High \( T_c \) superconductivity due to coexisting wide and narrow bands: A fluctuation exchange study on the Hubbard ladder as a test case

Kazuhiko Kuroki\(^1\), Takaumi Higashida\(^1\), and Ryotaro Arita\(^2\*)

\(^1\) Department of Applied Physics and Chemistry, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan
\(^2\) Department of Physics, University of Tokyo, Hongo 7-3-1, Tokyo 113-0033, Japan

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We propose that when the Fermi level lies within a wide band and also lies close to but not within a coexisting narrow band, high \( T_c \) superconductivity may take place due to the large number of interband pair scattering channels and the small renormalization of the quasiparticles. We show using fluctuation exchange method that this mechanism works for the Hubbard model on a ladder lattice with diagonal hoppings. From this viewpoint, we give a possible explanation for the low \( T_c \) for the actual hole doped ladder compound, and further predict a higher \( T_c \) for the case of electron doping.

The discovery of high \( T_c \) superconductivity in the cuprates, followed by discoveries of various unconventional superconductors, has brought up renewed fascination for the search of high \( T_c \) superconductors, for which a theoretical guiding principle is highly desired. One way to attack this problem is to theoretically search for lattice structures that provide good conditions for Cooper pairing. Ladder-like structures may be considered as a candidate for this, but up to now, \( T_c \) in the actual hole doped ladder compound \( \text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41} \) (14-24-41) remains to be around \( \approx 12 \) K which is low compared to the layered cuprates. In this context, we have previously proposed a high \( T_c \) mechanism due to disconnected Fermi surfaces, which can in fact be realized with a ladder-like lattice structure with a larger hopping integral in the rung direction than in the leg direction but up to now there exist no actual materials (or methods) to realize the situation we have proposed. In the present study, we propose a different mechanism for high \( T_c \) superconductivity in systems with coexisting narrow and wide bands, which may be realized in actual ladder compounds with electron doping.

Our idea is as follows. Let us consider a system where the Fermi level \( E_F \) lies within a band with a moderate width (we call this “the wide band A”) and also lies close to, but not within, a narrow band (“band B”). If the amplitude of the pair scattering processes from band A to band B is strong enough, the pairing instability may become very large because (i) the sign change of the gap, necessary for repulsive pairing interactions, occurs between the bands, so that there are no gap nodes on the Fermi surface, and (ii) there is a huge number of interband pair scattering channels due to the narrow character of band B (see the bottom of the right panel in Fig.1). Another point to be stressed here is that the Fermi level is not within the narrow band, so that the renormalization of the quasiparticles at the Fermi level is not so large as to strongly suppress superconductivity. Systems with coexisting wide and narrow bands may be reminiscent of models consisting of wide \( s \) or \( p \) bands and narrow \( d \) or \( f \) bands, but in that case, the amplitude of the interband (interorbital) pair scattering processes may not be so large because of the different character of the orbitals. Here we consider systems with one orbital per site, where the multiplicity of the bands originates from the lattice structure rather than the multiplicity of the orbitals at each site, so that the pairing interaction can be strong, originating from the large on-site repulsion.

The above condition for the energy bands can most simply be satisfied in a tightbinding model on a ladder lattice with diagonal hoppings shown in Fig.1. The Hamiltonian of this model is given in momentum space as

\[
H_{\text{kin}} = \sum_{k \sigma} (c^\dagger_{k \sigma}, d^\dagger_{k \sigma}) \begin{pmatrix}
-2t_l \cos k & -2t' \cos k - t_r \\
-2t' \cos k - t_r & -2t_l \cos k
\end{pmatrix}
\begin{pmatrix}
c_{k \sigma} \\
d_{k \sigma}
\end{pmatrix}
\]

where \( c_{k \sigma} \) and \( d_{k \sigma} \) annihilate an electron with spin \( \sigma \) at wave number \( k \) on the left and right legs, respectively, and \( t_l, t_r, \) and \( t' \) are the hopping integrals in the leg, rung, and diagonal directions, respectively. The dispersion of...
the two bands are given as \( \varepsilon_{\pm}(k) = -2(t_1 \pm t') \cos k \mp t_r \).

When \( t' = 0 \) (Fig. 1 top of the right panel), the two bands have identical dispersions with a level offset of \( 2t_2 \), while one of the bands (band B) is narrower than the other (band A) in the presence of \( t' \), and becomes perfectly flat for \( t' = \pm t_1 \) (Fig. 1 bottom of the right panel).

Here, we consider the on-site interaction \( (U) \) term in addition to the above kinetic energy terms, and also take into account the trellis-like lattice structure of the actual cuprate ladder compounds, where the ladders are weakly coupled by diagonal hoppings \( t_{ij} \). We estimate the superconducting transition temperature of this Hubbard model using the combination of the fluctuation exchange method (FLEX) and the Eliashberg equation, which has been successfully applied to the problem of layered high \( T_c \) cuprates. The values of \( U, t_r, t_i \) will be fixed at \( U = 6t_i, t_r = t_i, \) and \( t_i = 0.25t_2 \) throughout the study. We define the site filling \( n \) as \( n = \text{[number of electrons]/[number of sites]} \), so when the bands are both fully filled, the band filling is \( n = 2 \).

In the two-band version of FLEX, the Green's function \( G \), the susceptibility \( \chi \), the self-energy \( \Sigma \), and the superconducting gap function \( \phi \) all become \( 2 \times 2 \) matrices, e.g., \( G_{lm}(k, i\varepsilon_n) \), where \( l, m \) specify the two sites in a unit cell. The orbital-indexed matrices for Green's function and the gap functions can be converted into band-indexed ones with a unitary transformation. As for the spin susceptibility, we diagonalize the spin susceptibility matrix and concentrate on the larger eigenvalue, denoted as \( \chi \).

The actual calculation proceeds as (i) Dyson’s equation is solved to obtain the renormalized Green’s function \( G(k) \), where \( k \equiv (k, i\varepsilon_n) \) denotes the 2D wavevectors and the Matsubara frequencies, (ii) the effective electron-electron interaction \( V^{(1)}(q) \) is calculated by collecting RPA-type bubbles and ladder diagrams consisting of the renormalized Green’s function, namely, by summing up powers of the irreducible susceptibility \( \chi_{\text{irr}}(q) = -\frac{1}{\pi} \sum_k G(k + q)G(k) \) (\( N \): number of \( k \)-point meshes), (iii) the self energy is obtained as \( \Sigma(k) \equiv \sum_q G(k - q)V^{(1)}(q) \), which is substituted into Dyson’s equation in (i), and these procedures are repeated until convergence is attained.

We determine \( T_c \) as the temperature at which the eigenvalue \( \lambda \) of the linearized Eliashberg equation, \( \lambda \phi_{lm}(k) = -\frac{T}{N} \sum_{k' < l m'} V^{(1)}(k - k')G_{ll'}(k')G_{mm'}(-k')\phi_{lm'}(k') \), reaches unity. Here the pairing interaction \( V^{(2)}(q) \) for singlet pairing is given by \( V^{(2)}(q) = U + \frac{2}{9}U^2\chi_{\text{irr}}(q)/(1 - U\chi_{\text{irr}}(q)) - \frac{2}{9}U^2\chi_{\text{irr}}(q)/(1 + U\chi_{\text{irr}}(q)) \).

Throughout the study, we take up to \( 64 \times 64 \) \( k \)-point meshes and the Matsubara frequencies \( \varepsilon_n \) from \( -(2N_c - 1)\pi T \) to \( (2N_c - 1)\pi T \) with \( N_c \) up to 8192 in order to ensure convergence at low temperatures.

We now move on to the results. We first show the \( t' \) dependence of \( T_c \) for \( n = 1.25 \). We consider the case of \( t' < 0 \) since this is the realistic choice of sign for the cuprates. In Fig. 3(a), we plot \( T_c \) as a function of \( -t' \).
for $n = 1.25$. It can be seen that $T_c$ takes its maximum around $-t' = t_1$, where band B is flat. There, $T_c$ almost reaches $0.08t_1$, which is extremely high if $t_1$ is assumed to be of the order of few hundred meV as in the cuprates.

To trace back the origin of this high $T_c$, we look into the Green’s functions, spin susceptibility and the gap functions for $-t' = 0.95t_1$ and $n = 1.25$. In Fig. 4, we plot $|G_{u,l}(k_x, k_y, i\pi T)|^2$, $\chi(k_x, k_y, 0)$, and $\phi_{u,l}(k_x, k_y, i\pi T)$ viewed from the direction of the $k_x$ axis. Here, we display the results for $G$ and $\phi$ in the band representation, where $u$ and $l$ denote the upper and lower portions of the bands as shown in the inset of Fig. 4(a). Since bands A and B intersect with each other, the wide band A (the narrow band B) consists of the upper (lower) band around $k_y = \pm \pi$ and the lower (upper) band around $k_y = 0$. In the Green’s functions, the two peak-like structures seen around $k_y = \pm \pi/4$ is due to the Fermi level crossing, while the narrow structure (noted as N.B.) owes to the flatness of band B. Since the volume of the Fermi surface (the length $2k_F$) is $\simeq \pi/2$, the wide band A is nearly quarter filled, and thus the narrow band is fully filled, i.e., the Fermi level lies above the narrow band. The spin susceptibility has a broad structure again due to the flatness of band B, which enhances the number of pair scattering channels due to spin fluctuations. The gap function changes sign between band A and band B, but there is no sign change within each band, as expected in our intuitive picture.

In Fig. 5(b), we fix $-t'$ at 0.95$t_1$ and show the band filling dependence of $T_c$, which takes its maximum around $n = 1.25$. This result shows that $T_c$ becomes low when $n$ is too large, that is, when the Fermi level lies too far above the narrow band since this will make the system close to a purely single band model. $T_c$ also goes down when the Fermi level comes too close to or within the

FIG. 4: Color online. (a) $|G_{\alpha}(k_x, k_y, i\pi k_y T)|^2$, (b) $\chi(k_x, k_y, 0)$, (c) $\phi_{\alpha}(k_x, k_y, i\pi k_y T)$ for $n = 1.25$, $t' = -0.95t_1$, and $T = 0.08t_1$ viewed from the direction of the $k_x$ axis. The thickness of the curves represents the dispersion in the $k_y$ (the length $2k_F$) axis. Here, we display the results for $G$ and $\phi$ in the band representation, where $u$ and $l$ denote the upper and lower portions of the bands as shown in the inset of Fig. 4(a).

FIG. 5: Plots similar to Fig. 4 for $n = 0.9$ and $t' = -0.95t_1$.

FIG. 6: $T_c$ plotted as a function of $n$ for $t' = -0.4t_1$. 
narrow band B.

In fact, when the Fermi level is within the narrow band, we find a \( t' \) dependence that is completely the opposite to what is seen in Fig. 3(a). In Fig. 3(c), we plot the eigenvalue \( \lambda \) of the Eliashberg equation for \( n = 0.99 \) at \( T = 0.05t_1 \). In this case, a finite \( T_c \) is not obtained for all of the \( t' \) values, so we plot \( \lambda \) for a fixed temperature instead of \( T_c \). As seen in the figure, \( \lambda \) takes its minimum around \(-t' = t_1\). In this case, the Fermi level is within band B as can be seen from the Green’s function shown in Fig. 3(a). Namely, the length between the two peaks is about 0.7\( \pi \) (which is in fact larger than the case of \( n = 1.25 \) meaning that the band is not rigid), so that both of the bands has to be partially occupied. We can see in Fig. 3(a) that the Green’s functions are small (the quasiparticle renormalization is strong) compared to those in Fig. 3(a), so this should suppress \( T_c \). Moreover, the gap function (Fig. 3(c)) changes sign within the wide and the narrow bands near the Fermi surface, and this also should work destructive against superconductivity. The sign change in the gap means that contributions from the pair scattering interactions within the narrow (and the wide) band are large, which is a consequence of the Fermi level crossing of the narrow band with a large density of states. This means that the peak structure in the susceptibility (Fig. 3(b)) originates from both interband and intraband scattering processes.

The above results suggest that superconductivity with high \( T_c \) may be obtained in the ladder compounds for the case of electron doping. The condition for the maximum \( T_c \), \(-t' \approx t_1\), is of course unrealistic for the cuprate ladders, but we notice in Fig. 3 that the enhancement of \( T_c \) remains even if we deviate from \(-t' = t_1\), and relatively high \( T_c(\sim 0.04t_1) \) is obtained even below \(-t' = 0.5t_1\). Note that \( t' \) should be around \( t' \approx -0.4t_1 \) in the actual cuprate ladder compounds, assuming that \( t' \) has values similar to those for the layered cuprates such as YBa\(_2\)Cu\(_3\)O\(_y\).

To look in more detail into the possibility of high \( T_c \) superconductivity for realistic values of the hopping integrals, we plot in Fig. 4 the band filling dependence of \( T_c \) for \(-t' = 0.4t_1\). \( T_c \) is not calculated near \( n = 1 \) because (i) antiferromagnetic fluctuations strongly develop at high temperatures so that \( T_c \) is not obtained, and in any case, (ii) FLEX loses its validity in the vicinity of half filling, where a Mott transition should take place. We find that a maximum \( T_c \) of \( \sim 0.05t_1 \), which is still considerably high, is reached at around \( n = 1.3 \), namely, when a large amount of electrons is doped. By contrast, for hole doping (\( n < 1 \)), \( T_c \) turns out to be much smaller, namely, of the order 0.001\( t_1 \), which is of the same order as the \( T_c(\sim 12K) \) for the actual 14-24-41 compound. The origin of the difference between the electron doped and the hole doped cases, can again be traced back to the Green’s functions, the spin susceptibility, and the gap functions, in which the characteristic features seen for \( t' = -0.95t_1 \) (Fig. 4) still remain to some extent. The details on this point will be published elsewhere.

We have seen that our high \( T_c \) mechanism due to coexisting narrow and wide bands works for a ladder system. Now, an interesting question is to ask how general this mechanism is. We have in fact found similar results for the Hubbard model on a lattice where a pair of square lattices with in-plane nearest neighbor hoppings \( (t) \) is coupled by out-of-plane vertical \( (t_v) \) and diagonal \( (t') \) hoppings. The Hamiltonian of this model is given as These results seem to suggest that the present mechanism is likely to work on two band lattices having the Hamiltonian of the form

\[
H_{\text{kin}} = \sum_{\mathbf{k},\sigma} \left( \epsilon^{\dagger}_{\mathbf{k},\sigma} d^{\dagger}_{\mathbf{k},\sigma} \left( \frac{\epsilon_{\mathbf{k}}}{\alpha \epsilon_{\mathbf{k}} + \beta \epsilon_{\mathbf{k}}} \right) \right) \left( \frac{\epsilon_{\mathbf{k},\sigma}}{d_{\mathbf{k},\sigma}} \right),
\]

where \( \alpha \) and \( \beta \) are constants. Here, a flat band coexists with a wide band for \( \alpha = \pm 1 \) (\( \epsilon_{\mathbf{k}} = -2t_1 \cos k \) for the ladder, and \(-2t(\cos k_x + \cos k_y) \) for the coupled planes). It would be an interesting future problem to investigate the validity of the present superconducting mechanism in a more wide class of models where wide and narrow bands coexist.

To summarize, we have proposed a mechanism for high \( T_c \) superconductivity in a two band system where wide and narrow bands coexist. When the Fermi level lies close to but not within the narrow band, \( T_c \) becomes higher as the flatness of the narrow band increases, while completely the opposite takes place when the Fermi level is within the narrow band. From this viewpoint, we have given a possible explanation for the rather low \( T_c \) for the actual hole doped 14-24-41 ladder compound, and have further predicted a higher \( T_c \) for the case of electron doping. As for the 14-24-41 compound, recent NMR experiments have observed a coherence peak and an unchanged Knight shift across \( T_c \). As for the presence of the coherence peak, the singlet gap function obtained in our study can be consistent with the experiments since the gap does not change its sign on the Fermi surface. As for the unchanged Knight shift, we believe further investigation is necessary, but even this is due to spin-triplet pairing originating from effects not included in the present study (e.g., phonons), we have to explain why \( T_c \) of the singlet pairing is even lower than 12K. The present viewpoint can still be relevant for answering this question, and we believe that the prediction for a higher \( T_c \) in the case of electron doping remains valid.

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Present address: Max Planck Institute for Solid State Research, Heisenbergstr. 1, Stuttgart 70569, Germany

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12 The Fermi level can be brought below and close to the narrow band in the hole doped case, but for \( t' < 0 \), this occurs when holes are significantly doped away from half filling so that the band filling is very small. In such a case, \( T_c \) enhancement due to electron correlation effects cannot be expected.
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