Superconductivity in a two-band Hubbard model

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(Received 3 January 1990; revised manuscript received 28 March 1990)

As a model for high-T_c superconductors, a two-band Hubbard model is proposed. When the Coulomb interactions are introduced between the α and β orbitals, an effective attraction of carriers in the β (doped) band is shown to arise in an appropriate condition. The quantum Monte Carlo method is used to confirm the occurrence of Cooper pairing in finite two-band Hubbard systems. The attraction, which also appears in the density-density correlation, enhances the on-site singlet Cooper pair-pair correlation in the β band and suppresses the antiferromagnetic spin-spin correlation in the α band. The criterion for the pairing and the nature of the pairing are discussed. Thus we provide a mechanism of superconductivity specific to strongly correlated two-band systems.

I. INTRODUCTION

The mechanism of high-T_c superconductivity has become one of the most challenging problems in solid-state physics, since the high-T_c copper oxides were discovered by Bednorz and Müller.[1] A body of experimental indications suggests electronic mechanisms for the occurrence of the superconductivity arising from strong electron correlation.

After a pioneering suggestion to this effect by Anderson,[2] the Hubbard model, a prototype of the strongly correlated electron system, has been a subject of intensive theoretical study. Experimental results[3] show that the superconductivity appears just after the antiferromagnetic spin ordering is suppressed in the phase diagram versus the doping level, and this is considered to be an indication that strong electron correlation is a key factor.

Since the simple, single-band Hubbard model seems to suffice for the mechanism in terms of the resonating-valence-bond picture,[2] numerical studies for the model have been performed by a number of authors[4–6] with the direct diagonalization method for small systems or the conventional quantum Monte Carlo method at finite temperatures in one dimension (1D) and two dimensions (2D). Recently Sorella *et al.*[7] have proposed a novel quantum Monte Carlo method that enables us to obtain the ground state for systems of a size intractable by direct diagonalization. The method has been applied to the Hubbard model by Sorella *et al.*[7] and also by Imada and Hatsugai[8] and White *et al.*[9] These results do not support unambiguously the occurrence of superconductivity, or more precisely, the tendency towards Cooper pairing, in the single-band Hubbard model. In simplified models such as the t-J model, some enhanced pairing has been obtained. However, this has been explained[10] as an essential difference between the t-J and the original Hubbard models. The carrier-carrier attraction is overestimated in the t-J model as compared with the Hubbard model.

From the early stage of the theoretical study of high-T_c copper oxides, on the other hand, several theories suggest that the existence of more than one orbital per CuO unit is essential for superconductivity. The existence of O $2p$ orbitals has been explicitly considered in various models.[11–23] Numerical studies for models including O $2p$ (the d-p model) indicate that there is a slight enhancement of superconducting susceptibility, but the results have not been conclusive. The problem of superconductivity is also ambiguous for other models such as the "coupled spin-fermion model," in which one of the bands has degenerated into a spin system or Kondo centers rather than a fermion system.

In this paper we propose a new mechanism of Cooper pairing *specific to a strongly correlated two-band system.* Our study is motivated by an observation that a two-band model in its original Hubbard form should be required for the electronic structure, especially for doped bands, as is indeed shown from the present results. The idea is numerically confirmed by the Sorella quantum Monte Carlo method. A brief account of the present work has been published elsewhere.[24] The present study also gives an insight for the long-standing question of whether superconductivity can arise from purely repulsive interactions. Muttalib and Emery have addressed this problem using a two-band Luttinger model for spinless fermions as a model for fluctuating-valence systems, organic superconductors, and heavy-electron superconductors.[25] They have concluded that superconductivity can exist in the Luttinger model with only repulsive interactions. The present work shows that superconductivity can exist in the Hubbard model.

II. FORMULATION

Usually the term "multiband Hubbard model" is used in a loose sense, in which models considering oxygen $2p$ orbitals in addition to copper $3d$ orbitals are also called multiband models. When the coupling among different orbitals is hybridization alone, introduction of multiple orbitals amounts to taking molecular-orbital basis functions.

Instead, we consider here a two-band model in which there are two orthogonal (molecular) orbitals on each site with inter-orbital as well as intra-orbital electron-electron interactions. A typical model along this line proposed by

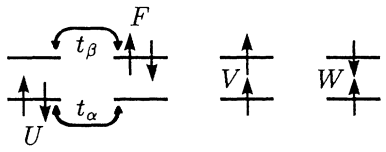

FIG. 1. The two-band Hubbard-model Hamiltonian.

Aoki and Kamimura[15] considers hybridized Cu $3d-$O $2p$ orbitals of different symmetries such as a_{1g} and b_{1g}. The model Hamiltonian is given, in the standard notation, by

$$H=\sum_{\nu=\alpha,\beta}\sum_{\langle i,j\rangle}\sum_{\sigma}t^{\nu}(c_{i\sigma}^{\nu\dagger}c_{j\sigma}^{\nu}+\text{H.c.})+\sum_{\iota,\mu,\nu}U_{\mu\nu}n_{\iota\uparrow}^{\mu}n_{\iota\downarrow}^{\nu}+\sum_{i\sigma}(U_{\alpha\beta}-J)n_{i\sigma}^{\alpha}n_{i\sigma}^{\beta}-J\sum_{i\sigma}c_{i\sigma}^{\alpha\dagger}c_{i-\sigma}^{\alpha}c_{i-\sigma}^{\beta\dagger}c_{i\sigma}^{\beta}\ , \tag{1}$$

where $\langle i,j\rangle$ are nearest-neighbor Cu-O units, α,β label orbitals, and σ is the spin. Here t^{α} (t^{β}) is the transfer energy in the α (β) band, $U_{\alpha\beta}$ is the on-site Coulomb repulsion between the α and β orbitals, and J is the intra-atomic exchange energy.

To simplify the model to some extent, here we neglect the exchange processes to obtain

$$H=\sum_{\nu=\alpha,\beta}\sum_{\langle i,j\rangle}\sum_{\sigma}t^{\nu}(c_{i\sigma}^{\nu\dagger}c_{j\sigma}^{\nu}+\text{H.c.})+\sum_{\iota}(Un_{\iota\uparrow}^{\alpha}n_{\iota\downarrow}^{\alpha}+Fn_{\iota\uparrow}^{\beta}n_{\iota\downarrow}^{\beta})+\sum_{i,\sigma}(Wn_{i\sigma}^{\alpha}n_{i-\sigma}^{\beta}+Vn_{i\sigma}^{\alpha}n_{i\sigma}^{\beta}) \tag{2}$$

in which the interaction terms only contain number operators. Here U (F) is the repulsion within the α (β) orbital and V (W) is the inter-orbital repulsion for the parallel (antiparallel) spins with $V=W-J$ (Fig. 1). We assume no hybridization (transfer) between the molecular orbitals on different sites.[26] Thus the number of electrons in each band remains constant, and the difference in the energy levels of orbitals is only implicitly taken into account in that we assume the α band is (half) filled, while the doped carriers go into the β band.

From theoretical estimates,[27] magnitudes of parameters for individual atomic orbitals are transfer energy $|t|\sim 1$ eV, on-site Hubbard repulsions ~ 10 eV for copper $3d$ and ~ 5 eV for oxygen $2p$ orbitals, and intra-atomic exchange interaction $J\sim 1.5$ eV. Since we are considering interaction among electrons in molecular orbitals, interaction parameters should be modified from these atomic values. Specifically, different molecular orbitals with different symmetries and spatial extensions should have different Coulomb repulsions ($F\neq U$, etc.) in general. We have studied this model for various values of parameters to explore the possibility of superconductivity.

III. METHOD

We have adopted the quantum Monte Carlo method for the ground state as described and applied to the single-band Hubbard model by Imada and Hatsugai.[8] To apply the method to the two-band Hubbard model, we must perform the Hubbard-Stratonovich transformation for the interorbital interaction terms such as

$$\exp(-\Delta\tau Vn_{i\sigma}n_{j\sigma'})=\tfrac{1}{2}\sum_{s=\pm 1}\exp\left[2as(n_{i\sigma}-n_{j\sigma'})-\frac{\Delta\tau V}{2}(n_{i\sigma}+n_{j\sigma'})\right], \tag{3}$$

$$a=\tanh^{-1}\left[\tanh\left[\frac{\Delta\tau V}{4}\right]\right]^{1/2}$$

in addition to the transformation for the intra-orbital interaction terms. Thus the number of Stratonovich variables, which is six per site in the present case, increases as the number of bands increases. The ground state of the free-electron system is employed as the trial state. Periodic boundary conditions are imposed.

Here we study one-dimensional systems. This is motivated by two reasons: First, the negative sign problem in the quantum Monte Carlo algorithm, which becomes serious for two-dimensional systems, is not encountered in 1D as far as we consider the closed-shell electron number $(4N+2)$ (N stands for integer) in each band. Second, the nature of superconductivity in 1D has been established as will be described, so that we can readily study the occurrence of Cooper pairing in 1D as far as we consider mechanisms that do not require two dimensionality.

In 1D no true long-range order exists. However, as is pointed out by Popov,[28] we can look at the correlation of order parameters to identify the ordering such as superconductivity even in 1D. This can be illustrated for the one-dimensional attractive Hubbard model with attractive ($U<0$) on-site interactions. There exists superconductivity in this system, and correlation as a function of $r=r_i-r_j$ evolves as

free electron $\rightarrow$ interacting electron

$$\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle\sim 1/r\rightarrow\sim e^{-r/\xi}\ , \tag{4a}$$

$$\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}c_{j\downarrow}c_{j\uparrow}\rangle\sim 1/r^2\rightarrow\sim 1/r^{\gamma}\ \ (\text{Cooper pairing})\ , \tag{4b}$$

$$\langle(n_i-\langle n_i\rangle)(n_j-\langle n_j\rangle)\rangle\sim 1/r^2\rightarrow\sim 1/r^{1/\gamma}\ \ (\text{CDW})\ , \tag{4c}$$

as is rigorously shown from the conformal field theory by Bogoliubov and Korepin,[29] where $\gamma=1$ for the half-filled band. For $U\neq 0$, the pairing correlation has a slow, power-law decay, while $\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$ damps exponentially. This implies that the electron pair of size ξ has a long-range correlation, hallmarking superconductivity in 1D. For the less-than-half-filled case, $\frac{1}{2}<\gamma<1$ with $\gamma-1$ being a function of doping, i.e., the decay of the pairing correlation becomes slower, while that of the charge-density wave (CDW) becomes more rapid.

In this study, we have also looked at the following correlation functions in real space for each band to identify the magnetic and pairing properties: the Green's function,

$$\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle ,$$

the density-density correlation,

$$\langle (n_{i\uparrow}+n_{i\downarrow})(n_{j\uparrow}+n_{j\downarrow}) \rangle ,$$

spin-spin correlation,

$$\langle S_i^z S_j^z \rangle = \tfrac{1}{4} \langle (n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow}) \rangle ,$$

and the correlation of the Cooper pairing,

$$\langle (c_{i\uparrow}^{\dagger} c_{i+\delta\downarrow}^{\dagger} - c_{i\downarrow}^{\dagger} c_{i+\delta\uparrow}^{\dagger})(c_{j+\delta\downarrow} c_{j\uparrow} - c_{j+\delta\uparrow} c_{j\downarrow}) \rangle ,$$

for the on-site pairing ($\delta=0$) and nearest-neighbor pairing ($\delta=1$). For the pair-pair correlation, $\langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{j\downarrow} c_{j\uparrow} \rangle$ differs from $\langle c_{i\uparrow} c_{i\downarrow} c_{j\downarrow}^{\dagger} c_{j\uparrow}^{\dagger} \rangle$ only at $r_i = r_j$ by

$$\begin{aligned} \langle c_{i\uparrow} c_{i\downarrow} c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} \rangle &= \langle n_{i\uparrow} n_{i\downarrow} \rangle - \langle n_i \rangle + 1 \\ &= \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow} \rangle - \langle n_i \rangle + 1 , \end{aligned}$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$. For $r=0$, the density-density correlation function becomes

$$\langle (n_{i\uparrow}+n_{i\downarrow})^2 \rangle = 2\langle n_{i\uparrow} n_{i\downarrow} \rangle + \langle n_i \rangle .$$

In plotting these correlation functions at $r=0$, only the value of the terms proportional to $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ are shown in the figures for clarity. For the nearest-neighbor pairing, a similar convention is employed also for $r_i - r_j = 1$. Lattice constant is taken to be unity in plotting correlation functions in real space.

IV. RESULTS FOR THE TWO-BAND HUBBARD MODEL

Before performing the simulation, we have considered whether there exists a mechanism, specific to the two-band Hubbard model, favoring effective attractions among carriers. Here we propose such a mechanism as is intuitively illustrated in Fig. 2. We consider doped carriers in the β band on top of the α band, which is assumed to be half filled or nearly half filled. When two carriers are apart, the total interaction energy is $u_i + u_j$ ($u_i = U$, V, or W) in each configuration, so that the interaction energy becomes at least $2V$ (with $V \le W \le U$). When the two carriers are on the same site, on the other hand, the cost of energy is $U+F$ if we deplete electrons in the α band from the site. Thus, when $2V > U+F$, the two carriers have the lowest interaction energy when they are on the same site, so that an effective on-site attraction of carriers arises. The effect of kinetic energies will be discussed in the next section.

From this consideration, we have performed the quantum Monte Carlo study for $U \ge W \ge V \ge F$ with $U+F \lesssim 2V$. Unless otherwise indicated, we consider a 22-site system with 22 electrons in the α band (half filled) and 6 electrons in the β band (doped), and $t^{\alpha} = t^{\beta} = -1$ is assumed.

We have first checked the validity of the quantum Monte Carlo method for the two-band Hubbard model by comparing the Monte-Carlo result with the exact diagonalization result for a four-site (eight-orbital) system with two electrons in each band. The two results, shown in Table I, coincide within numerical accuracy. We have then simulated the 22-site two-band Hubbard model in 1D, in which the convergence is confirmed by varying Trotter decomposition. The computation takes 7 h on the Hitac $S820$ for $U=V=W=3$. Simulation for larger U, V, W requires finer Trotter decomposition, and thus a longer computer time.

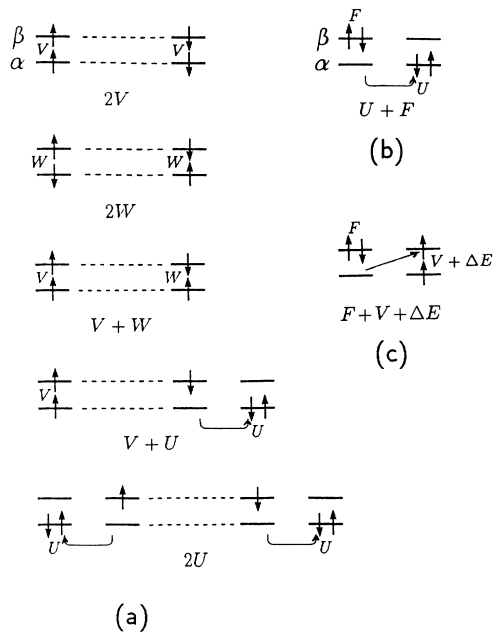

FIG. 2. (a) For two carriers in the β band apart, interaction energy is $u_i + u_j$ ($u_i = U$, V, or W) in any configuration. (b) For the two carriers on the same site, the cost of energy is $U+F$ if electrons in the α band is depleted from the site. (c) Shows the situation in which inter-orbital transfer is allowed.

The result for the β-band density-density correlation, the β-band pairing correlation, and the α-band spin-spin correlation are shown for the extreme case of $U=V=W$ in Fig. 3 and for general $U > V, W$ in Fig. 4. The result shows the following.

TABLE I. Comparison of the exact and quantum Monte Carlo (QMC) results for a four-site (eight-orbital) two-band Hubbard system with two electrons in each band for $U=3.0$, $W=V=2.5$, $F=0.5$. The errors due to Monte Carlo sampling (statistical errors) are shown. Results also have systematic errors of few percent due to Trotter decomposition. $F=0.5$.

	Exact	QMC
β-band		
density-density correlation		
$\lvert i-j \rvert = 0$	0.641	0.641±0.001
$\lvert i-j \rvert = 1$	0.1249	0.1241±0.0003
$\lvert i-j \rvert = 2$	0.109	0.110±0.001
β-band		
on-site pairing correlation		
$\lvert i-j \rvert = 0$	0.282	0.282±0.002
$\lvert i-j \rvert = 1$	0.233	0.233±0.002
$\lvert i-j \rvert = 2$	0.210	0.212±0.003

(i) The density-density correlation is enhanced around $r=0$. This indicates effective attraction of carriers in the β band.

(ii) The amplitude of the spin-singlet, on-site (within the same molecular orbital) Cooper pairing in the β band is enhanced over the value for the free-electron system, and the enhancement has a long tail in real space. The attractive density-density correlation and the enhanced Cooper pairing increase when the condition $2V > U+F$ is better satisfied. More precisely, the enhancement, which is large for the extreme case of $U=V=W$, is considerable even when V and W are reduced to $U/2$.

(iii) In these situations, the antiferromagnetic spin-spin correlation in the α band is drastically suppressed and only a short-range (nearest-neighbor) antiferromagnetic correlation survives.

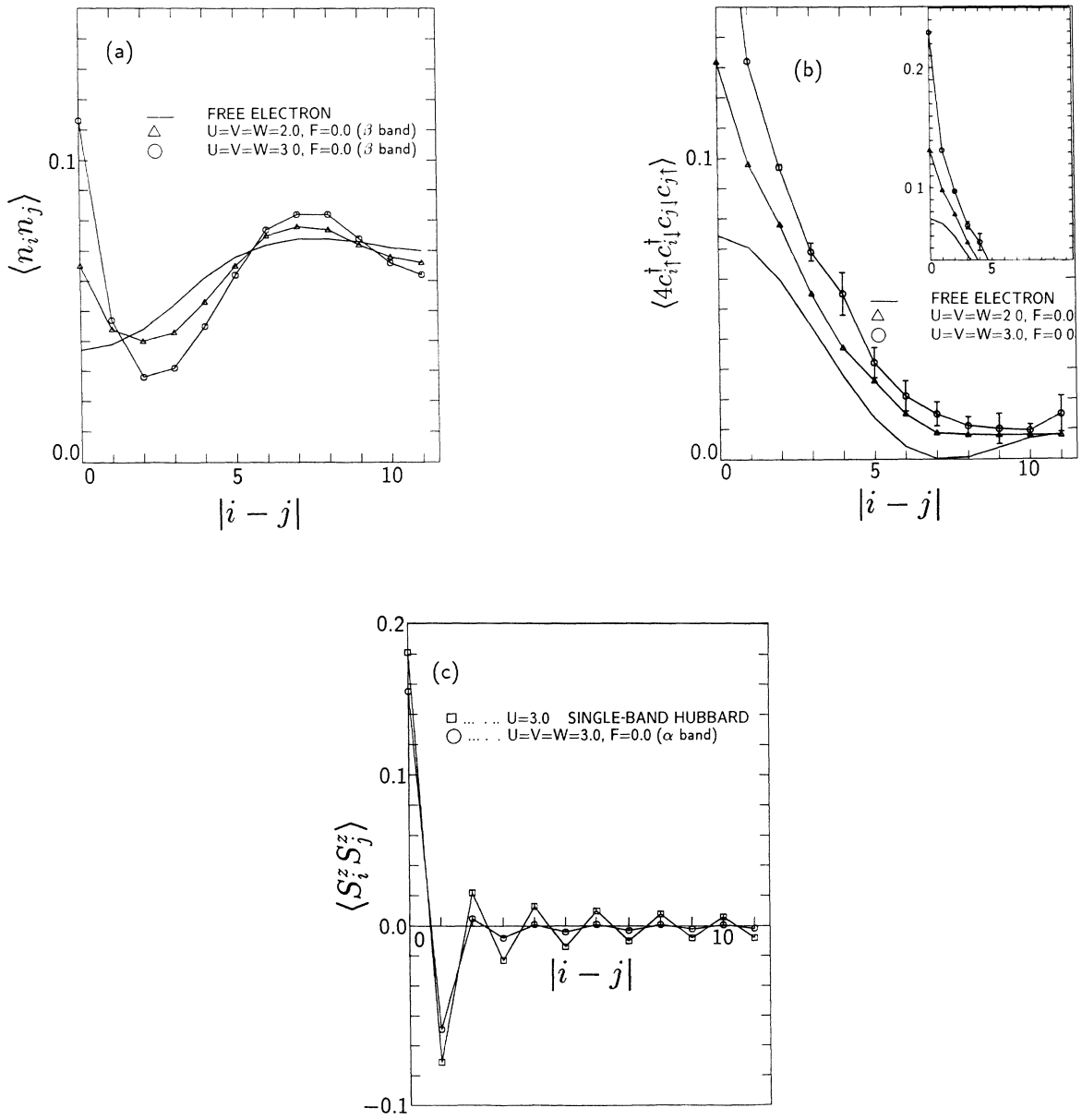

FIG. 3. The quantum Monte Carlo result for the density-density correlation in the β band (a), correlation of the singlet, on-site Cooper pairing amplitude in the β band (b), the spin-spin correlation in the α band (c) for a 22-site two-band Hubbard model in 1D with 22 electrons in the α band and 6 electrons in β. Here the interaction is $U=W=V=2(\Delta)$ or $3(\circ)$ with $F=0$, and $t^{\alpha}=t^{\beta}=-1$. The solid curve represents the free-electron result. The spin-spin correlation in the single-band Hubbard model with $U=3$ is shown by $\square$ for comparison in (c). Error bars in the QMC result are indicated when they are larger than the size of the symbols. The error is mainly the statistical error from Monte Carlo sampling. The error due to the Trotter decomposition is $\sim O((\beta/LT)^2U)$, for which we have taken $(\beta/LT)^2U=0.018$ with $\beta=17$, $LT=220$ for $U=3$. Inset for (b) shows the behavior around $r=0$.

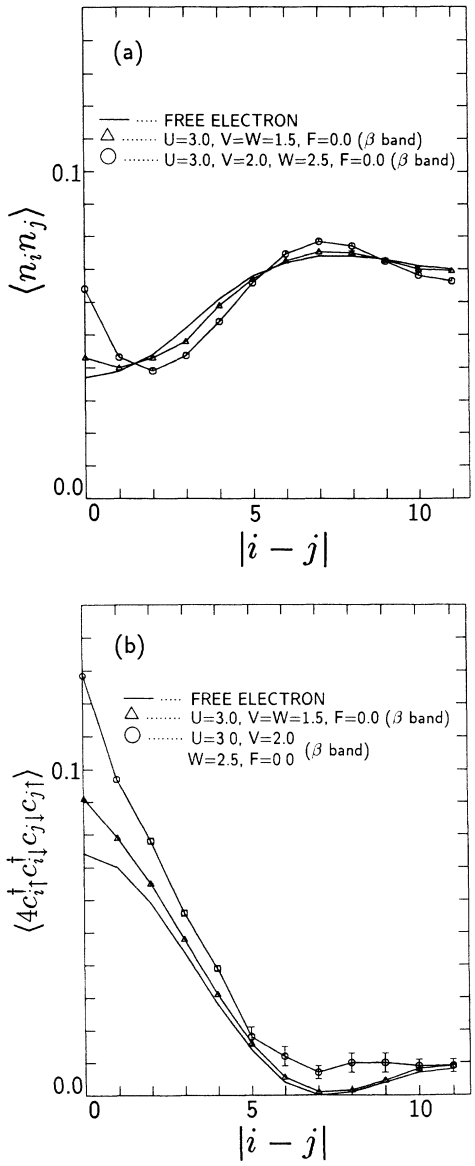

FIG. 4. The quantum Monte Carlo result for the density-density correlation in the β band (a), and correlation of the singlet, on-site Cooper pairing amplitude in the β band (b) for $U=3.0$, $V=2.0$, $W=2.5$ (○), and $U=3.0$, $V=W=1.5$ (△).

V. DISCUSSION

A. Pairing criterion

1. Effect of kinetic energies and energy level offsets

We have shown clear evidence for enhanced Cooper pairing with a systematic dependence on U, V, and W, in which correlated motions of electron in the β and α orbitals are essential. The condition, $2V > U+F$, for the appearance of effective attraction only considers interaction energies. If we include the kinetic energies, the condition should be corrected as

$$2V-b > U+F-a \tag{5}$$

with $a \sim O(t)$, $b \sim O(t)$. First note that U in Fig. 2 should correspond to an energy, U^*, required to put an electron in the $(N-1)$-site system rather than onto a single site, so that we first have to replace U with $U^*=U-a$ [$a \sim O(t)$]. Similar correction is required for the energy of two separate carriers in its lowest configuration, which is reduced to $2V-b$ due to the motion of electrons in the α band with $b \sim |t|$ for $V \simeq U$. When $V < U^*$, an electron in the α orbital does not gain interaction energy by hopping to other occupied sites, so b should be smaller. In the extreme case in which intra- and inter-orbital interactions coincide ($U=V=W$), the gain from the kinetic energy is larger, and the criterion reduces to $2U^* > U^*+F$, i.e., $b=2a$. Thus the correction terms such as b are dependent on U, V, W in general. For the two carriers on the same site, on the other hand, the energy is estimated to be U^*+F in any situation. From the Bethe-ansatz exact solution by Lieb and Wu[30] we have

$$U^* = U - 2|t| - 4\sum_{n=1}^{\infty}(-1)^n[(t^2+\tfrac{1}{4}n^2U^2)^{1/2}-\tfrac{1}{2}nU] \tag{6}$$

for the half-filled one-dimensional single-band Hubbard model. We can see that $a=U-U^*$ is an increasing function of U with $a=1.2|t|$ for $U=3$.

For the case of $U=3$, $V=W=1.5$, $F=0$, an enhanced Cooper pairing occurs (Fig. 4). This result confirms the preceding argument, since the corrected criterion, Eq. (5), may be satisfied in this case even though $2V > U+F$ is not. Equation (5) also explains the result that the behavior of density-density and enhanced pairing correlation is similar for $U=V=W=2$ (Fig. 3) and for $U=3$, $W=2.5$, $V=2$ (Fig. 4). While $2V-(U+F)$ is different for these two cases, $(2V-b)-(U+F-a)$ can be similar.

We have also studied the case in which $F \neq 0$. For a fixed $2V-(U+F)$, the case of $U > V, W$ favors the pairing over the $U=V=W$ case from the preceding discussion. If we look at the result (Fig. 5) for two cases with $(U,V,W,F)=(2,2,2,0.5)$ and $(3,2.5,2.5,0.5)$ with the same $2V-(U+F)$, the latter case has more enhanced pairing, which confirms the foregoing argument. The enhancement, however, occurs only around $|r_i-r_j| \sim 0$ in these two cases. This subtlety is discussed in Sec. V A 3 following.

For atomic orbitals in a single atom such as the fivefold d orbitals, the matrix elements of the Coulomb and exchange interactions satisfy a certain relation.[31] For molecular orbitals, however, these interactions must be calculated for each configuration of the molecular orbital unit. For two spatially extended molecular orbitals with large mutual overlap, for instance, V is expected to be large and criterion (5) is favored. A detailed study for the molecular orbitals in cuprates is planned to be published elsewhere.[32]

When we introduce hybridization between different orbitals, we must consider inter-orbital transfer processes with the energy difference, ΔE, of the two orbitals. In this case we can shift the α electron onto a β orbital in the neighboring site [Fig. 2(c)] at the cost of ΔE[~ 1 eV

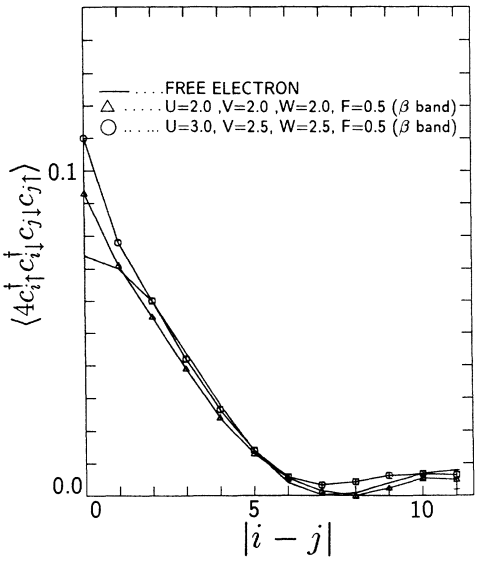

FIG. 5. The quantum Monte Carlo result for the correlation of the singlet, on-site Cooper pairing amplitude in the β band for $(U,V,W,F)=(2,2,2,0.5)$ ($\triangle$) and (3,2.5,2.5,0.5) ($\circ$).

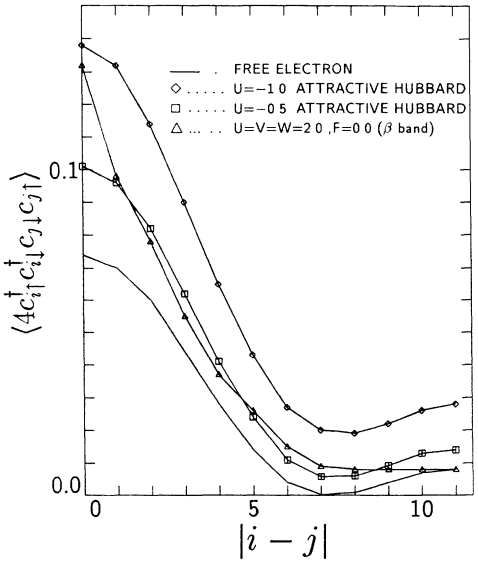

FIG. 6. The two-band Hubbard model with $(U,V,W,F)=(2,2,2,0)$ ($\triangle$), for which $(2V-b)-(U+F-a)\sim 1.0$, is compared with the attractive Hubbard model with $U=-0.5$ and -1.0. Here the QMC result for the on-site spin-singlet pairing correlation is plotted.

(Ref. 33)] plus the interband interaction V if that is energetically favorable. Equation (5) now reads

$$\min[2V-d,2(V+\Delta E)-e]>F+\min(U^*,V+\Delta E-c)\ ,$$

where c,d,e depend on the strength of hybridization as well as on t^{α},t^{β}, and we can make a similar observation for the pairing. The quantum Monte Carlo study can in principle be extended to these hybridized models.

2. *Magnitude of the effective attraction*

From the preceding discussion, it might be tempting to define an effective attraction,

$$U_A=(2V-b)-(U+F-a)\ .$$

However, we should like to stress that the present two-band model naturally differs considerably from the attractive Hubbard model with $U=-U_A$ due to quantum processes involving the two bands. To show this quantitatively, we compare in Fig. 6 the attractive Hubbard model with $U=-1$ and the two-band Hubbard model for $U=V=W=2$, $F=0$ for which $a\sim 2b\sim 2$ ($U_A=1$). The pair-pair correlation in the latter model, although it resembles that of the former around $r=0$, starts to deviate for larger r and approaches the result for the attractive Hubbard model with a smaller attraction ($U=-0.5$).

3. *Dependence on the band filling*

A Cooper pair has, in general, a finite spatial extent, which is determined by the many-body processes involving both charge and spin degrees of freedom. In deriving the attraction in an intuitive picture in Fig. 2, we have neglected the effect of overlapping of pairs, so that, for finite concentrations of carriers, the pairing criterion [Eq. (5)] should depend on the doping. Another way of saying this is that since the pairing of carriers in the β band is highly correlated with the motion of α carriers through the inter-orbital interactions, a finite concentration of β carriers necessarily causes modification of the α band, which in turn modifies the β band properties.

To explore the dependence on the band filling, we have varied the filling of the β band. For 10 electrons in 22 sites for the β band on top of 22 electrons in 22 sites for the α, in which the number of β carriers are increased from 6 (previous figures), the case of $U=V=W=2$, $F=0$ still exhibits a strongly enhanced pairing. Rather, the effect of doping is best illustrated for the most subtle case studied so far, in which $U=3.0$, $V=W=2.5$, $F=0.5$. In this case, we have seen that the result for 6 electrons in 22 sites (Fig. 5) shows an enhancement around $r=0$ but suppression for $r\geq 3$. This can be interpreted as the above-mentioned effect of overlapping of pairs. The result for various band fillings (Fig. 7) indeed shows that, as the filling of the β band is decreased from 10 electrons in 22 sites to 6 electrons in 26 sites, the enhancement in the pairing correlation is recovered.

4. T_c

An electronic mechanism of high-T_c superconductivity must explain why $T_c\sim 100$ K is so low in real materials, given electronic energies of order of eV. We envisage the following.

(i) As seen in Sec. V A 1 the present pairing mechanism reflects a balance of interaction and kinetic energies (and energy-level offset). In real high-T_c materials, subtle energy differences may be realized.

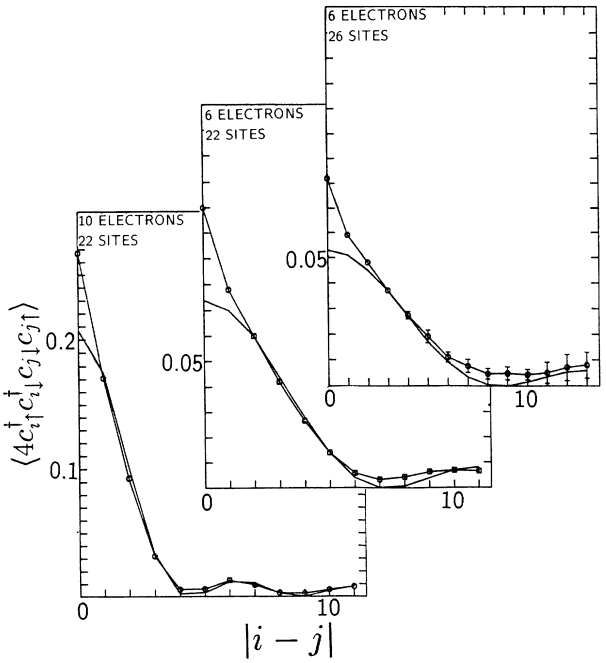

FIG. 7. The result for various fillings for $U=3.0$, $V=W=2.5$, $F=0.5$.

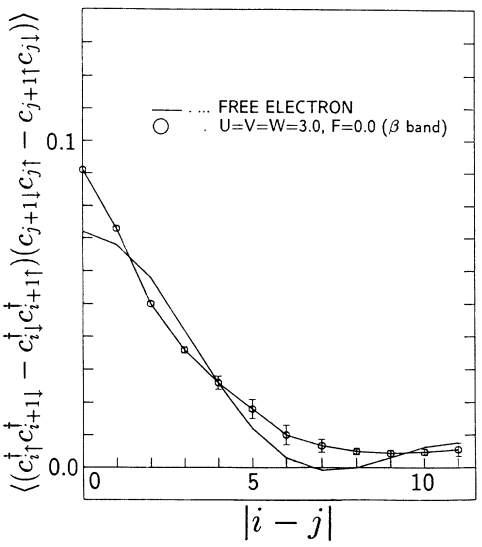

FIG. 8. The correlation function for the nearest-neighbor spin-singlet pairing for $U=V=W=3$, $F=0$.

(ii) The pairing energy and T_c do not necessarily coincide, especially when the Bardeen-Cooper-Schrieffer (BCS) picture is not guaranteed as in the superconductors with electronic mechanisms. T_c in the three-dimensional attractive Hubbard model has been estimated only in the $|U|\to\infty$ limit.[34] For the one-dimensional attractive Hubbard model, the Bethe-ansatz solution by Bogoliubov and Korepin[29] gives the exact expression for the superconductivity energy gap at $T=0$ as

$$\Delta=2[(t^2+U^2)^{1/2}-|t|]$$

for small densities of carriers. For $|t|\sim 1$ eV and $U\sim -0.1$ eV, for instance, Δ, which is a measure of T_c, becomes $\sim 0.1|U|\sim 100$ K. If we naively combine (i) and (ii), an effective attraction

$$(2V-b)-(U+F-a)\sim 0.1 \text{ eV}$$

could give $T_c\sim 100$ K, but the situation may not be so straightforward, since the two-band model can considerably differ from the attractive Hubbard model as we have emphasized.

B. Pairing correlation

1. Intraband correlation

We have seen a clear enhancement of the on-site pairing in Fig. 3. If we turn to the nearest-neighbor pairing correlation (Fig. 8), there is some enhancement over the free-electron value. This is reasonable if we note that the carrier-carrier attraction in the β band envisaged in Fig. 2 extends to nearest neighbors due to quantum effect as is also reflected in the density-density correlation in Figs. 3 and 4. Detailed discussion of the pairing correlation would require the study of the spatial extension of the pair.

In the analysis of the attractive Hubbard model,[29] the fast (exponential) decay rate of the Green's function in real space [Eq. (4a)] is related to the size of the pairing, while the pairing correlation has a power-law decay. The result for the Green's function in the present case (Fig. 9) also exhibits a fast decay.

2. Interband correlation

Another point is, despite the correlated motion of β and α orbital carriers, the Cooper pair considered here is

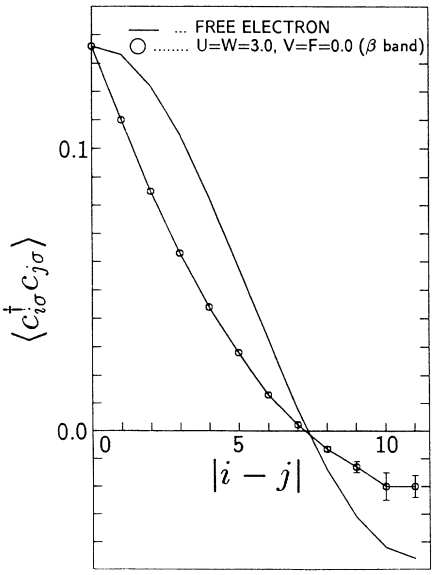

FIG. 9. The Green's function, $\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$, for $U=V=W=3$, $F=0$.

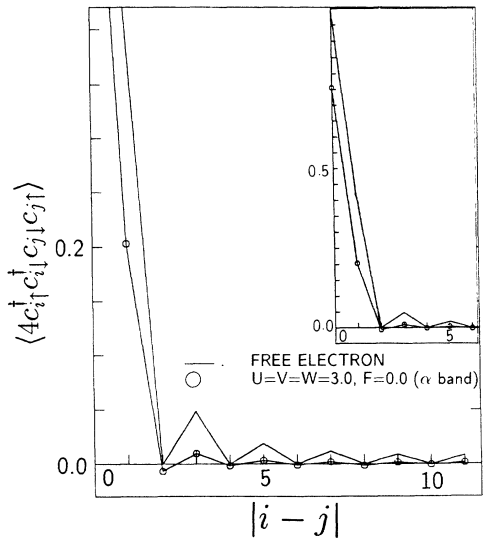

FIG. 10. The correlation function for the on-site spin-singlet pairing within the α band for $U=V=W=3$, $F=0$. The inset shows the behavior around $r=0$.

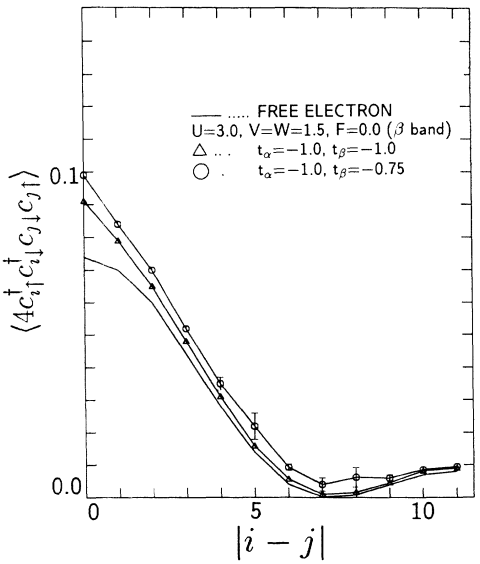

FIG. 11. The correlation function for the on-site spin-singlet pairing for $U=3.0$, $V=1.5$, $W=1.5$, $F=0$ with $t^{\alpha}=-1.0$ and $t^{\beta}=-0.75$.

constructed only from carriers in the doped band as far as we neglect hybridization, i.e., no enhanced pairing is shown (Fig. 10) for $\langle c_i^{\alpha\dagger}c_i^{\alpha\dagger}c_j^{\alpha}c_j^{\alpha}\rangle$ (spin indices dropped). This is physically reasonable, since, although the holes (depleted electrons) in the α orbital just at a site of paired β electrons (Fig. 2) resemble paired holes, α carriers experience repulsions at a majority of sites where paired β electrons are absent.

The inter-orbital pair-pair correlation,

$$\langle c_i^{\alpha\dagger}c_i^{\beta\dagger}c_j^{\beta}c_j^{\alpha}\rangle ,$$

is not enhanced, either. This is already seen in the inter-orbital density-density correlation, $\langle n_i^{\alpha}n_j^{\beta}\rangle$, which coincides with the pair-pair correlation at $r_i-r_j=0$. $\langle n_i^{\alpha}n_i^{\beta}\rangle$ is shown to be reduced to 0.14 for $U=W=V=3$ from the free-electron value of 0.27 for the 6 (22) electrons in the β (α) band in the 22-site system. Thus the carriers in α and β bands are subject to repulsively correlated motion as one would expect.

3. *Effect of band widths*

We have also studied the effect of band widths ($t^{\alpha}\neq t^{\beta}$ in general). For the attractive Hubbard model, the only relevant parameter is the dimensionless $|U/t|$, so that, for a fixed U, the superconductivity is stronger for smaller t. We have examined whether the Cooper pairing becomes more enhanced as t^{β} is reduced in the present model. The result for $t^{\beta}=-0.75$ (Fig. 11) shows that that is indeed the case. This is in sharp contrast with the case (such as the Hund's coupling case shown below) with no pairing enhancements, in which reduction of $|t|$ is shown to make the pairing correlation more suppressed.

C. Other correlation functions

In the result for the density-density correlation in real space, there is an oscillation, which can be regarded as corresponding to a CDW correlation. (The oscillation for the free-electron case is a Fermi-surface effect for a partially filled band.) The coexistence of the pairing and CDW correlations in the present model is physically reasonable, since a similar situation arises in the attractive Hubbard model as explicitly shown by Eq. (4). Another example from the half-filled extended Hubbard model[35] shows that the case of on-site attraction and vanishing nearest-neighbor repulsion is just the boundary between the superconducting and CDW phases in the phase diagram. For the half-filled case there is also Nagaoka's work,[36] in which a transformation of the repulsive and attractive Hubbard models maps spin-density wave state in the former into a state with both pairing and CDW amplitudes in the latter. Some additional interactions, such as off-site interactions, could stabilize either superconductivity or CDW, as is the case with the single-band extended Hubbard model with attractive interactions.[35] To determine whether an instability towards superconductivity in the thermodynamic limit exists in the present model would require a study of the asymptotic form of the correlation function with size-dependence (scaling) studies.

The destruction of the spin-spin correlation with doping in the present two-band model is consistent with experimental results for high-T_c materials.[37] The destruction of the spin correlation also occurs in the single-band Hubbard model.[7–9] An example of the quantum Monte Carlo result for the latter model is shown in Fig. 12 for 26 electrons in a 26-site system (half-filled case) and for 26 electrons in a 28-site system (less-than-half-filled case). The antiferromagnetic spin-spin correlation is interrupted by holes for only a slight level of doping. In the present model, the destruction of the spin-spin correlation in the a band comes from the paired-off spins as depicted in Fig. 2, in which the pairing in the β band ac-

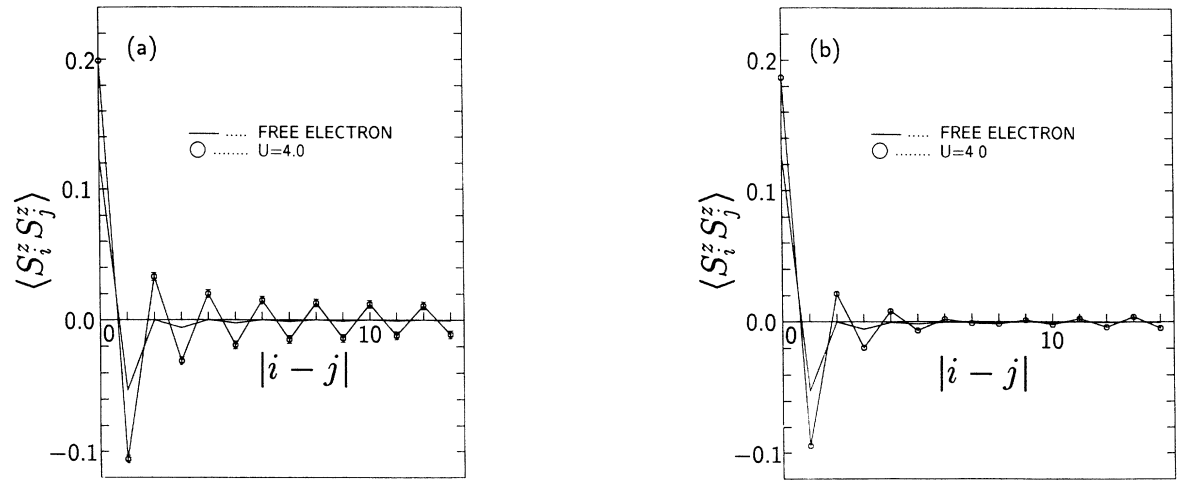

FIG. 12. The quantum Monte Carlo result for the spin-spin correlation in the single-band Hubbard model for 26 electrons in a 26-site chain (half filled) (a) and 26 electrons in a 28-site chain (less than half filled) (b). The interaction is $U=0$ (solid line) and 4 (○).

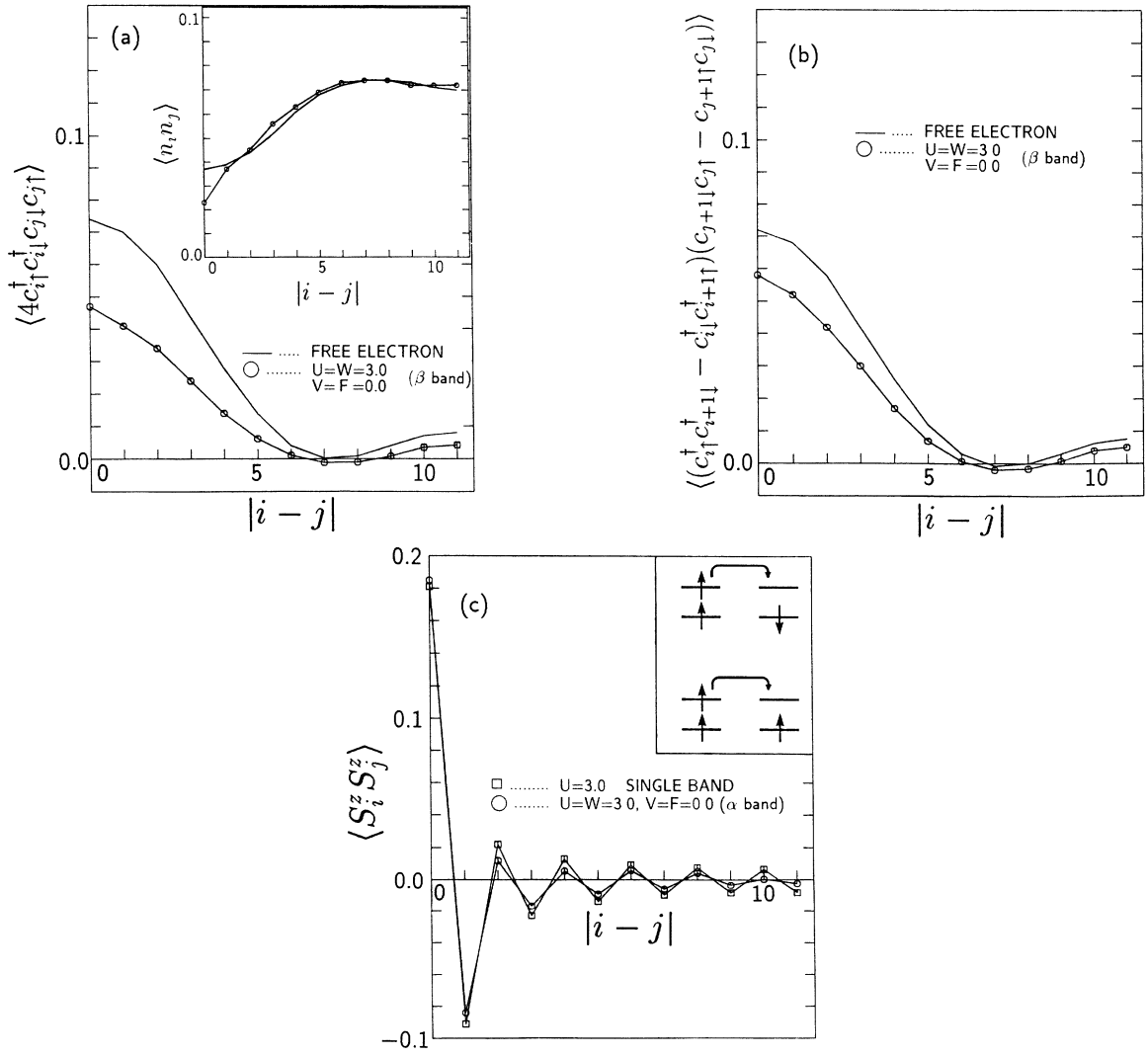

FIG. 13. The correlation of the on-site spin-singlet pair (a), nearest-neighbor spin-singlet pair (b), and the spin-spin correlation (c) for the Hund's coupling case with $U=3$, $V=0$, $W=3$, $F=0$. The density-density correlation is shown in the inset of (a) and electron configurations are shown in the inset of (c) to indicate that the destruction of antiferromagnetic correlation favors the kinetic energy.

companies both unoccupied and doubly occupied sites in the α band. Thus the destruction has a different physical origin from that in the single-band Hubbard model.

D. Necessity of two bands

The two-band pairing mechanism proposed in this paper provides a clear example of the essential difference between the two-band Hubbard model and simplified models such as a coupled spin-fermion model. The mechanism proposed here rests only upon the introduction of two bands in the Hubbard model, and does not require, *per se,* two dimensionality either, except that the effect of kinetic energy differs in 2D.

The present mechanism does not even require a direct spin-spin coupling of different orbitals such as the Hund's coupling as is shown from the enhanced pairing for the situation in which $V=W$ (vanishing intra-atomic exchange with inter-orbital interactions being independent of spin). For comparison, we have also studied the strong Hund's coupling case,

$$U\sim W,\ F=V=0\ ,$$

where electrons in the β orbital are free unless they meet an α electron of opposite spin on a same site. In this case, β electrons experience an effective repulsion mediated by the α band, which is easily shown by comparing the energies of electron configurations with a diagram similar to Fig. 2. The repulsion is confirmed by the density-density correlation [inset of Fig. 13(a)], and the Cooper pairing (on-site and nearest-neighbor) is suppressed accordingly [Figs. 13(a) and 13(b)]. The spin-spin correlation in the α band tends to be destroyed when the β band is doped [Fig. 13(c)]. This is because, in the presence of a strong Hund's coupling, the β electrons can gain kinetic energy when the antiferromagnetic correlation in the α band becomes weaker [inset of Fig. 13(c)].

An effect of two bands on the usual phonon-mediated superconductor has been studied within the BCS formalism by several authors.[38] For instance, Kondo shows that, in a BCS pairing Hamiltonian in which the β band has a positive BCS Δ parameter for $|\varepsilon_k-\mu|<\hbar\omega_D$ as well as a negative Δ for the α band and a negative interband (α-β) transfer of Cooper pairs, the BCS estimate for T_c increases with the interband transfer. By contrast, the present model is remarkable in that the superconductivity itself comes from purely repulsive, electron-electron interactions in the original Hamiltonian.[39]

As mentioned in the Introduction, Muttalib and Emery[25] have examined the two-band extension of the one-dimensional Luttinger model, in which only the electrons around the Fermi energy are considered. From the g-ology (for various coupling constants between the electrons at E_F) for spinless fermions, they have shown that the model can be mapped into a system of bosons when backward scattering involving the two bands are neglected. When a certain condition is met, spin and charge degrees of freedom decouple in the boson system, and the model is solvable. From this it is shown that the criterion in terms of the g-ology for superconductivity with intraband pairing can be satisfied for entirely repulsive interactions. The present study shows unambiguously that a two-band *Hubbard* model can embody superconductivity. It is interesting, especially for two-band systems, to ask whether the Luttinger model and the Hubbard model are of the same universality class, where the effects of backward scattering, etc., are subtle in comparing the two models. The criterion for superconductivity obtained for the Luttinger model has quite a different form from the criterion for the Hubbard model given here, and it would be an interesting future problem to probe their relation.

An interesting point about two-band models is the effect of hybridization. We can study the problem also by the quantum Monte Carlo method, which accommodates models with hybridization. One indication that the introduction of hybridization may not incur drastic suppression of superconductivity is the following. When hybridization is turned on, the band filling of each band will change. We have looked into the case in which the band filling of the α band rather than the β band is varied. The Monte Carlo result (Fig. 14) shows that even when the α-band filling deviates from half-filling to 26 electrons per 22 sites, the Cooper pairing correlation does not change appreciably.

In the normal phase of highly correlated electrons, the problem of whether the Fermi-liquid picture applies has been a central issue.[40] Both the g-ology and numerical results indicate a power-law singularity in the momentum distribution.[40] Here we show the result (Fig. 15) for the momentum distribution for the case in which the Cooper pairing is enhanced. As for the α band, we can see that the distribution at E_F becomes steeper when the interband interactions are turned on. This is consistent with the picture shown in Fig. 2, since producing unoccupied sites in the α band may be viewed as a deviation from the half filling, which then enhances the singularity at E_F. If

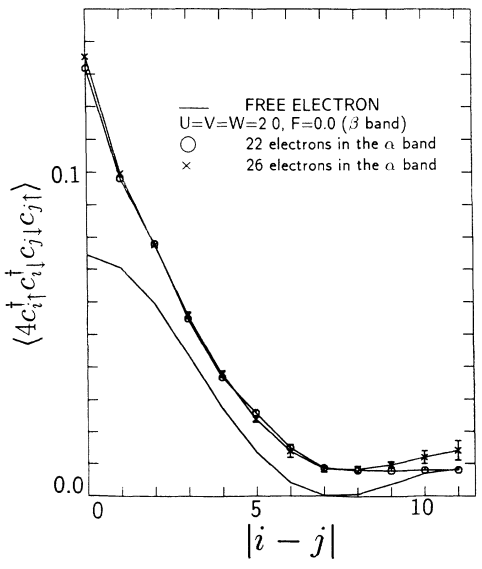

FIG. 14. The effect of changing the α-band filling from half filling with 22 electrons in 22 sites ($\circ$) to 26 electrons in 22 sites ($\times$).

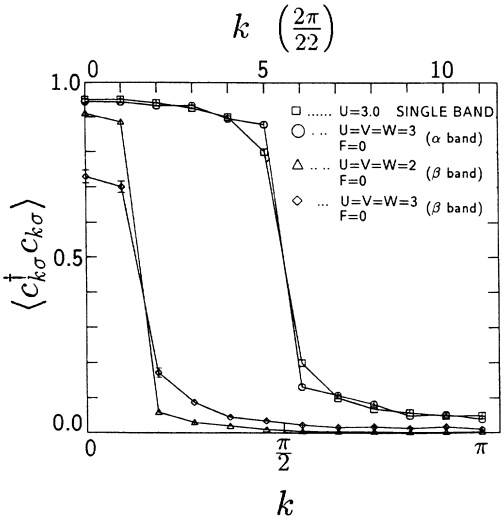

FIG. 15. The quantum Monte Carlo result for the momentum distribution for the α band ($\circ$) with $U=V=W=3$ compared with the result for the single-band Hubbard model (22 electrons in 22 sites) with $U=3$ ($\square$). For the β band, the momentum distribution for $U=V=W=2$ ($\triangle$) and $U=V=W=3$ ($\Diamond$) is shown.

we look at the β band, the distribution is smeared with the smearing being larger for larger interactions. In the BCS picture, the momentum distribution,

$$|v_{\mathbf{k}}|^2=\frac{1}{2}\left[1-\frac{\xi_{\mathbf{k}}}{(\Delta^2+\xi_{\mathbf{k}}^2)^{1/2}}\right],$$

in the superconducting phase resembles the Fermi distribution for $T=T_c$.[41] Here $\xi_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\mu$. It is an interesting problem to identify the nature of the condensate occurring in electron models such as the attractive Hubbard or present two-band Hubbard models. There is also a possibility that a two-band Hubbard model can explain temperature-dependent Hall conductivity, which is experimentally observed.[42] These serve as future problems.

In summary, we have proposed a two-band Hubbard model, which is shown to embody a novel mechanism for an enhanced Cooper pairing as confirmed by the quantum Monte Carlo result.

ACKNOWLEDGMENTS

We would like to thank Dr. L. A. Takhtajan for illuminating discussions and Dr. V. E. Korepin for sending us Ref. 29 prior to its publication. We are also indebted to Professor S. Sorella, Professor M. Imada, and Dr. Y. Hatsugai for sending us Refs. 7 and 8, respectively, prior to their publication. Thanks are also due to Professor M. Wadati, Professor T. Eguchi, Professor H. Kamimura, Professor M. Kohmoto, and Dr. D. Ko, Dr. I. Morgenstern, Dr. J. Suzuki, Dr. Y. Hatsugai, and Dr. S. Tsuneyuki for valuable discussions. Numerical calculations were done on HITAC S-820 in the University of Tokyo computer center.

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