonaga-Luttinger liquid state against randomness.

We next discuss the model II. The Hamiltonian is given by

$$
H = -t \sum_{i,\sigma} c_i^{\dagger} c_{i+1,\sigma} + u \sum_{i} c_i^{\dagger} c_i + J_4 \sum_{i} S_{i,\uparrow} \cdot S_{i,\downarrow} + J_d \sum_i S_{d,i} \cdot S_{d,i+1} + J \sum_i S_{c,i} \cdot S_{d,i},
$$

where $J_d$ is the anti-ferromagnetic exchange interaction $(J_d > 0)$ and other notations are the same as those of eq. (3). The charge degree of freedom for $d$-electrons is completely frozen in this model, which may approximately describe the system in which the energy levels of electrons composing the $S = 1$ state are largely separated. In the strong-coupling limit at half-filling, this Hamiltonian also reduces to the $S = 1$ Heisenberg model.

In order to properly describe symmetry of the system away from half-filling at the fixed point, non-Abelian bosonization [3, 4] is more suitable than Abelian bosonization because two chains decouple at the fixed point and SU(2) symmetry of each chain should be retained as we will see below. By applying non-Abelian bosonization formula to the spin sector, we can write down the Hamiltonian in a continuum limit for the case away from half-filling as

$$
H = H_c + H_s
$$

$$
H_c = \int dx \left[ \frac{v_c(c)}{2k_F(c)} (\partial_x \phi_c)^2 + \frac{v_c(c) k_F(c)}{2} \Pi_c(c) \right]
$$

$$
H_s = \int dx \frac{2\pi v_c}{3} [J_{cL} \cdot J_{cL} + J_{cR} \cdot J_{cR}]
$$

$$
+ \int dx \frac{2\pi v_d}{3} [J_{dL} \cdot J_{dL} + J_{dR} \cdot J_{dR}]
$$

$$
+ J_m \int dx [J_{cL} \cdot J_{cL} + J_{cR} \cdot J_{cR}]
$$

$$
+ J_{ir} \int dx [J_{cL} \cdot J_{dL} + J_{cR} \cdot J_{dR}],
$$

where $J_{cL}$ and $J_{dL}$, etc., are the current operators for spinons of $c$- and $d$-electrons, which satisfy SU(2) Kac-Moody algebra, and initially we have $J_m = J_{ir} = J$. Here we dropped irrelevant oscillating terms. In general, spinons of $c$- and $d$-electrons have different velocities, $v_c$ and $v_d$. From the operator product expansion of level-1 SU(2) Kac-Moody algebra, we obtain the scaling equations for couplings $J_m$ and $J_{ir}$,

$$
\frac{dJ_m}{dl} = 0, \quad \frac{dJ_{ir}}{dl} = \frac{J_{ir}^2}{2\pi(v_c + v_d)}.
$$
Thus the last term of $H_s$ is marginally irrelevant for $J < 0$. The $J_m$-term just renormalizes the velocities of spinons and does not break SU(2) symmetry in each chain. Hence at the low-energy fixed point there exist one massless mode in the charge sector described by $c = 1$ Gaussian theory and two massless modes in the spin sector described by level-1 SU(2) Wess-Zumino-Witten theory \cite{Affleck}, and consequently there is no spin gap away from half-filling. Therefore doping holes in this model drastically changes characteristic properties of spin excitations, in contrast to the model I. We note that the existence of two massless spin modes is also contrasted to the Kondo lattice model with the antiferromagnetic coupling $J > 0$ where only one massless spin mode with a large Fermi surface exists \cite{I}. At this fixed point, two kinds of spinons have different pseudo-Fermi surfaces. Therefore correlation functions involving spin excitations show singularities at two different points reflecting the existence of two pseudo-Fermi surfaces. For example, the spin correlation function for the total spins, $S_i(x) = S_c(x) + S_d(x)$, is given by

$$<S^z_i(x)S^z_j(0)> \sim \frac{A_0}{x^2} + \frac{A_1 e^{2k_F x}}{x^\alpha} + \frac{A_2 e^{i\pi x}}{x} + c.c.$$ (18)

where $A_0$, $A_1$, and $A_2$ are some constants, and the exponent of the second term is given by $\alpha = 1 + K_c^{(c)}$. Here we omitted logarithmic corrections due to marginal operators. Thus the form factor of the spin correlation function may exhibit two structures in the momentum space at $q = 2k_F$ and $\pi$.

The effects of randomness on the model II can also be investigated. In this model, two chains are decoupled at the fixed point. Then the problem is simply divided into two parts; the 1D Hubbard model and the 1D $S = 1/2$ Heisenberg model with site randomness. For the former problem, according to Giamarchi and Schulz \cite{T}, the Anderson localization takes place for repulsive interaction. For the latter problem, if the on-site correlation between localized $d$-electrons is sufficiently strong, the site randomness does not affect the exchange interaction $J_d$ so much, and hence the massless spin mode can survive, although the system may be of the glass state if we additionally include randomness for exchange interaction.

Comparing the results for the models I and II, which exhibit quite different behaviors upon doping, we can say that characteristic properties of hole-doped Haldane systems strongly depend on whether the energy levels of electrons consisting the $S = 1$ state are nearly degenerate, or largely separated.

According to the experimental results of ref. [2], low-energy excited states below the spin gap appear upon doping, and localization occurs in transport properties. These seem to be consistent with the model II with random potential. We think that the model II may effectively describe low-energy properties of the doped Haldane system $Y_{2-x}Ca_xBaNiO_5$ for larger doping regions, though hole-doping has been realized in a way different from the present model [2].

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