Superconductivity in the three-leg Hubbard ladder: a Quantum Monte Carlo study

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Abstract

Quantum Monte Carlo method is used to look into the superconductivity in the three-leg Hubbard ladder. The enhanced correlation for the pairing across the central and edge chains, which has been predicted in the weak-coupling renormalization as an effect of coexistence of gapful and gapless spin modes, is here shown to persist for intermediate interaction strengths.

74.20.Mn and 71.27.+a
There is an increasing fascination toward strongly correlated electrons on ladders. This has been kicked off by the pioneering works [1,2], which have proposed that the ladder at half-filling should be a spin liquid with gapful spin excitations for an even number of chains, while odd-numbered chains should be antiferromagnetic (AF) with gapless spin excitations. This property, which is reminiscent of Haldane’s conjecture [1,3,4] for the one-dimensional (1D) AF Heisenberg model for integer and half-odd-integer spins, have been confirmed by numerical calculations [5,6]. Experimentally the ladders realized in cuprates indeed exhibit a spin liquid behavior when two-legged, while a three-leg system shows an AF behavior. [7]

This has led to an expectation that a doping of the ladder with carriers will produce an interchain singlet superconductivity in an even-numbered ladder associated with the persistent spin gap, while an odd-numbered ladder should have the usual $2k_F$ spin-density wave (SDW) reflecting the gapless spin excitations. [8] The superconductivity in two-leg ladders has indeed been confirmed by the perturbational renormalization group for weak-coupling repulsive interactions. [8,9] Most of the numerical calculations for $t - J$ ladder models also support the dominant pairing correlation. [8,10,11] The numerical results for the Hubbard ladder models [17,18] are less conclusive, but some of the controversies have recently been resolved from Quantum Monte Carlo (QMC) calculations, where the pairing correlation is indeed enhanced in Hubbard ladders. [20] Experimentally a occurrence of superconductivity is reported for a cuprate recently [21].

Now, whether the ‘even-odd’ conjecture for superconductivity continues to be valid for triple chains has to be tested. In fact, we [22] and Schulz [23] have independently calculated the correlation functions in the three-leg Hubbard ladder within the weak-coupling theory and have found similar results. The message obtained there is that an odd number (three) of legs can in fact superconduct, providing a counter-example of the even-odd conjecture. A key is that gapless and gapful spin excitations coexist in a three-leg ladder. This has been analytically shown from the correlation functions starting from the phase diagram given by Arrigoni [24], who has enumerated the number of gapless and gapfull modes with the perturbative renormalization-group technique in the weak-coupling limit. The coexisting
gapful and gapless modes gives rise to a peculiar situation where a specific pairing across the central and edge chains (that is roughly a d-wave pairing) is dominant, while the $2k_F$ SDW on the edge chains simultaneously shows a subdominant but still long-tailed (power-law) decay associated with the gapless spin mode. In other words, the dominant superconductivity only requires the existence of gap(s) in not all but some of the spin modes when there are multiple of them.

However, there is a serious question about these weak-coupling approaches. First, only for an infinitesimally small coupling is the weak-coupling theory guaranteed to be valid in principle. Furthermore, when there is a gap in the excitation, the renormalization flows into a strong-coupling regime, so that the weak-coupling (perturbational) theory might break down even for small $U$. Hence it is imperative to study the problem from an independent numerical method, especially for an intermediate strength of the Hubbard $U \sim t$. Although such a study comparing the numerical result for $U \sim t$ with the weak-coupling theory has been done for the two-leg system, this does not necessarily serve to enlighten the situation in the three-leg case, where gapless and gapful modes coexist. This is exactly our motivation for the present study, which reports an extensive QMC calculation for three-leg Hubbard ladder. The result indeed turns out to exhibit an enhancement of the pairing correlation even for finite coupling constant, $U/t = 1 \sim 2$.

The Hamiltonian of the three-leg Hubbard model is given by in standard notations as

$$H = -t \sum_{\mu \sigma} (c_{\mu i \sigma}^{\dagger} c_{\mu i+1 \sigma} + \text{h.c.}) + t_\perp \sum_{i \sigma} (c_{a i \sigma}^{\dagger} c_{b i \sigma} + c_{b i \sigma}^{\dagger} c_{g i \sigma} + \text{h.c.}) + U \sum_{\mu i} n_{\mu i \uparrow} n_{\mu i \downarrow},$$

where $t(t_\perp)$ is the intra- (inter-) chain hopping, $i$ labels the rung while $\mu = \alpha, \beta, \gamma$ labels the leg (with $\beta$ being the central one). In the momentum space we have

$$H = \sum_{k \sigma} \left( -2t \cos(k) - \sqrt{2} t_\perp \right) a_{1k \sigma}^{\dagger} a_{1k \sigma} + 2t \sum_{k \sigma} \cos(k) a_{2k \sigma}^{\dagger} a_{2k \sigma}$$
\[ + \sum_{k} \left( -2t\cos(k) + \sqrt{2}t_\perp \right) a_{\sigma}^{\dagger}a_{\sigma}^{\dagger}a_{\sigma}a_{\sigma}^{\dagger} + U \sum \text{(terms of the form } a_{\sigma}^{\dagger}a_{\sigma}^{\dagger}aa). \]  

(2)

Here \( a_{jk\sigma} \) annihilates an electron with lattice momentum \( k \) in the \( j \)-th band (\( j = 1, 2, 3 \)), where \( a_{jk\sigma} \) is related to \( c_{\mu k\sigma} \) (the Fourier transform of \( c_{\mu i\sigma} \)) through a linear transformation,

\[
\begin{pmatrix}
  c_{\alpha k\sigma} \\
  c_{\beta k\sigma} \\
  c_{\gamma k\sigma}
\end{pmatrix}
= \begin{pmatrix}
  \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\
  \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\
  \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2}
\end{pmatrix}
\begin{pmatrix}
  a_{1k\sigma} \\
  a_{2k\sigma} \\
  a_{3k\sigma}
\end{pmatrix}.
\]  

(3)

If we first recapitulate the weak-coupling theory [22-24], the pair hopping process \( (a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}a_{3\downarrow}a_{3\uparrow} + \text{h.c.}) \) between the first and third bands and the backward-scattering processes within the first or third band become relevant scattering processes. As a result, two spin modes and one charge mode become gapful. This leaves one spin mode and two charge modes gapless, which are characterized by critical exponents, \( K_{\sigma^2}^* (= 1 \text{ for the spin independent interaction}) \) and \( K_{\rho^2}^*, K_{\rho^3}^*, \) respectively [22]. We can recognize that the first (third) band is analogous to the bonding (anti-bonding) band in the two-leg ladder, while the second band is analogous to the single 1D (Luttinger-liquid like) system.

The correlation of the intraband singlet pairing within the first or third band, \( \sum_{\sigma} (a_{1k\sigma}a_{1k-\sigma} - a_{3k\sigma}a_{3k-\sigma}) \), decays like \( r^{-1/2} \) at large distances. This pair, when expressed in a real space via the inverse Fourier transform, is an interchain singlet pair across the central chain and an edge chain, \( \hat{O}_i = (c_{\alpha i\sigma} + c_{\gamma i\sigma})c_{\beta i-\sigma} - (c_{\alpha i-\sigma} + c_{\gamma i-\sigma})c_{\beta i\sigma}. \) All the \( K_{\rho}^* \)'s should tend to unity in the limit of vanishing interaction, where the interchain superconductivity has an exponent of 1/2 while the density wave correlations have exponents of at least 2. [22,23] Thus the pairing correlation is identified as the most dominant. In the weak-coupling renormalization, however, we have to make a reasoning: ‘the pair hopping process and the backward scattering process flow, in the weak-coupling renormalization, into the strong-coupling regime upon our integrating out the high-energy modes, which results in a formation of the gaps’. Thus the validity of the weak-coupling scheme has to be tested as stressed above. This problem should be especially subtle when gapful and gapless modes
Here we employ the projector Monte Carlo method \[26\] to look into the ground state pairing correlation function \( P(r) \equiv \langle O_j^\dagger O_{j+r} \rangle \). We assume periodic boundary conditions along the chain direction, \( c_{N+1} \equiv c_1 \), where \( N \) is the number of rungs. We only consider here the case where the intra- and inter-band Umklapp processes are irrelevant because that is the case where the above mentioned result obtained by weak-coupling theory is valid. The details of the QMC calculation are similar to those for our calculation for the two-leg case. \[20\] Specifically, the negative sign problem makes the QMC calculation feasible for \( U \leq 2t \). We set \( t = 1 \) hereafter.

In the two-leg case with a finite \( U \), we have found an interesting property for finite systems: the pairing correlation is enhanced in agreement with the weak-coupling theory only when the one-electron energy levels of the bonding and anti-bonding bands lie close to each other around the Fermi level (which is certainly the case with an infinite system). \[20\] When the levels are misaligned (for which a 5\% change in \( t_\perp \) is enough), the enhancement of the pairing correlation dramatically vanishes. In the weak-coupling theory, ratio of the spin gap to the level offset is assumed to be infinitely large at the fixed point of the renormalization flow, so that the level offset has to be small for the effect of the spin gap to be detectable in a finite system.

We have found that this applies to the three-leg ladder as well, i.e., the pairing correlation is enhanced when the one-electron levels of the first and third bands lie close to each other. Hence we concentrate on such cases hereafter.

We first show in Fig. 1 the result for \( P(r) \) for \( t_\perp = 0.92 \) with \( U = 1 \) with the band filling \( n = 0.843 = 86 \) electrons/(34 rungs \( \times \) 3 sites). For this choice of \( t_\perp \) the levels in first and third bands lie close to each other around the Fermi level with the level offset being as small as 0.01. We can see that there exists a large enhancement over the \( U = 0 \) result at large distances. This is the key result of this paper.

Although it is difficult to determine the decay exponent of \( P(r) \), we can fit the data by supposing a trial function as expected from the weak-coupling theory as we did in the
two-leg case \[20],

\[ P(r) = \frac{1}{\pi^2} \sum_{d=\pm} \left\{ cr_d^{-1/2} + (2-c)r_d^{-2} \right. \\
- \left. \left[ \cos(2k_{F1}r_d) + \cos(2k_{F3}r_d) \right]r_d^{-2} \right\}. \quad (4) \]

Here \( k_{F1}(k_{F3}) \) is the non-interacting Fermi wave number of the first (third) band, while a constant \( c \), which should vanish for \( U = 0 \), is here least-square fit (by taking logarithm of the data) as \( c = 0.05 \). Since we assume the periodic boundary condition, we have to consider contributions from both ways around, so there are two distances between the 0-th and the \( r \)-th rung, i.e., \( r_+ = r \) and \( r_- = N - r \). The overall decay should be \( 1/r^2 \) as in the single-chain case, while the term \( c/r^{1/2} \), the dominant correlation at large distances, is borrowed from the weak-coupling result. \[22,23\] The QMC result for a finite \( U = 1 \) fits to the trial form (solid line in Fig.1) surprisingly accurately. A finite \( U \) may give some corrections to these functional forms, but even when we best-fit the exponent itself as \( c/r^{\alpha} \) in place of \( c/r^{1/2} \), we obtain \( \alpha < 0.7 \) with a similar accuracy.

In Fig.2, we show the result for a larger interaction \( U = 2 \). The result again shows the enhanced pairing correlation at large distances. However, the enhancement is slightly reduced than the \( U = 1 \) case. This is consistent with the weak-coupling theory, in which \( K_\rho^* \)'s should be a decreasing function of \( U \).

Finally, we study if the presence of band 2 around \( E_F \) can be detrimental to superconductivity. In Fig.3, we make the one-electron energy levels of all the three bands lie close to each other around the Fermi level. This is accomplished here for \( t_\perp = 0.685 \) and the band filling \( n = 0.719 = 82 \) electrons/(38 rungs \( \times \) 3 sites). The highest occupied level of the second band then lies between that of the first band and the lowest unoccupied level of the third band (lying above the highest occupied level of the first band by as small as 0.01, inset of Fig.3).

The result in Fig.3 for \( U = 1 \) shows that the pairing correlation is enhanced as well. Thus we may consider that the second band does not hinder the superconductivity in other bands. This is also consistent with the weak-coupling theory, in which all of the scattering
processes connected with the second band are irrelevant. The fit of the correlation function to the trial one is again excellent with $c = 0.03$.

It is intriguing to investigate how the intermediate-$U$ regime (which is shown in the present study to be similar to the weak-coupling situation) would cross over to the large-$U$ Hubbard model. It is also important to study the pairing correlation function in the three-leg $t - J$ ladder in order to clarify similarities and differences between $t - J$ and Hubbard ladders, since the former with an infinitesimal $J \sim t^2/U$ is an effective Hamiltonian of the latter with large $U$. The crossover to larger (especially odd) numbers of legs in the Hubbard model is also of interest.

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FIGURES

FIG. 1. The QMC result for the pairing correlation function, $P(r)(\bullet)$, plotted against the real space distance $r$ in a three-leg Hubbard ladder with 34-rung having 86 electrons for $U = 1$ with $t_\perp = 0.92$. The dashed line is the non-interacting result for the same system size, while the straight dashed line represents $\sim r^{-2}$. The solid line is a fit to a trial function (see text).

FIG. 2. A similar plot as in Fig.1 for $U = 2$.

FIG. 3. A similar plot as in Fig.1 for a 38-rung system having 82 electrons for $U = 1$ with $t_\perp = 0.685$. The inset schematically depicts the positions of energy levels for the non-interacting case.
Fig. 1
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Fig.2
