Correlation functions in the three-chain Hubbard ladder

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In order to check whether odd-numbered Tomonaga-Luttinger ladders are dominated by antiferromagnetic correlations associated with gapless spin excitations, correlation functions of the doped three-chain Hubbard model are obtained with the bosonization at the renormalization-group fixed point. The correlation of the singlet superconducting pairing across the central and edge chains is found to be dominant, reflecting two gapful spin modes, while the intraedge spin-density-wave correlation, reflecting the gapless mode, is only subdominant. This implies that, when there are multiple spin modes, a dominant superconductivity can arise from the presence of *some* spin gap(s) despite the coexistence of power-law correlated spins. [S0163-1829(96)52338-6]

Recently, a wealth of experimental and theoretical results indicate that interacting electrons on multiple chains, or ladders, are an interesting realm of correlated systems. An increasing fascination toward them has been kicked off by an ''even-odd'' conjecture by Rice *et al.*, who have proposed that the ladder, at half filling, with even number of chains should be a spin liquid reflecting the absence of gapless spin excitations, while odd-numbered chains should be antiferromagnetic (AF) reflecting the presence of gapless spin excitations.[1–3] This is reminiscent of Haldane's conjecture[4,5] for the one-dimensional (1D) AF Heisenberg model for integer and half-odd-integer spins.

When the system is doped with carriers, it is usually supposed that an even-numbered ladder should exhibit the interchain singlet superconductivity as expected from the persistent spin gap, while an odd-numbered ladder should have the usual $2k_F$ spin-density wave (SDW) reflecting the gapless spin excitations. In 1D, an interacting electron system may be described by the Tomonaga-Luttinger liquid.[6] Thus intensive analytical studies have been performed by extending the Tomonaga-Luttinger model analysis to the two-chain ladders. These analytical calculations support the superconductivity in double chains within the perturbational renormalization-group analysis for weak repulsive interactions.[7–11] To be more precise, the correlation of the interchain pairing is dominant and much stronger than that of the subdominant $4k_F$ charge-density wave (CDW) in the above calculations. On the other hand, numerical calculations performed directly for the two-chain t-J and Hubbard models have also been performed, although the phase diagram including the strong-coupling regime has not been conclusive.[12–16]

Experimentally, cuprates $SrCu_2O_3$ and $Sr_2Cu_3O_5$ are investigated as prototypes of two and three-chain systems, respectively.[17] The two-chain system indeed shows a spin-liquid behavior characteristic of a finite spin-correlation length, while the three-chain system shows an AF behavior.

Theoretically, however, whether the ''even-odd'' conjecture continues to be valid for triple chains remains an open question. In fact, Arrigoni has looked into the triple chains having weak interactions by using the usual perturbational renormalization-group technique to conclude that gapless and gapful spin excitations *coexist* there.[18] Namely, he has actually enumerated the numbers of gapless charge and spin modes on the phase diagram spanned by the doping level and the interchain electron-tunneling strength. He found that, at half filling, one gapless spin mode exists for the interchain hopping comparable with the intrachain hopping, in agreement with some experimental results and theoretical expectations. Away from the half filling, on the other hand, one gapless spin mode is found to remain at the fixed point in the region where the fermi level intersects all the three bands in the noninteracting case. From this, Arrigoni argues that the spin-spin correlation should decay as a power law.

On the other hand, his result also indicates that two gapful spin modes exist in addition. While the existence of a gapful spin mode crudely favors a singlet superconductivity (SS), we are in fact faced here with an intriguing problem of what happens when gapless and gapful spin modes coexist, since it may well be possible that the presence of gap(s) in *some* out of multiple spin modes may be sufficient for a dominance of superconductivity. This has motivated us, in the present work, to actually look at the correlation functions using the bosonization method at the fixed point away from half filling. Since we have the cuprate ladder in mind, we concentrate on the open boundary condition (OBC) across the chain, where the central chain is inequivalent to the two edge chains. We find that the interchain SS pairing between the central and edge chains is the dominant correlation, which is indeed realized due to the presence of the two gapful spin modes. On the other hand, the SDW correlation, which has a power law for the intraedge chain reflecting the gapless spin mode, is only subdominant.

We start from the Hamiltonian,

$$H = H_0 + H_{\rm int}, \tag{1}$$

$$H_0 = \sum_{irk\sigma} \epsilon_k a^\dagger_{irk\sigma} a_{irk\sigma} - t \sum_{rk\sigma} (a^\dagger_{\alpha rk\sigma} a_{\beta rk\sigma} + a^\dagger_{\beta rk\sigma} a_{\gamma rk\sigma} + \text{H.c.}). \tag{2}$$

Here $a^{\dagger}_{irk\sigma}$ creates an electron with lattice momentum k and spin σ on right ($r=R$) or left ($r=L$) going branch in the ith chain ($i=\alpha,\beta,\gamma$, with β being the central one), ϵ_k the kinetic energy of each chain, and t the interchain hopping. The one-electron part, H_0, may be diagonalized by a linear transformation,

$$\begin{pmatrix} a_{\alpha rk\sigma} \\ a_{\beta rk\sigma} \\ a_{\gamma rk\sigma} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{2}}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{\sqrt{2}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} c_{1rk\sigma} \\ c_{2rk\sigma} \\ c_{3rk\sigma} \end{pmatrix} \tag{3}$$

resulting in

$$H_0=\sum_{rk\sigma} [(\epsilon_k-\sqrt{2}t)c^{\dagger}_{1rk\sigma}c_{1rk\sigma}+\epsilon_k c^{\dagger}_{2rk\sigma}c_{2rk\sigma} + (\epsilon_k+\sqrt{2}t)c^{\dagger}_{3rk\sigma}c_{3rk\sigma}]. \tag{4}$$

Hereafter we linearize the band structure around the fermi points as usual and neglect the difference in the fermi velocities of three bands, which will be acceptable for the weak-hopping case.[19] We focus on the case in which all of three bands are away from half filling.

The part of the Hamiltonian, H_d, that can be diagonalized in the bosonization only includes forward-scattering processes in the band picture, and has the form

$$H_d=H_{\rm spin}+H_{\rm charge},$$

$$H_{\rm spin}=\sum_i \frac{v_{\sigma i}}{4\pi}\int dx\left[\frac{1}{K_{\sigma i}}(\partial_x\phi_{i+})^2+K_{\sigma i}(\partial_x\phi_{i-})^2\right], \tag{5}$$

$$H_{\rm charge}=\sum_i \frac{v_{\rho i}}{4\pi}\int dx\left[\frac{1}{K_{\rho i}}(\partial_x\chi_{i+})^2+K_{\rho i}(\partial_x\chi_{i-})^2\right].$$

Here ϕ_{i+} is the spin phase field of the ith band, χ_{i+} is the diagonal charge phase field, while $\phi_{i-}(\chi_{i-})$ is the field dual to $\phi_{i+}(\chi_{i+})$, $K_{\sigma i}(K_{\rho i})$ the correlation exponent for the $\phi(\chi_i)$ phase with $v_{\sigma i}(v_{\rho i})$ being their velocities. For the Hubbard-type interaction, we have $v_{\sigma i}=v_F$, $K_{\sigma i}=1$ for all i's, while $v_{\rho 1}=v_F$, $v_{\rho 2}=v_F\sqrt{1-4g^2}$, $v_{\rho 3}=v_F\sqrt{1-g^2/4}$, $K_{\rho 1}=1$, $K_{\rho 2}=\sqrt{(1-2g)/(1+2g)}$, $K_{\rho 3}=\sqrt{(1-g/2)/(1+g/2)}$, where $g=U/2\pi v_F$ is the Hubbard U interaction made dimensionless.

The diagonalized charge field $\chi_{i\pm}$ is linearly related to the initial charge field $\theta_{i\pm}$ of the ith band as

$$\begin{pmatrix} \theta_{1\pm} \\ \theta_{2\pm} \\ \theta_{3\pm} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \end{pmatrix} \begin{pmatrix} \chi_{1\pm} \\ \chi_{2\pm} \\ \chi_{3\pm} \end{pmatrix}, \tag{6}$$

where $\theta_{i\pm}$ and $\phi_{\pm}$ are related to the field operator for electrons $\psi_{ir\sigma}$ as

$$\psi_{i+(-)\sigma}(x)=\frac{\eta_{i+(-)\sigma}}{2\pi\Lambda}\exp\left\{\pm ik_{iF}x\pm\frac{i}{2}\{\theta_{i+}(x)\pm\theta_{i-}(x) + \sigma(\phi_{i+}(x)\pm\phi_{i-}(x))\}\right\}. \tag{7}$$

Here $\eta_{ir\sigma}$'s are Majorana fermion operators (or Haldane's U operators)[20] which ensure the anticommutation relations between electron operators through the relation, $\{\eta_{ir\sigma},\eta_{i'r'\sigma'}\}_+=2\delta_{ii'}\delta_{rr'}\delta_{\sigma\sigma'}$, $\eta^{\dagger}_{ir\sigma}=\eta_{ir\sigma}$.

There are still many scattering processes corresponding to the backward scattering and pair tunneling scattering processes between two bands, which cannot be treated exactly. Arrigoni examined the effect of such scattering processes by the diagrammatic perturbational renormalization group technique. He found that the backward-scattering interactions within the first or the third band turn from positive to negative as the renormalization is performed and that the pair tunneling processes between the first and third bands also become relevant. At the fixed point the Hamiltonian density, H^*, then takes the form, in term of the phase variables,

$$H^*=-\frac{g_b(1)}{\pi^2\Lambda^2}\cos[2\phi_{1+}(x)]-\frac{g_b(3)}{\pi^2\Lambda^2}\cos[2\phi_{3+}(x)] + \frac{2g_{ft}(1,3)}{\pi^2\Lambda^2}\cos[\sqrt{2}\chi_{1-}(x)]\sin\phi_{1+}(x)\sin\phi_{3+}(x), \tag{8}$$

where $g_b(1)$, $g_b(3)$ are negative large quantities and $g_{ft}(1,3)$ is a positive large quantity.[21]

This indicates that the phase fields ϕ_{1+}, ϕ_{3+}, and χ_{1-} are long-range ordered and fixed at $\pi/2$, $\pi/2$, and $\pi/\sqrt{2}$, respectively, which in turn implies that the correlation functions that contain ϕ_{1-}, ϕ_{3-}, and χ_{1+} fields decay exponentially. The renormalization procedure will affect the velocities and the critical exponents for the gapless fields, $\chi_{2\pm}$, $\chi_{3\pm}$, and $\phi_{2\pm}$, so that we should end up with renormalized v^*'s and K^*'s.

In principle, the numerical values of renormalized v^*'s and K^*'s for finite g may be obtained from the renormalization equations as has been attempted for a double chain by Balents and Fisher,[10] although it would be difficult in practice. However, at least in the weak-coupling limit, $g\to 0$, to which our treatment is meant to fall upon, we will certainly have $v^*\simeq v_F$ and $K^*\simeq 1$ for *gapless* modes even after the renormalization procedure.

Now we are in position to calculate the correlation functions. The two-particle correlation functions which include the following two particle operators in the band description show power-law decay:

(1) operators constructed from two operators only in the second band (since the charge and spin phases are both gapless, electrons in this band should have the usual Luttinger-liquid behavior),

(2) order parameters of singlet superconductivity in the first or third bands, $\psi_{1+\uparrow(\downarrow)}\psi_{1-\downarrow(\uparrow)}$, $\psi_{3+\uparrow(\downarrow)}\psi_{3-\downarrow(\uparrow)}$.

As a result, the order parameters that possess power-law decays should be the following, where we also give the exponents:

(A) The correlations within each of the two edge (α and γ) chains or across the two edge chains:

(a) $2k_F$ CDW, $O_{\text{intra CDW}}=\psi^\dagger_{\alpha(\gamma)+\uparrow}\psi_{\alpha(\gamma)-\uparrow}$; $O_{\text{inter CDW}}=\psi^\dagger_{\alpha(\gamma)+\uparrow}\psi_{\gamma(\alpha)-\uparrow}$,

(b) $2k_F$ SDW, $O_{\text{intra SDW}}=\psi^\dagger_{\alpha(\gamma)+\uparrow}\psi_{\alpha(\gamma)-\downarrow}$; $O_{\text{inter SDW}}=\psi^\dagger_{\alpha(\gamma)+\uparrow}\psi_{\gamma(\alpha)-\downarrow}$,

(c) singlet pairing (SS), $O_{\text{intra SS}}=\psi_{\alpha(\gamma)+\uparrow}\psi_{\alpha(\gamma)-\downarrow}$; $O_{\text{inter SS}}=\psi_{\alpha(\gamma)+\uparrow}\psi_{\gamma(\alpha)-\downarrow}$,

(d) triplet pairing (TS), $O_{\text{intra TS}}=\psi_{\alpha(\gamma)+\uparrow}\psi_{\alpha(\gamma)-\uparrow}$; $O_{\text{inter TS}}=\psi_{\alpha(\gamma)+\uparrow}\psi_{\gamma(\alpha)-\uparrow}$,

(B) The singlet pairing across the *central* chain (β) and an edge chain, $O_{\text{central SS}}=\psi_{\alpha(\gamma)+\uparrow}\psi_{\beta-\downarrow}$.

In the band picture we can rewright $O_{\text{central SS}}$ as primarily comprising $O_{\text{central SS}}\sim\psi_{1+\uparrow}\psi_{1-\downarrow}-\psi_{3+\uparrow}\psi_{3-\downarrow}$. We may thus call this paring d-wave-like in a similar sense as in the two-chain case, in which a pair is called d-wave when the pairing within the bonding band and that within antibonding band enter with opposite signs.[9,14]

Thus the edge-chain SDW correlation has a power-law decay, while the SDW correlation within the central chain decays exponentially since it consists of the terms containing ϕ_{1-} and/or ϕ_{3-} phases. Although we calculate the case away from half filling, the SDW correlation should obviously be more enhanced at half filling. NMR experiments at half filling[17] show that the nuclear-spin relaxation rate $1/T_1$ which is represented by the imaginary part of the dynamical susceptibility increase with decreasing temperature for the three-chain cuprates in contrast to the two-chain case. This is consistent with the present result, since the experiments should detect the total SDW correlation of all the chains.

Intraedge or interedge correlation functions have to involve forms bilinear in c_2 in Eq. (3). They are described in terms of the second band θ_2, which does not contain χ_1 [Eq. (6)], a phase-fixed field. Thus the edge-channel correlations are completely determined by the character of the second band (the Luttinger-liquid band), while the other phase fields, being gapful, are irrelevant. The final result for the edge-channel correlations at large distances, up to $2k_F$ oscillations, is as follows regardless of whether the correlation is intraedge or interedge:

$$\begin{aligned}
&\langle O_{\text{CDW}}(x)O^\dagger_{\text{CDW}}(0)\rangle\sim x^{-(1/3)\,(K^*_{\rho2}+2K^*_{\rho3})-K^*_{\sigma2}},\\
&\langle O_{\text{SDW}}(x)O^\dagger_{\text{SDW}}(0)\rangle\sim x^{-(1/3)\,(K^*_{\rho2}+2K^*_{\rho3})-(1/K^*_{\sigma2})},\\
&\langle O_{\text{SS}}(x)O^\dagger_{\text{SS}}(0)\rangle\sim x^{-(1/3)\,[(1/K^*_{\rho2})+(2/K^*_{\rho3})]-K^*_{\sigma2}},\\
&\langle O_{\text{TS}}(x)O^\dagger_{\text{TS}}(0)\rangle\sim x^{-(1/3)\,[(1/K^*_{\rho2})+(2/K^*_{\rho3})]-(1/K^*_{\sigma2})}.
\end{aligned}\tag{9}$$

By contrast, if we look at the pairing $O_{\text{central SS}}(x)$ across the central chain and one of the edge chains, this pairing, which circumvents the on-site repulsion and is linked by the resonating valence bonding between the neighboring chains, is expected to be stronger than other correlations as in the two-chain case. The correlation function for $O_{\text{central SS}}(x)$ is indeed calculated to be

$$\langle O_{\text{central SS}}(x)O^\dagger_{\text{central SS}}(0)\rangle\sim x^{-(1/3)\,[(1/K^*_{\rho2})+(1/2K^*_{\rho3})]},\tag{10}$$

In the weak (infinitesimal) interaction limit, all the K^*'s tend to unity, where the SS exponent becomes as small as 1/2 while the exponents of other correlations tend to 2. Thus, at least in this limit, the central SS correlation dominates over the others.[22] The duality relation (in which the pairing and density-wave exponents are reciprocal of each other[11]) is similar to that in the two-chain case, in which the interchain-SS exponent is 1/2 while the exponent of the $4k_F$ CDW is 2.

In summary, we have studied correlation functions using the bosonization method at the renormalization-group fixed point away from half filling. We found that the dominant correlation is the interchain singlet pairing across the central chain and either of the edge chains. The key message is that there is an example where the dominance of superconductivity only requires the existence of gap(s) in some spin mode, despite the coexistence of a power-law spin-spin correlation, when there are multiple modes. It would be interesting to further look into how the situation for the single, double, triple,..., chains crosses over to the two-dimensional system.

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[22] Mathematically, the reason why the exponents for the edge-channel SS correlations have to be greater than that for $O_{\text{central SS}}$ is that O_{SS} contains a summation $\psi_{1+\uparrow}\psi_{1-\downarrow}+\psi_{3+\uparrow}\psi_{3-\downarrow}$, which is proportional to $\cos(\chi_{1-}/\sqrt{2})\sim 0$, while $O_{\text{central SS}}$ is the subtraction, $\psi_{1+\uparrow}\psi_{1-\downarrow}-\psi_{3+\uparrow}\psi_{3-\downarrow}$, which is proportional to $\sin(\chi_{1-}/\sqrt{2})\sim 1$. This is the same mechanism by which the interchain SS becomes dominant (while the intrachain SS decays exponentially) in a two-chain system.