

Superconductivity in the Two-Chain Hubbard Model Including the Interchain Coulomb Interaction

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Recently, two-chain (2C) systems have been extensively studied from theoretical, computational and experimental points of view. We have been studying the 2C Hubbard model^{1,2)} because this model is the most basic one for the Coulomb-origin mechanism of superconductivity. In terms of the bonding and antibonding orbitals on the rung this model can be rewritten into a two-band model of the type originally proposed by J. Kondo,³⁾ and appearance of an SC state has been strongly indicated by numerical studies,^{1,2)} when the interchain transfer energy has an appropriate value, presumably due to the interband electron-pair transfer generated by the on-site Coulomb repulsion. In trying to apply this mechanism to real ladder systems there is a suspicion that the SC state may be suppressed by an appreciable interchain Coulomb interaction, because it weakens the interband pair-transfer effect and strengthens the intraband Coulomb repulsion. In this paper we study this problem by means of Lanczos exact-diagonalization method. We find that the SC phase preserves its region tenaciously against the increase of the interchain repulsion. This feature is remarkable and removes the problem in obtaining superconductivity in real 2C systems.

The 2C Hubbard model is given by

$$H = H_0 + H_1, \quad (1)$$

$$H_0 = t_d \sum_{l,\sigma} (c_{1l\sigma}^\dagger c_{2l\sigma} + \text{H.c.}) + t \sum_{j=1}^2 \sum_{l,\sigma} (c_{j l \sigma}^\dagger c_{j, l+1, \sigma} + \text{H.c.}), \quad (2)$$

$$H_1 = U_0 \sum_{j=1}^2 \sum_l c_{j l \uparrow}^\dagger c_{j l \uparrow} c_{j l \downarrow}^\dagger c_{j l \downarrow}, \quad (3)$$

where $c_{j l \sigma}^\dagger$ ($c_{j l \sigma}$) is the creation (annihilation) operator of an electron with spin σ at the l th site along the j th chain ($j=1,2$), t is intrachain transfer energy and t_d is interchain transfer energy. By bringing in the bonding and antibonding combinations $a_{j l \sigma} = (c_{1 l \sigma} +$

$(-1)^j c_{2 l \sigma})/\sqrt{2}$, $j = 1, 2$, on the l th rung and making the Fourier transformation, H_0 is diagonalized into two bands with dispersions, $2t \cos k + (-1)^j t_d$, $j = 1, 2$. In terms of new operators $a_{j l \sigma}$, H_1 is rewritten into four terms; intraband Coulomb term with coupling constant U_j , $j = 1, 2$, interband Coulomb term with U' , interband pair-transfer term with K and interband exchange term with L . All coupling constants are equal, i.e., $U_1 = U_2 = U' = K = L = U_0/2$. The pair-transfer term with K transfers a pair of electrons with up and down spins from one band to the other. This process promotes a BCS-like pairing against the opposing intraband Coulomb terms with U_j . Fortunately, K is as large as U_j , which we interpret to bring about an SC state which has been strongly indicated in numerical studies in a band situation where the upper band is touching the Fermi level lying in the lower band.^{1,2)}

In this paper, we bring into this 2C Hubbard model the interchain Coulomb interaction with coupling constant V_d defined by

$$H_2 = V_d \sum_{l\sigma\sigma'} c_{1l\sigma}^\dagger c_{1l\sigma} c_{2l\sigma'}^\dagger c_{2l\sigma'}. \quad (4)$$

When we rewrite H_2 in terms of $a_{j l \sigma}$ operators, we get similar interaction terms as stated above with slightly modified constants: $U_1 = U_2 = U' = (U_0 + V_d)/2$, $K = L = (U_0 - V_d)/2$. Here K promoting pairing diminishes but U_j opposing pairing enlarges, both leading to weakening of pairing. Our problem is to what extent the superconductivity is weakened by the interchain Coulomb interaction. We apply the Lanczos exact-diagonalization method to this extended model in order to get the ground-state energy. We treat ten electrons on the lattice having six rungs, or 2×6 sites, with antiperiodic boundary condition along the chain. Obtaining the ground-state wave function $|g\rangle$ by means of the conjugate-gradient method, we have calculated the following SC-pair correlation functions:

$$P_{s-} = \langle g | \Delta_-^\dagger \Delta_- + \text{H.c.} | g \rangle, \quad (5)$$

$$P_{s-}(m) = \sum_l \langle g | \Delta_-^\dagger(l) \Delta_-(l+m) | g \rangle / N, \quad (6)$$

where pair operators are defined by

$$\Delta_- = \sum_l \Delta_-(l) / \sqrt{N}, \quad (7)$$

$$\Delta_-(l) = a_{1l\downarrow} a_{1l\uparrow} - a_{2l\downarrow} a_{2l\uparrow} = c_{1l\downarrow} c_{2l\uparrow} - c_{1l\uparrow} c_{2l\downarrow}. \quad (8)$$

$\Delta_-(l)$ annihilates a singlet pair on the l th rung. In Fig. 1, we show P_{s-} and $P_{s-}(m)$ for the case of $U_0 = 8$ and $V_d = 2$. The unit of energy is t .

We see that when $0.91 \lesssim t_d \lesssim 1.35$, P_{s-} is clearly enhanced in Fig. 1(a). The SC correlation enhancement is more pronounced in the P_{s-} vs m curves in Fig. 1(b). We interpret this region as SC phase as in the previous works.^{1,2)} We varied the value of parameters, i.e., U_0 , V_d and t_d , and obtained the SC phase diagram shown in Fig. 2. The SC region was checked to exist at least up to $V_d = 15$. For negative V_d the SC region extends in t_d at small U_0 . We see that the SC state survives against interchain Coulomb repulsion quite tenaciously.

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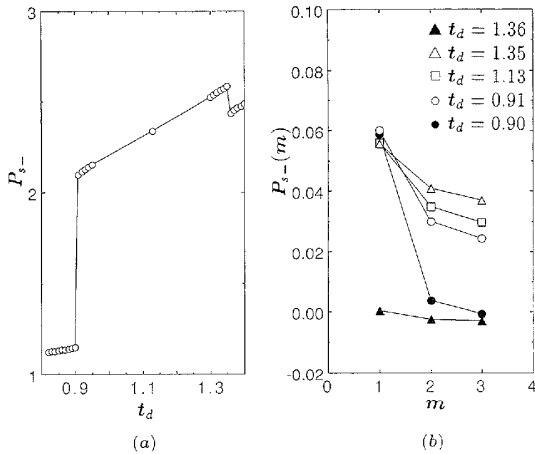


Fig. 1. (a) t_d dependence of correlation function P_{s-} in the case of 2×6 sites, 10 electrons, $V_d = 2$ and $U_0 = 8$. (b) SC pair correlation function $P_{s-}(m)$ against the separation m of pairs in the same case. Open and filled symbols correspond to the SC and non-SC state, respectively.

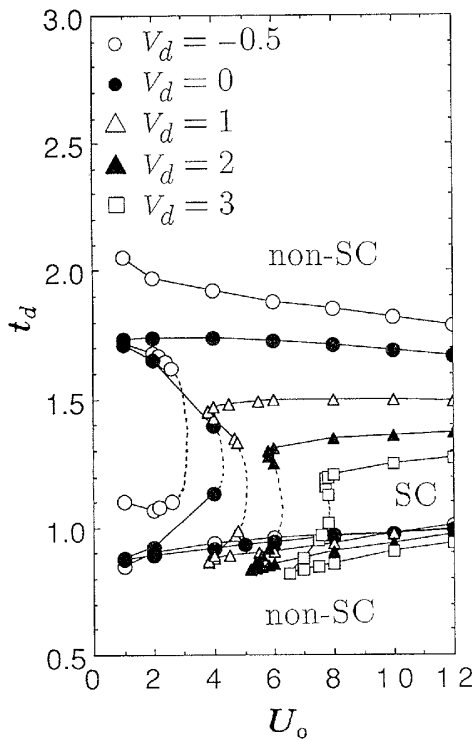


Fig. 2. SC phase diagram in the case of 2×6 sites, 10 electrons of each V_d . When V_d becomes large, the SC region is shifted to larger values of U_0 and becomes smaller but survives tenaciously. Dotted curves are the guide for the eyes.

For fixed U_0 the SC region disappears when V_d exceeds $\sim 0.4U_0$ for $U_0 \sim 8$. The ratio of the upper bound for V_d to U_0 increases with increasing U_0 .

At $U_0 = 8$ we have checked that the SC state is a spin singlet state (SS), the non-SC state in the region of larger t_d is a triplet state (TS) and the non-SC state in the region of smaller t_d is singlet (SS). This indicates that the system has a spin gap phase in a wide region covering the SC phase as known in the 2C Hubbard model,⁴⁾ although the present system size is too small to conclude about this state.

Now we consider why the SC state survives tenaciously against the interchain Coulomb interaction. We calculate the difference between the lowest SS and TS energies when a pair of electron is on a rung separated from the surrounding. It is given by $4t_d^2/(U - V_d)$ for $V_d \ll U_j$. Since it is larger than in the absence of V_d , SS is more stabilized against TS. As seen from the rewritten interaction, existence of singlet pairs on the rungs should help the pair transfer process with K work efficiently and the SC phase resist against V_d . We can see the stabilization of SS in another way, transforming this model to a 2C t - J model. Following the transformation of the Hubbard model to the t - J model,⁵⁾ we get the 2C t - J model for the present case, with the exchange constant along the chain $J = 4t^2/U$ and that for the rung $J_d = 4t_d^2/(U - V_d)$. The interchain Coulomb interaction remains, making a difference to the pure t - J model. With finite positive V_d , J_d for the rung increases, stabilizing the SS on the rung. We consider that this singlet stabilizing effect partly cancels detrimental effects of V_d to the SC phase such as chasing away of the electron pair on the rung and weakening of the transfer of singlet pairs. The above consideration is in accord with the fact that even when we brought in the nearest neighbor Coulomb interaction along the chain instead of V_d , the modification of the SC phase was much smaller than in the interchain Coulomb case.

In summary, we have calculated the 2C Hubbard model including the interchain Coulomb interaction with coupling constant V_d and obtained a result indicating that the SC phase survives in a large region $V_d \lesssim 0.4U_0$ from exact diagonalization calculations. This wideness of the SC phase against V_d is suggested to come from an effect of V_d stabilizing the singlet state on each rung which partly cancels detrimental effects of V_d .

- 1) K. Yamaji and Y. Shimoi: Physica C222 (1994) 349.
- 2) K. Yamaji, Y. Shimoi and T. Yanagisawa: Physica C235-240 (1994) 2221.
- 3) J. Kondo: Prog. Theor. Phys. 29 (1963) 1.
- 4) R. M. Noack, S. R. White and D. J. Scalapino: Europhys. Lett. 30 (1995) 163.
- 5) C. Gros, R. Joynt, T. M. Rice: Phys. Rev. B36 (1987) 381.