Ground-state phase diagram of the one-dimensional $t$-$J_s$-$J_\tau$ model at quarter filling

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We study the ground state of the one-dimensional “$t$-$J_s$-$J_\tau$ model”, which is a variant of the $t$-$J$ model with additional channel degree of freedom. The model is not only a generalization of the $t$-$J$ model but also an effective model of the two-channel Kondo lattice model in the strong coupling region. The low energy excitations and correlation functions are systematically calculated by the density matrix renormalization group (DMRG) method and the ground-state phase diagram at quarter filling consisting of Tomonaga Luttinger liquid, spin-gap state, channel-gap state, insulator, and phase separation is determined. We find that weak channel fluctuations stabilize the spin-gap state, while strong channel fluctuations lead to the transition to the insulator.

I. INTRODUCTION

Fluctuations of quantum degree of freedom are important feature of microscopic systems, which give rise to plenty of interesting phenomena. In condensed matter physics, spin fluctuations play an important role to realize various quantum states, such as spin liquid and superconductivity. One of minimal theoretical models containing both of spin and charge degrees of freedom is the $t$-$J$ model. The model was originally proposed to describe high-$T_c$ superconductivity [1], and its one-dimensional model has been studied to understand the fundamental properties of the strongly correlated systems. Although this model include only kinetic energy term and the exchange energy term, various quantum state including spin-gap state have been found [2], and it is interesting to investigate whether new quantum states appear when we include additional interactions existing in more realistic systems. One simple extension is the inclusion of repulsive interaction $V$ between the neighboring electrons. It has been reported that the repulsive interaction $V$ stabilizes the spin-gap phase at quarter filling [3], but other new states have not yet been obtained. Another approach to extend the $t$-$J$ model is to add new degrees of freedom of electrons.

Praseodymium contained in cage-shaped composite, such as PrTi$_2$Al$_2$, has non-Kramers doublet as the crystal-field ground state [4, 5]. The theoretical model of such materials is the two-channel Kondo lattice model (TCKLM) [6, 7], which has multiple degree of freedom associated with the non-Kramers doublets. As a simplest model of interacting electron systems consisting of multiple degree of freedom, we propose “$t$-$J_s$-$J_\tau$ model”, which is not only an extension of $t$-$J$ model but also an effective model of the TCKLM in the strong coupling region.

In this paper we study the ground state properties of the model by the DMRG method, and investigate the effect of the channel degree of freedom to the ground state. The obtained results show that the spin-gap state is stabilized by weak channel fluctuations, while strong channel fluctuations lead to the transition to the insulator.

II. MODEL

The model we study here is the following “$t$-$J_s$-$J_\tau$ model”:

\[
H_{t,J_s,J_\tau} = -t \sum_{i \sigma} (a_{i \sigma}^\dagger b_{i+1, \sigma}^\dagger a_{i+1, \sigma} + h.c.) + J_s \sum_i S_i \cdot S_{i+1} + J_\tau \sum_i \tau_i \cdot \tau_{i+1} + V \sum_i n_i n_{i+1},
\]

where $a_{i \sigma}^\dagger$ and $b_{i \sigma}^\dagger$ are the creation operators of particles and “holes” at the $i$-th site with spin $\sigma$ and channel $\alpha$, respectively. The empty and double occupancy of $a_{i \sigma}^\dagger$ and $b_{i \sigma}^\dagger$ are inhibited. This model is equivalent to the extended $t$-$J$ model in the limit of $J_\tau = 0$. The spin and channel-pseudospin operators are defined as $S_i = \frac{1}{2} \sum_{\sigma \sigma'} a_{i \sigma}^\dagger \sigma \sigma' a_{i \sigma'}$ and $\tau_i = \frac{1}{2} \sum_{\alpha \alpha'} b_{i \alpha}^\dagger \alpha \alpha' b_{i \alpha'}$, respectively. We define the number operator of the particles as $n_i = \sum_\sigma a_{i \sigma}^\dagger a_{i \sigma}$. This model is derived from the TCKLM,

\[
H_{\text{TCKLM}} = -\tilde{t} \sum_{i \sigma \alpha} (c_{i \sigma \alpha}^\dagger c_{i+1, \sigma \alpha} + h.c.) + \tilde{J} \sum_{i \sigma \sigma' \alpha} \bar{S}_i \cdot (c_{i \sigma \sigma'}^\dagger c_{i \sigma \sigma'}),
\]

as follows: assuming that the number of conduction electrons per local spins $n_s$ satisfies $1 \leq n_s \leq 2$, the effective Hamiltonian in the strong coupling region is given by the second-order perturbation of $1/J$ from the limit $J/t = \infty$.

In this case, $a_{i \sigma}^\dagger$ and $b_{i \sigma}^\dagger$ are the composite particles defined as $a_{i \sigma}^\dagger = \frac{1}{\sqrt{2}} (2c_{i \sigma}^\dagger e_{i \sigma}^\dagger f_{i \sigma}^\dagger - c_{i \sigma}^\dagger e_{i \sigma}^\dagger f_{i \sigma}^\dagger - c_{i \sigma}^\dagger e_{i \sigma}^\dagger f_{i \sigma}^\dagger)$.
and \( b_{i\alpha}^\dagger = \frac{1}{\sqrt{2}} \left( c_{i\alpha \uparrow}^\dagger f_{i\downarrow}^\dagger - c_{i\alpha \downarrow}^\dagger f_{i\uparrow}^\dagger \right) \), respectively, as schematically represented in Fig. 1. The transfer integral \( t \) in Eq. (1) is given as \( t = \frac{3}{4} \tilde{t} \) and the effective interactions are

\[
J_s = \frac{1504 t^2}{135 J}, \quad J_\tau = \frac{64 t^2}{9 J}, \quad \frac{J_\tau}{J_s} \approx 0.64. \tag{4}
\]

The interactions \( J_s \) and \( J_\tau \) are the two largest terms obtained by the perturbation expansion and the other ones including next-nearest hopping are ignored. The neglected long range interactions are expected to suppress the phase separation caused by the above two interactions. Instead of treating all of such terms explicitly, we consider the repulsion term \( V \) to suppress the phase separation. Note that when \( n_c = 1 \), which corresponds to the absence of the \( a^\dagger \) particles \( (n = 0) \), the model is reduced to the Heisenberg model of channel degree of freedom [7].

In this study, we analyze the ground state of the Hamiltonian of Eq. (1) with equal number of particles and holes \( n = 1/2 \) (quarter filling, \( k_F = \pi/4 \)). This filling corresponds to \( n_c = 3/2 \) in the TCKLM. Throughout this paper, we fix the nearest-neighbor interaction \( V \) as \( V/t = 0.8 \), and take the transfer integral \( t \) as the units of energy.

### III. Method

We use the density matrix renormalization group (DMRG) method [8, 9] to analyze the ground states of the Hamiltonian of Eq. (1). In this method, the accuracy of the ground-state wave function is systematically controlled by the number of keeping states \( m \). We increase \( m \) up to 400 to see the convergence of the results, where the truncation error is less than \( 10^{-5} \). The system size is in the range of 128–192.

To suppresses the finite size effect caused by the open boundary conditions used in the DMRG calculation, we apply the sine square deformation (SSD) [10] to the Hamiltonian. Since the SSD reproduces the bulk response to an external field [11], we use this property to obtain the excitation gap of the infinite system.

### IV. Result

We first study the elementary excitations of the model to clarify how the interactions modify the low energy.
properties of the system. We calculate the excitation gap for the charge ($\Delta_n$), spin ($\Delta_s$), and channel ($\Delta_r$) degrees of freedom in the parameter space of $J_s-J_r$. Figure 2 shows the excitation gaps obtained along the line defined by Eq. (4). With decreasing the parameter $J$ of the TCKLM (with increasing $J_s$ and $J_r$ of the $t$-$J_s$-$J_r$ model), the spin excitation gap first opens, and then, the charge and channel gaps open.

These successive transitions show the presence of the spin-gap phase. To further confirm the spin-gap phase, we systematically calculate the excitation gaps for various $J_s$ and $J_r$ and determine the ground-state phase diagram of the $t$-$J_s$-$J_r$ model. Figure 3 shows the phase diagram, in which five phases appear: metallic phase (M; no excitation gap), spin-gap phase (SG; only the spin gap opens), channel-gap phase (ChG: only the channel gap opens), insulating phase (I; gap opens for all excitations), and phase separation (PS). From the diagram, it is obvious that the line of TCKLM pass through the spin-gap phase.

As shown in Fig. 3, the transition lines are symmetric with respect to the line of $J_s = J_r$. This arises from the invariance of the Hamiltonian of Eq. (1) under the transformation $(a^\dagger_{ij}, a^\dagger_{i1}, b^\dagger_{i1}, b^\dagger_{i2}) \rightarrow (b^\dagger_{i1}, b^\dagger_{i2}, a^\dagger_{i1}, a^\dagger_{i2})$ with the exchange of $J_s$ and $J_r$ except for the difference in chemical potential. As long as we focus on the quarter filling (i.e. equal number of particles and holes), this transformation gives a completely equivalent ground state. Thus we only need to determine the transition points in the region of $J_s \geq J_r$. In the parameter sets we studied, the direct transition between the metallic phase and the insulating phase occurs only on the line of $J_s = J_r$. This implies the existence of a quantum tetra-critical point.

A. Metallic phase

We first focus on the metallic phase in the region of weak interaction, where all the excitations are gapless and each degree of freedom behaves as Tomonaga-Luttinger liquid (TLL) [12, 13]. As shown in Fig. 4, the correlation functions defined by

$$g(r) = \langle X_j X_{j+r} \rangle - \langle X_j \rangle \langle X_{j+r} \rangle,$$  

(5)

$$X_j = \begin{cases} n_j & \text{(for charge)} \\ S^z_j & \text{(for spin)} \\ \tau^z_j & \text{(for channel)}. \end{cases}$$

(6)

decay in power law $r^{-\alpha}$. For spin and channel degrees of freedom, the exponent is $\alpha \sim 1.6$ at $J = 9$, which is almost consistent with the prediction of TLL theory $\alpha = 1 + K_p$, where the Luttinger parameter $K_p$ is determined as $K_p \sim 0.5$ from the slope of the Fourier components of the charge correlation function $N(q)$ near $q = 0$ [2, 14, 15]. The $J_s$ dependence of $N(q)$ defined by

$$N(q) = \frac{1}{L} \sum_{i,j=1}^{L} e^{i q (x_i - x_j)} (\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle),$$

(7)

also shows that the period of the charge correlation function clearly changes from $4k_F$ (2 site) to $2k_F$ (4 site) with the increase in $J_s$ and $J_r$ as presented in Fig. 5.

When $J_s$ exceeds a critical value, the system undergoes the transition to the spin-gap phase. At $J_r = 0$, the critical value of $J_s$ is close to the band width $4t$. Figure 3 shows that this critical value becomes smaller with the increases in $J_r$, which indicates the interaction acting on the channel degree of freedom stabilizes the spin-gap phase. We note that the critical value is insensitive to $V$ when $V$ is sufficiently smaller than $4t$.

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**FIG. 4.** Correlation functions in the metallic phase at $J_s = 1.2$ and $J_r = 0.71$ ($J = 9.0$).

**FIG. 5.** Fourier components of the charge correlation function. Central $L = 152$ sites of 192-site system are used to suppress the boundary effects. The dominant wavelength changes from $4k_F$ to $2k_F$ with the decrease in $J_s$ and $J_r$. 
B. Spin-gap phase

As discussed above, the increase in \(J_s\) and \(J_r\) enhances the spin gap, which make the slope of the exponential decay of the spin correlation-function steeper as shown in Fig. 8(a). For the charge and channel correlation-functions, the power law behavior is confirmed as seen in Fig. 8(b). The power-law exponent of the charge correlation-function slightly decreases with the increase in the spin gap.

C. Insulating phase

We finally investigate the insulating state. In the insulating phase, all the excitations have finite energy gap and the correlation functions decay exponentially as shown in Fig. 8 where we find almost the same slope although the charge gap is much smaller than the spin gap. We think this is a result of alternating product state wave function of the spin and channel singlets as shown later.

To find the symmetry braking order of the insulating phase, we calculate several local expectation values. Figure 8 shows site dependence of the local densities and nearest-neighbor correlations defined as

\[
s_i = \langle S_{i-1/2}^z S_{i+1/2}^z \rangle - \langle S_{i-1/2}^z \rangle \langle S_{i+1/2}^z \rangle,
\]

\[
s_r = \langle \tau_{i-1/2} \tau_{i+1/2}^z \rangle - \langle \tau_{i-1/2}^z \rangle \langle \tau_{i+1/2} \rangle,
\]

where \(i\) is the center position of the two operators. We find the charge density \(n_i\) has \(2k_F\) (4-site) oscillation, whereas the spin and channel densities \(\langle S_i^z \rangle\) and \(\langle \tau_i^z \rangle\) keep zero everywhere. In addition, the nearest-neighbor correlations strongly correlate with the charge density oscillation. These results suggest that the insulating phase is a product state of spin and channel singlets, as schematically shown in Fig. 8. The spin-gap state is then considered as a state only spin degree of freedom form singlet pairs.

As shown in Fig. 8, the transition to the insulating state and the opening of the channel gap simultaneously occur in the region of \(J_s > J_r\). With the increase in \(J_s\) from 0, the critical value of \(J_r\) which opens the channel gap decreases from almost the band width of \(4t\) to \(t\) but never goes down to 0, which indicates the cooperation of the spin and channel degrees of freedom is essential for the emergence of the insulating phase.

Here we comment on the effect of the nearest-neighbor repulsion \(V\). This term is added to effectively include the higher order interactions existing in the original
TCKLM, which suppress the transition to the phase separation. As the nearest-neighbor repulsion leads to the metal-insulator transition in the extended Hubbard model at quarter filling\cite{16,17}, this may affect the phase diagram. However the insulating state caused by the nearest-neighbor repulsion $V$ is characterized by the $4k_F$ (2 sites) charge densities, which is clearly different from the insulating state found in the present study, where only $2k_F$ (4 sites) oscillation appears. We therefore think the repulsion term is not essential in the present analysis.

V. CONCLUSION

We have studied the ground states of the $t$-$J_s$-$J_\tau$ model, which is a minimal model consisting of multiple degrees of freedom. The low energy excitations of the spin, charge and channel degrees of freedom have been calculated by the DMRG method with the SSD, and it has shown that the phase transition occurs from the metallic state to the spin-gap or channel-gap state when the exchange interactions exceeds almost the band width, roughly $\sqrt{J_s^2 + J_\tau^2} \sim 4t$. For the symmetric case of $J_s = J_\tau$, however, direct transition to the insulating state takes place. These results imply that weak channel fluctuations stabilize the spin-gap state of the $t$-$J$ model while strong channel fluctuations lead to the transition to the insulating state which is characterized by the alternating product state of the spin and channel singlets.

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