A possible phase diagram of a t-J ladder model

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Abstract

We investigate a t-J ladder model by numerical diagonalization method. By calculating correlation functions and assuming the Luttinger liquid relation, we obtained a possible phase diagram of the ground state as a function of $J/t$ and electron density $n$. We also found that behavior of correlation functions seems to consist with the prediction of Luttinger liquid relation. The result suggests that the superconducting phase appear in the region of $J/t \sim 0.5$ for high electron density and $J/t \sim 2.0$ for low electron density.

Keywords: t-J ladder model, spin gap, electronic structure, phase diagram, superconductivity
Low-dimensional antiferromagnetic systems attract much interest due to the possible relevance to high-$T_c$ superconductivity. In particular, ladder systems which show a finite spin gap are extensively studied now. For example, recent measurements of the magnetic susceptibility and/or the nuclear relaxation rate of $\text{SrCu}_2\text{O}_3$ and $(\text{VO})_2\text{P}_2\text{O}_7$ indicate that these materials are described weakly coupled ladder models with spin-gap\cite{1, 2, 3}. Many theoretical works also have been performed on Heisenberg of ladder models and the spin gap up to order of exchange energy is found\cite{4, 5, 6}. Recently, It is claimed that the spin-gap survives against light hole doping and it vanishes for heavy doping in $t$-$J$ ladder models by numerical diagonalization method.\cite{7, 8, 9} Hayward et al. gave numerical evidence of superconductivity in $t$-$J$ ladders for sufficiently large exchange energy $J$ by a density matrix renormalization method\cite{10}.

If the low energy behavior of the ladder system can be described as that of one-dimensional (1D) system, an approach of the 'Luttinger liquid' theory will be useful. In the Luttinger liquid theory, some relations have been established as universal relations\cite{11, 12}. They supplied us with unambiguous and important information about not only one-band electronic systems but complicated 2-band systems\cite{13}.

Hayward and Poilblanc\cite{14} discussed the Luttinger liquid behavior of a $t$-$J$ ladder model and give a possible phase diagram of a critical exponent $K_\rho$ which characterizes the algebraic decay of correlation functions in the Luttinger liquid theory. However, it is not clear whether or not exponents of correlation functions given by the Luttinger liquid relation consist with the behavior of correlation functions calculated by the numerical method\cite{10}.

In this letter, we reexamine the critical exponent and Luttinger liquid behavior of $t$-$J$ ladder by numerical diagonalization method. We find that a prediction of the Luttinger liquid theory consists with the behavior of the correlation functions of $t$-$J$ ladder. Using the exponent, we determine a superconducting region on the possible phase diagram.

The $t$-$J$ ladder Hamiltonian is written as

$$H = -t \sum_i \left( c_{i,\alpha}^\dagger c_{i+1,\alpha} + h.c. \right) - t \sum_i \left( c_{i,1,\sigma}^\dagger c_{i,2,\sigma} + h.c. \right) + J \sum_{i,\alpha} \left( S_{i,\alpha} \cdot S_{i+1,\alpha} - \frac{1}{4} n_{i,\alpha} n_{i,\alpha} \right) + J \sum_i \left( S_{i,1} \cdot S_{i,2} - \frac{1}{4} n_{i,1} n_{i,2} \right),$$

(1)

where $c_{i,\sigma}^\dagger$ is the electron creation operator with spin $\sigma$ on a rung $i$ of ladder.
and $S_{i,\alpha}$ is the spin operator made of $c_{i,\alpha,\sigma}^\dagger$ and $c_{i,\sigma,\alpha}$. Here, $\alpha(=1,2)$ labels the two legs of the ladder and $n_{i,\alpha} = \sum_\sigma c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma}$. $J$ is exchange energy between the nearest neighbor sites and $t$ stands for the transfer energy, which will be set to be unity hereafter in the present study. We take account of the infinite on-site repulsion by removing states with doubly occupied sites from the Hilbert space.

We numerically diagonalize the Hamiltonian up to 20 sites (10 unit cells) using the standard Lanczos algorithm. We use the periodic boundary condition for $N_e = 4m + 2$ and anti periodic boundary condition for $N_e = 4m$, where $N_e$ is the total number of electrons and $m$ is an integer. We also use the open boundary condition to calculate correlation functions because we are able to take more points in correlation functions. The filling $n$ is defined by $n = N_e/(2N_u)$, where $N_u$ is the total number of unit cells (each unit cell corresponds to a rung).

The chemical potential $\mu(N_e, N_u)$ is defined by

$$\mu(N_e, N_u) = \frac{E_0(N_e + 1, N_u) - E_0(N_e - 1, N_u)}{2},$$

where $E_0(N_e, N_u)$ is the total ground state energy. When the charge gap vanishes in the thermodynamic limit, the uniform charge susceptibility $\chi_c$ is obtained from

$$\chi_c(N_e, N_u) = \frac{2/N_u}{\mu(N_e + 1, N_u) - \mu(N_e - 1, N_u)}.$$

It is noted that our definition of the $\chi_c$ is larger than that of previous works\[9, 14\] by a factor of 2 since we use the charge susceptibility $\chi_c$ per rung rather than per site.

In the model which is isotropic in spin space, exponents of various types of correlation functions are determined by the critical exponent $K_\rho$. For single band model, the Luttinger liquid theory predicts that Superconducting (SC) correlation function is dominant for $K_\rho > 1$ (attractive case), whereas Charge or Spin Density Wave (CDW or SDW) correlation is dominant for $K_\rho < 1$ (repulsive case). In the case of non-interacting fermion systems, the exponent $K_\rho$ is always unity.

On the other hand, the bosonization method\[15, 16\] shows that two-chain model with a small interchain hopping has a spin-gaped phase and SC and
"4k_F" CDW correlations decay as $\sim r^{-\frac{2k_F}{r}}$ and $\sim r^{-2K\rho}$ respectively (SDW and "2k_F" CDW correlations decay exponentially). Hence, SC correlation is dominant for $K\rho > 0.5$.

When we apply the above relations to the t-J ladder, we should pay attention to the filling of electrons in the t-J ladder. For low density region, we should adopt the relation for the single band model since electrons fill in only the lower band of the t-J ladder. For high density region, we can expect the relation for two-chain model to be useful.

It is convenient to introduce a critical exponent $\tilde{K}\rho$ which is related to the usual critical exponent $K\rho$ by the relations,

$$\tilde{K}\rho = \frac{\pi}{2} v_c \chi_c,$$  \hspace{1cm} (4)

$$v_c = \frac{N_u}{2\pi} (E_1 - E_0),$$ \hspace{1cm} (5)

where $E_1 - E_0$ is the lowest charge excitation energy. For low density, our definition of the $\tilde{K}\rho$ is equivalent to that of the exponent $K\rho$ \cite{11, 17}. When electrons are filled in only lower band, we should define the $K\rho$ of a multi-band model as above. Another definition of $K\rho$ in previous works \cite{3, 14} is misleading in applying the Luttinger liquid relation to t-J ladder at low density. On the contrary, for high density, the $\tilde{K}\rho$ is larger than the $K\rho$ by a factor of 2 since we use the $\chi_c$ given by eq.(3). Considering the $\chi_c$ and $K\rho$ of a non-interacting ladder system, it is easily understood.

In both the low density and the high density cases, we expect that the superconducting correlations dominate for $\tilde{K}\rho > 1$.

We can also determine the $\tilde{K}\rho$ by the Drude weight $D$

$$\tilde{K}\rho = \pi (\frac{\chi_c D}{2})^{1/2},$$ \hspace{1cm} (6)

$$D = \frac{1}{2N_u} \frac{\partial^2 E(\phi)}{\partial \phi^2}.$$ \hspace{1cm} (7)

where $E(\phi)$ is the total energy of the ground state as a function of flux $\phi$. Using these two independent equations of the $\tilde{K}\rho$, we can check the consistency of the Luttinger liquid relations.\cite{18}

To investigate the band structure of the t-J ladder model, we show the chemical potential $\mu$ (Fermi energy $E_F$ at the $T = 0$) as a function of electron
filling $n$ in Fig.1. For a non-interacting ladder model, band structure is given as

$$E^\pm(k) = 2t\cos(k) \pm t$$  \hspace{1cm} (8)

where $k$ is a wave vector. When $n$ is smaller than 0.5, electrons are filled in only lower band $E^-(k)$. At $n = 0.5$, lower and upper bands begin to fill with electrons simultaneously. The slope of $\mu$ is equal to zero and the value of the charge susceptibility $\chi_c$ diverges at $n = 0.5$, where the slope of $\mu$ corresponds to $2/\chi_c$. Thus, the divergence of $\chi_c$ signifies a change in the electronic state of non-interacting systems.

On the other hand, $\chi_c$ of t-J ladders seems to be finite at $n = 0.5$ for $J<1.0$. If the divergent point of $\chi_c$ exists, it may move to more high density. In contrast to non-interacting fermion ladder, we expect that the ground state of t-J ladder continues from low density over $n = 0.5$. In fact, points of $n = 0.5$ for $J<1.0$ belongs to the spin-gapless region, which is yield by Ref.\[8\]. Roughly speaking, Ref.\[8\] shows that the spin-gap phase appears at high density and large $J$ and the remainder is the gapless phase.

It is interesting to see that the $n$-dependence of $\mu$ at $J/t = 2$ almost corresponds to that of non-interacting ladder system in low electron density. It suggests that the electronic state of non-interacting system resembles that of t-J ladder in this parameter region. To confirm the above, we calculate the density-density correlation function on the same leg $C_{CDW}(R) = <n_{0,\alpha}n_{R,\alpha}> - <n_{0,\alpha}><n_{R,\alpha}>$ of both systems, where $R$ is distance from one of ends of the system. In Fig.2(a), we show $C_{CDW}(R)$ for 18-site systems with 4-electrons under the open boundary condition. Correlation functions of both systems are very close to each other. We also get similar results for singlet pairing and spin-spin correlation functions of the same systems.

These results show that low energy behavior of t-J ladder is approximately described as non-interacting system. It also indicates that the correlation exponent $\tilde{K}_\rho (= K_\rho)$ is close to unity. The direct numerical calculation of $\tilde{K}_\rho$ by eq.(4) shows $\tilde{K}_\rho \approx 1.0$ for $N_s = 18$ system with $N_e=4$. It reminds us that the wave function of a single chain t-J model at $t = J/2$ is close to projected Fermi liquid\[19\] and the exponent $K_\rho$ becomes unity in the low density limit\[17\]. Therefore, the properties of t-J ladder are close to that of the single band model. It suggests that the existence of upper band $E^+(k)$ is irrelevant to the low energy behavior of t-J ladder in the low electron density region\[16\].
Next, we consider the case of high electron density. For \( J = 1 \), we can also compare a behavior of correlation functions and the value of \( \tilde{K}_\rho(= 2K_\rho) \). Recently, Hayward et al. calculated correlation functions by using the density-matrix renormalization-group method at \( J/t = 1 \) and \( n = 0.8 \). Their results show that a pairing correlation is longer range than other correlations, decaying slower than \( \sim R^{-1} \). The power of the density-density correlation function seems to be \(-2\) or slightly larger.

If we assume \( \tilde{K}_\rho \sim 1.5 \) in this case, the powers of correlation functions can be explained with the 'duality' relation which is introduced by Nagaosa and Oshikawa\([20]\); the powers of paring and density-density correlations are obtained as \( \sim 0.7 \) and as \( \sim 1.5 \) respectively. It is consist with the value of \( \tilde{K}_\rho \sim 1.4 \), which is obtained from the Luttinger liquid relation for the \( N_s = 20 \) site system with 16 electrons. These results suggest that the Luttinger liquid relation holds for t-J ladder.

Furthermore, we calculate the pairing correlations and density-density correlations for another system. Figs.3 show the rung-rung pairing correlation function \( C_{SC}(R) = \langle \Delta_0\Delta_0^\dagger \rangle \), where \( \Delta_0^\dagger = (c_{R,1,\uparrow}^\dagger c_{R,2,\downarrow}^\dagger - c_{R,1,\downarrow}^\dagger c_{R,2,\uparrow}^\dagger) \) and the density-density correlation function \( C_{CDW}(R) \) for \( N_s = 16 \) site system at \( n=12/16 \). For \( J = 0.5 \), both correlation functions seem to decay as \( \sim R^{-1} \) as shown in Fig.3(a). For \( J = 1.5 \), pairing correlations decay slower than the density-density correlations; the former seems to decay as \( \sim R^{-0.5} \) or more rapidly and the later seems to decay as \( \sim R^{-2} \) as shown in Fig.3(b).

Although the system size is not sufficiently large to get exponents of correlation functions precisely, the powers of both correlation functions seem to satisfy the duality relation. At least, the behavior of correlation functions suggests that the paring correlations dominate others for \( J/t > 0.5 \). Using eq.(6), the critical exponent \( \tilde{K}_\rho \) is obtained as \( \sim 1.0 \) and \( \sim 2.0 \) for \( J = 0.5 \) and \( J = 1.5 \) respectively. It consists with the behavior of correlation functions and indicates the validity of the Luttinger liquid relation for two-chain model.

In the limit of \( J \to 0 \), the situation is complicated. Nagaoka ferromagnetic state is known to appear at the ground state of finite systems\([4]\). However, a very small \( J \) lifts the ferromagnetic state and changes the ground state to singlet. If the Nagaoka ferromagnetic phase exists in the thermodynamic limit, the phase may be restricted to the region with very small \( J \). Thus, the lowest singlet state is not the true ground state at \( J = 0 \); nevertheless, we single it out as the relevant state at very small \( J \).
Fig.1 shows that the band structure of t-J ladder at $J = 0$ is close to that of non-interacting spinless fermions in the ladder model. In Fig.4, we compare the density-density correlation functions $C_{\text{CDW}}(R)$ of t-J ladder with that of spinless fermion ladder. It shows that both correlation functions are close to each other. Using the equations (6), the correlation exponent $\tilde{K}_\rho$ is estimated as $\sim 0.4\,[21]$, which is almost consist with the value of $K_\rho (= 0.5)$ of the spinless fermion system. The same situation is already found in a single chain t-J model for very small $J\,[22]$. This result indicates that we should apply not the relation for two-chain model but single-chain model contrary to expectation. Probably, only the upper band $E^+(k)$ is relevant to the low energy behavior and charge degree of freedom is reduced to that of spinless fermion system in the high density region at $J = 0$.

Finally, we examine the phase diagram of superconducting state in the $J$-$n$ plane with the exponent $K_\rho$. In Fig.5, we show the possible phase diagram of t-J ladder. When the $\tilde{K}_\rho (\chi_c)$ diverges, the uniform state becomes unstable and phase separation occurs. The boundary of phase separation agrees with the results of previous works\[4, 9\]. Fig.5 shows that the region of superconducting state appears at lower value of $J/t$ than a single chain case at high electron density. It seems to resemble the behavior in two-dimensional case. On the other hand, the behavior of the superconducting region at small electron concentration resembles that of a single chain\[17\]. Hayward et al.\[14\] also obtained the phase diagram in the $J$-$n$ plane, but their value of $K_\rho$ is smaller than $\tilde{K}_\rho$ by a factor 2. If the value of $K_\rho$ is doubled in their phase diagram, the result of $\tilde{K}_\rho$ agrees with ours.

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In the spin-gaped phase, the bosonization method shows that powers of the pairing correlation function $K_{sc}$ and that of "$4k_f$" CDW correlation function $K_{CDW}$ satisfy the equation $K_{sc}K_{CDW} = 1$. They call it the duality relation.

In the high density region, it is difficult to obtain $\chi_c$ precisely by using eq. (4) since frustration of antiferomagnetic configuration on the legs increases. Thus, we fit data of $\mu$ to a polynomial as a function of $n$ by the least square method and estimate the $\chi_c$ from differential coefficient of the polynomial. Using the above $\chi_c$, we calculated the $\tilde{K}_\rho$ by the eq.(6).

In the single chain model, the ground state is degenerate in the spin degree of freedom at the limit $J \to 0$ and the wave function is decoupled to charge sector and spin sector. Since charge component is equivalent to spinless fermion, the value of $K_\rho$ becomes 0.5.
Figure captions

Fig.1. The chemical potential $\mu$ as a function of the filling $n$ for various values of $J$. $\mu$ is calculated for $N_s = 12, 14, 16, 18, and 20$. The dashed line represents a non-interacting fermion ladder band and the broken line represents a spinless-fermion ladder band.

Fig.2. The density-density correlation functions $C_{CDW}(R)$ of t-J ladder and non-interacting fermion systems. $C_{CDW}(R)$ is calculated for the $N_s = 18$ sites system with 4 electrons. The dashed line has slope -2.

Fig.3. The rang-rang paring correlation function $C_{SC}(R)$ and the density-density correlation function $C_{CDW}(R)$ of the $N_s = 16$ sites system with 12 electrons (a) for $J/t = 0.5$ and (b) for $J/t = 1.5$.

Fig.4. The density-density correlation functions $C(R)_{CDW}$ of t-J ladder and non-interacting spinless-fermion systems. $C(R)_{CDW}$ is calculated for the $N_s = 18$ sites system with 16 electrons. The dashed line has a slope -1.5.

Fig.5. A possible phase diagram of the t-J ladder as a function of $J/t$ and electron density $n = N_e/N_s$. The circles represent results of $N_s = 16$ sites systems.