Enhancement of Pairing Correlation and Spin Gap through Suppression of Single-Particle Dispersion in One-Dimensional Models

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We investigate the effects of suppression of single-particle dispersion near the Fermi level on the spin gap and the singlet-pairing correlation by using the exact diagonalization method for finite-size systems. We consider strongly correlated one-dimensional models, which have flat band dispersions near wave number $k = \pi/2$, if the interactions are switched off. Our results for strongly correlated models show that the spin gap region expands as the single-particle dispersion becomes flatter. The region where the singlet-pairing correlation is the most dominant also expands in models with flatter band dispersions. Based on our numerical results, we propose a pairing mechanism induced by the flat-band dispersion.

KEYWORDS: flat band, single-particle dispersion, spin gap, superconductivity

One of the characteristic features of hole-doped high-$T_c$ cuprates is the emergence of flat single-particle dispersion near the X points [i.e., $k = (\pi, 0), (0, \pi)$]. This unusual flatness of the dispersion relation is ascribed to strong electronic correlations. A recent numerical study on the two-dimensional (2D) Hubbard model showed that the flat single-particle dispersion near the X points is related to the universality class of the Mott transition. Pairing instabilities of systems under this universality class were also studied elsewhere where the dynamical exponent $z$ changes from four to two for the 2D Hubbard and $t$-$J$ models when a two-particle hopping term is switched on. This shows potential instability of flat single-particle dispersions towards singlet-pair formation, if two-particle hopping processes are introduced.

Taking this into account, we consider a possible scenario for enhancing the pairing instability: In strongly correlated systems, the two-particle hopping process can mainly be controlled by the incoherent part of charge excitations independently of the coherent part of single-particle excitations, while such a coherent single-particle process may rather suppress the pairing susceptibility through damping and pair breaking processes. Therefore, if only the single-particle dispersion near the Fermi level is suppressed, the two-particle hopping process determined from the dispersive band far from the Fermi level would enhance the pairing instability.

In this letter, in order to confirm the occurrence of this scenario in a simplified situation, we introduce one-dimensional (1D) models that have flat single-particle dispersion near half filling. We clarify how the singlet-pairing correlation and the spin gap behave in the parameter space of our model.

We consider the Hubbard model with long-range hopping terms defined by the following Hamiltonian:

$$
\mathcal{H}_0 \equiv \mathcal{H}_{\text{Hub}} + \mathcal{H}_{\text{lrh}}, \quad (1a)
$$

$$
\mathcal{H}_{\text{Hub}} \equiv -t \sum_{\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (1b)
$$

$$
\mathcal{H}_{\text{lrh}} \equiv -t_3 \sum_{\sigma} (c_{i\sigma}^\dagger c_{i+3\sigma} + c_{i+3\sigma}^\dagger c_{i\sigma}) - t_5 \sum_{\sigma} (c_{i\sigma}^\dagger c_{i+5\sigma} + c_{i+5\sigma}^\dagger c_{i\sigma}) - t_7 \sum_{\sigma} (c_{i\sigma}^\dagger c_{i+7\sigma} + c_{i+7\sigma}^\dagger c_{i\sigma}). \quad (1c)
$$

We take hopping amplitude $t_i$ ($i = 3, 5, 7$) of the long-range hopping terms as (i) $t_3/t = 1/3, t_5/t = t_7/t = 0$, (ii) $t_3/t = 0.5, t_5/t = 0.1, t_7/t = 0$, and (iii) $t_3/t = 0.6, t_5/t = 0.2, t_7/t = 1/35$ in order to realize flat dispersion near half filling in the noninteracting case. With this tuning, the noninteracting dispersion around $q_0 = \pm \pi/2$ is suppressed up to $(q - q_0)^\nu$, where $\nu = 2, 4$ and 6 for (i), (ii) and (iii), respectively. The dispersion relations of these noninteracting models are shown in Fig. 1. The region of flat-band dispersion near half filling is allowed to expand further as the hopping range becomes longer.

Taking the limit of strong correlation (i.e. $U \to \infty$), we obtain the following effective Hamiltonian:

$$
\mathcal{H} \equiv \mathcal{H}_{t-J} + \mathcal{H}_{3\text{-site}} + \mathcal{H}_{\text{lrh}} + \mathcal{H}_{\text{longJ}}, \quad (2a)
$$

$$
\mathcal{H}_{t-J} \equiv -t \sum_{\sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+1\sigma} + \tilde{c}_{i+1\sigma}^\dagger \tilde{c}_{i\sigma}) + J \sum_{i} (S_i \cdot S_{i+1} - \frac{1}{4} n_{i\uparrow} n_{i+1\uparrow}), \quad (2b)
$$

$$
\mathcal{H}_{3\text{-site}} \equiv -\frac{J}{4} \sum_{\sigma} (\tilde{c}_{i-1\sigma}^\dagger n_{i-\sigma} \tilde{c}_{i+1\sigma} + \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+1\sigma} n_{i+\sigma} - \tilde{c}_{i-1\sigma} \tilde{c}_{i\sigma} \tilde{c}_{i+1\sigma} + \text{H.c.}), \quad (2c)
$$

$$
\tilde{H}_{\text{lrh}} \equiv -t_3 \sum_{\sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+3\sigma} + \tilde{c}_{i+3\sigma}^\dagger \tilde{c}_{i\sigma}).
$$
Here, $H_{\text{long},t}$ denotes the spin exchange and three-site terms originating from long-range hopping. In this letter, we mainly study the model defined by the Hamiltonian $H_{\text{dJ3I}} \equiv H_{tJ} + H_{3\text{-site}} + H_{\text{irh}}$ for simplicity. Later, we discuss the effects of $H_{\text{long},t}$ briefly. The operator $\tilde{c}_{i\sigma}^\dagger$ creates an electron with spin $\sigma$ at site $i$ in the subspace without double occupancy. The operators $S_i$ and $n_i$ are the spin and number operators at site $i$, respectively. Hereafter, the chain length and the number of electrons are denoted by $L$ and $N_e$, respectively. We set $t = 1$ as the energy unit.

We call models defined by $H_{\text{dJ3I}}$ with (i) $t_3 = 1/3$, $t_5 = t_7 = 0$, (ii) $t_3 = 0.5$, $t_5 = 0.1$, $t_7 = 0$, (iii) $t_3 = 0.6$, $t_5 = 0.2$, $t_7 = 1/3$, and (iv) $t_3 = t_5 = t_7 = 0$ as the $tJ_3$, $tJ_3t_5$, $tJ_3t_7$ and $tJ_3$ models, respectively. The $tJ_3$ model is nothing but the effective model of the strong-coupling limit of the Hubbard model up to the order $t^2/\tilde{U}$. The ground-state properties of this model were investigated in detail by Ammon, Troyer and Tsunetsugu. The aim of this study is to demonstrate that the suppression of single-particle hopping processes enhances singlet pair correlations. We show this enhancement by studying the effects of the above long-range hopping terms $H_{\text{irh}}$ on the singlet gap and the singlet-pairing correlation.

First, we show numerical results on the phase boundary between the Tomonaga-Luttinger (TL) liquid phase and the spin-gap (SG) phase. We employ the singlet-triplet level crossing method in order to determine the phase boundary. The effectiveness of this method has been demonstrated through the applications to 1D spin systems and electron systems. Using this method, we determine the critical point with high precision since the finite-size correction is only due to irrelevant fields with scaling dimension $x = 4$. This method is based on the assumption that the universality class of the phase transition is described by the level $k = 1$ SU(2) Wess-Zumino-Witten (WZW) model. In order to check the applicability of this method to our models, we have calculated the scaling dimension of the lowest singlet excitation ($x_s$) and that of triplet excitation ($x_t$) at wave number $k = 2k_F$. According to the renormalization-group analysis, the leading finite-size corrections of $x_s$ and $x_t$ near the critical point are written as

$$x_s = \frac{1}{2} + \frac{3}{4} \frac{y_0}{y_0 \log L + 1},$$

$$x_t = \frac{1}{2} - \frac{1}{4} \frac{y_0}{y_0 \log L + 1},$$

where $y_0$ is a coupling constant. As shown in Fig. 2, the value of $x_t \equiv (x_s + 3x_t)/4$ is very close to 1/2 and independent of the value of parameter $J$. This indicates that the low-energy physics of our models is described as that of the Tomonaga-Luttinger liquid, and that the transition belongs to the universality class of the $k = 1$ SU(2) WZW model. In fact, as shown in Fig. 3, the phase boundaries in clusters of length $L = 8, 10, 12, 14$ and 16 are scaled in single lines. This suggests that the size dependence is very small.

Figure 3 shows the phase boundaries between the TL liquid phase and the SG phase for the $tJ_3$, $tJ_3t_3$, $tJ_3t_5$ and $tJ_3t_7$ models. Clearly, the region of the SG phase expands further near half filling as the hopping range becomes longer. In other words, the suppression of the Fermi velocity enlarges the region of the spin-gap phase. This may be explained as follows: Generally, low-energy properties of fermionic systems are mainly determined by scattering processes near the Fermi level. The suppression of the Fermi velocity would have similar effects as the reduction of hopping amplitude $t$ on the low-energy physics, because the Fermi velocity is roughly proportional to $t$. The long-range hopping terms, which suppress the Fermi velocity, effectively decrease $t$, while they do not alter $J$ and the three-site terms. Then, they increase the effective $J/t$ for the $tJ_3$ model. In the large $J/t$ regime for the $tJ_3$ model, the spin excitation has an energy gap, because of the large two-particle hopping processes such as spin exchange and three-site hopping. Hence, the suppression of single-particle hopping processes due to the long-range hopping terms results in the enlargement of the spin-gap phase.

It should be noted that the spin-gap region extends only in the finite-doping regime, not at half filling. This is analogous to the behavior of high-$T_c$ cuprates and different from that of the dimerized model and the $t-J$ ladder model, respectively, where the spin gap opens not only in the finite-doping regime, but also at half filling. This difference results in different classes of proximity effects from Mott insulators and hence different pairing mechanisms. Our study provides some insight on this issue.

Next, we consider correlation functions. Generally, in 1D interacting systems, the long-range behavior of correlation functions is described by a single correlation exponent $K_\rho$. The correlation exponent $K_\rho$ is obtained as

$$K_\rho = \pi \sqrt{\frac{\sigma_0 n^2 \kappa}{2}},$$

where Drude weight of the ac conductivity $\sigma_0$ and compressibility $\kappa$ in finite-size systems are respectively defined as

$$\sigma_0 \equiv \frac{L}{2} \left( \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \right)_{\phi = 0},$$

$$\kappa \equiv \frac{L}{N_e^2 E_0(L N_e + 2) + 2 E_0(L N_e - 2) - 2E_0(L N_e)}.$$

Here, $E_0(\phi)$ denotes the ground-state energy of the system with twisted boundary conditions with phase factor $\phi$. $E_0(N_e)$ denotes the ground-state energy of the $N_e$-electron system of length $L$, and $n$ is the electron density defined by $n = N_e/L$. The long-range behavior of the singlet-pairing correlation function $P(r)$ is expressed in terms of $K_\rho$ as

$$P(r) \propto \frac{1}{r^{1+1/K_\rho}}$$

if the spin excitation is gapless, while $P(r) \propto 1/r^{1/K_\rho}$ in the spin gap phase. If $K_\rho$ is larger than one, the singlet-pairing correlation
is the most dominant among other correlation functions. We show the contour lines of $K_p = 1$ in Fig. 4. The region of $K_p > 1$ expands as the hopping range becomes longer. This means that the suppression of single-particle hopping enhances the singlet-pairing correlation.

Here, we briefly refer to the effects of the neglected terms in $H_{\text{long-J}}$ model. We consider the system defined by the following Hamiltonian:

$$H \equiv H_{\text{t-J}} + H_{\text{3-site}} + \tilde{H}_{\text{irh}} + H_{\text{lex-J}},$$

$$H_{\text{lex-J}} \equiv J_3 \sum_i (S_i \cdot S_{i+3} - \frac{1}{4} n_in_{i+3})$$

$$+ J_5 \sum_i (S_i \cdot S_{i+5} - \frac{1}{4} n_in_{i+5})$$

$$+ J_7 \sum_i (S_i \cdot S_{i+7} - \frac{1}{4} n_in_{i+7}),$$

where coupling constant $J_j$ is defined as $J_j = J \times t_j^2$ ($j = 3, 5$ and $7$). The spin-gap phase boundary and the contour line of $K_p = 1$ for the above model with $t_3 = 0.6, t_5 = 0.2, t_7 = 1/35$ are shown in Fig. 5. This shows that the long-range spin exchange interaction also enlarges the spin-gap region and the region of $K_p > 1$. The region of singlet pairs may be determined mainly by the following two factors: One is two-particle hopping processes, which enhance the coherent motion of electron pairs and prevent phase separation, and the other is antiferromagnetic fluctuations, which induce attractive interactions between up and down spins. For the $t$-$J$ model in the large $J$ regime, the spin-gap phase exists, but the antiferromagnetic fluctuations are so large that the spin-gap phase is confined in a narrow parameter regime due to instability resulting from phase separation.

For the $t$-$J$ model, single- and two-particle hopping processes are strong enough to prevent phase separation. However, since the larger single-particle hopping is accompanied by the three-site term, it requires a large $J$ to reach the region of $K_p > 1$. The numerical results shown in Fig. 5 indicate that the suppressed single-particle coherence together with preserved two-particle hopping and finite-range spin exchanges contribute to enhancing both the effective attractive interactions between up and down spins and the coherent pair motion.

Here, we consider possible realizations that may be described by the above models. An example is a three-chain system: The central chain is composed of atoms with $d$-orbitals where the Fermi level is located. The other two chains are composed of atoms with $\pi$-orbitals. These $\pi$-orbitals are designed to lie near the Fermi level and to overlap with the $d$-orbitals of the central chain. In such a system, electrons on $d$-orbitals can hop to a distant site by virtual hopping processes through the side chains. The low-energy physics may be described by the tJ3t3 model.

In summary, we have demonstrated that the suppression of the single-particle hopping processes near the Fermi level enlarges both the spin-gap region and the region for the dominance of the pairing. Based on the present results, we propose a possible scenario for a pairing mechanism: If the suppression of the single-particle hopping is sufficient, pairing correlations would be enhanced, which may lead to superconductivity.

Although the models investigated by us are specific and somewhat artificial, the underlying physics would be universal. The concept of flat-band induced pairing instability may be appropriate not only for one-dimensional models with long-range hopping terms, but also for models with short-range hopping terms in higher dimensions, if the single-particle hopping processes are sufficiently suppressed near the Fermi level close to the Mott insulator.

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Fig. 1. Dispersion relations of noninteracting models with long-range hopping terms, where $t_3/t$, $t_5/t$, $t_7/t$ take values of (i), (ii), (iii) in the text. The horizontal line corresponds to the Fermi level at half-filling. For comparison, the dispersion relation of the noninteracting model without long-range hopping terms is also plotted.

Fig. 2. Scaling dimension of the lowest singlet excitation ($x_s$) and that of triplet excitation ($x_t$) at $k = 2k_F$ for the $tJ_3t_7$ model at quarter-filling in a 16-site cluster. We also plot the quantity $x_r \equiv (x_s + 3x_t)/4$. 
Fig. 3. Phase boundary between the Tomonaga-Luttinger (TL) liquid phase and the spin-gap (SG) phase for the tJ3, tJ3t3, tJ3t5 and tJ3t7 models. The symbols are results for clusters of length $L = 8, 10, 12, 14$ and 16.

Fig. 4. Contour lines of $K\rho = 1$ for the tJ3, tJ3t3, tJ3t5 and tJ3t7 models in a 16-site cluster.

Fig. 5. Spin-gap phase boundary and the contour line of $K\rho = 1$ for the tJ3 model with the long-range spin exchange term. The spin-gap phase boundary and the contour line of $K\rho = 1$ for this model are represented by solid circles and a dash-dotted line, respectively. For comparison, we also plot those of the tJ3 model. The spin-gap phase boundary and the contour line of $K\rho = 1$ for the tJ3 model are represented by open circles and a dotted line, respectively.