High-T_c superconductivity due to coexisting wide and narrow bands: A fluctuation exchange study of the Hubbard ladder as a test case

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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 the 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.

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The discovery of high-T_c superconductivity in the cuprates,[1] followed by discoveries of various unconventional superconductors, has brought up renewed fascination for the search for 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. Ladderlike structures may be considered as candidates for this,[2] but up to now, the T_c in the actual hole-doped ladder compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ (14-24-41) remains around $\simeq$12 K,[3] 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 ladderlike lattice structure with a larger hopping integral in the rung direction than in the leg direction,[4] 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) a 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,p bands and narrow d,f bands, or models for MgB_2 comprising p_π and p_σ orbitals, but in those cases, 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 amplitude of the interband pair scattering can be strong, originating from the large on-site repulsion.

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

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

where $c_{k\sigma}$ and $d_{k\sigma}$ annihilate an electron with spin σ 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 is given as $\varepsilon_\pm(k)=-2(t_l\pm t')\cos k\mp t_r$. When $t'=0$ (Fig. 1, top of the right panel), the two bands have identical dispersions with a level offset of $2t_r$, while one of the bands (band B) is narrower than the other (band A) in the presence of t', and becomes perfectly flat for $t'=\pm t_l$ (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 trellislike lattice structure of the actual cuprate ladder compounds,[5,6] where the ladders are weakly coupled by diagonal hoppings t_i (Fig. 2). We estimate the superconducting transition temperature of this Hubbard model using a combination of the fluctuation exchange (FLEX) method and the Eliashberg equation, which has been applied to the problem of layered high-T_c cuprates.[7–9] The values of U, t_r, and t_i will be fixed at $U=6t_l$, $t_r=t_l$, and $t_i=0.25t_l$ throughout the study. We define the band filling n as $n=$(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 the FLEX method,[5] the Green's function G, the susceptibility χ, the self-energy Σ, and the superconducting gap function ϕ all become 2×2 matrices, e.g., $G_{lm}(\boldsymbol{k},i\varepsilon_n)$, where l, m specify the two sites in a unit cell. The orbital-indexed matrices for the 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 χ.

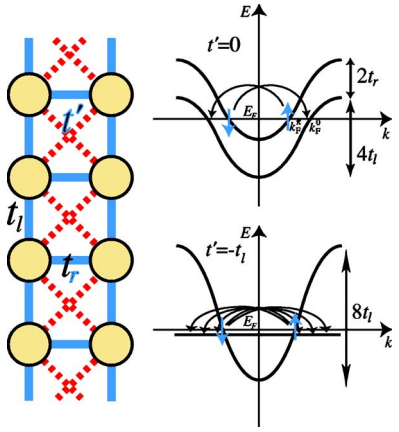

FIG. 1. (Color online) Left panel: The hopping integrals in the ladder lattice are shown. Right panel: the energy dispersion for the ladder lattice with $t'=0$ (top) and with $-t_l$ (bottom). The curved arrows show the pair scattering processes that give rise to superconductivity.

The actual calculation proceeds as follows: (i) Dyson's equation is solved to obtain the renormalized Green's function $G(k)$, where $k \equiv (\boldsymbol{k}, i\epsilon_n)$ denotes the two-dimensional (2D) wave vectors and the Matsubara frequencies; (ii) the effective electron-electron interaction $V^{(1)}(q)$ is calculated by collecting random-phase-approximation-(RPA-) type bubbles and ladder diagrams consisting of the renormalized Green's function, namely, by summing up powers of the irreducible susceptibility $\chi_{\rm irr}(q) \equiv -(1/N)\Sigma_k G(k+q)G(k)$ (N is the number of k-point meshes); (iii) the self-energy is obtained as $\Sigma(k) \equiv (1/N)\Sigma_q G(k-q)V^{(1)}(q)$, 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 λ of the linearized Eliashberg equation,

$$\lambda \phi_{lm}(k) = -\frac{T}{N}\sum_{k'l'm'} V^{(2)}_{lm}(k-k')G_{ll'}(k')G_{mm'}(-k')\phi_{l'm'}(k'),$$

reaches unity. Here the pairing interaction $V^{(2)}$ for singlet pairing is given by $V^{(2)}(q) = U + \frac{3}{2}U^2\chi_{\rm irr}(q)/[1-U\chi_{\rm irr}(q)] - \frac{1}{2}U^2\chi_{\rm irr}(q)/[1+U\chi_{\rm irr}(q)]$.

Throughout the study, we take up to 64×64 k-point meshes and the Matsubara frequencies ϵ_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.

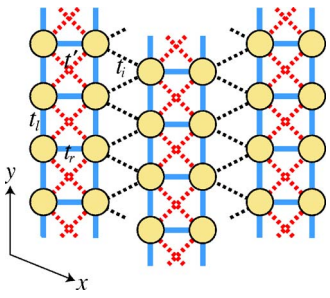

FIG. 2. (Color online) The trellis lattice adopted in the present study.

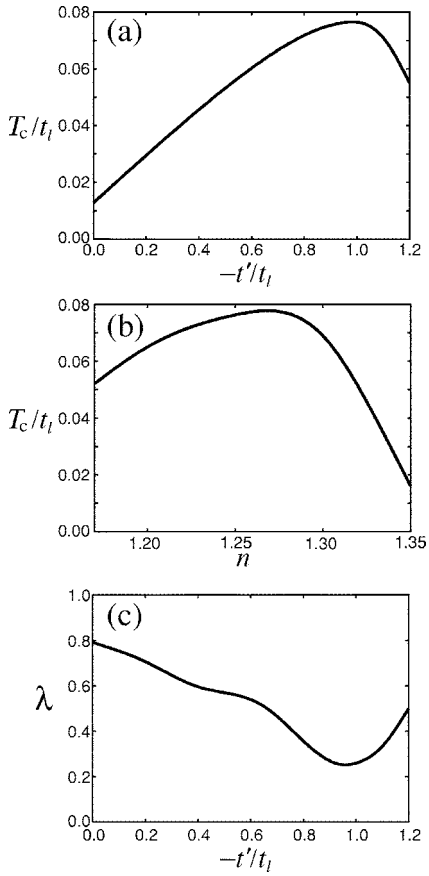

FIG. 3. T_c plotted as a function of (a) $-t'$ for $n=1.25$, and (b) n for $-t'=0.95t_l$. (c) The eigenvalue of the Eliashberg equation λ plotted as a function of $-t'$ for $n=0.9$ and $T=0.05t_l$.

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.[10] 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 $-t'=t_l$, where band B is flat. There, T_c almost reaches $0.08t_l$, which is extremely high if t_l is assumed to be of the order of a 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 gap functions for $-t'=0.95t_l$ 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 ϕ 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 peaklike structures seen around $k_y=\pm\pi/4$ are due to the Fermi level crossing, while the narrow structure (noted as N.B.) is owing 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 fluctua-

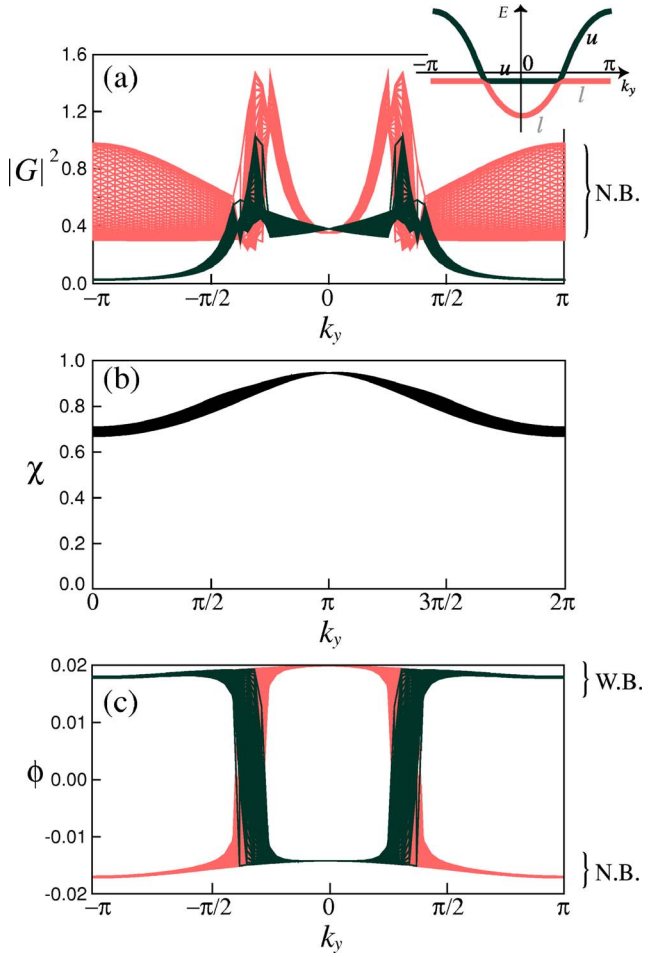

FIG. 4. (Color online) (a) $|G_\alpha(k_x,k_y,i\pi k_BT)|^2$, (b) $\chi(k_x,k_y,0)$, and (c) $\phi_\alpha(k_x,k_y,i\pi k_BT)$ for $n=1.25$, $t'=-0.95t_l$, and $T=0.08t_l$ viewed from the direction of the k_x axis. The thickness of the curves represents the dispersion in the k_x direction. In (a) and (c), quantities for $\alpha=u$ (upper band) and l (lower band) are shown by dark green and red (dark and light in print) curves, respectively, while N.B. (W.B.) denotes the portions corresponding to those for the narrow band B (wide band A). The relation between the narrow /wide bands and the lower /upper bands is shown in the inset of (a).

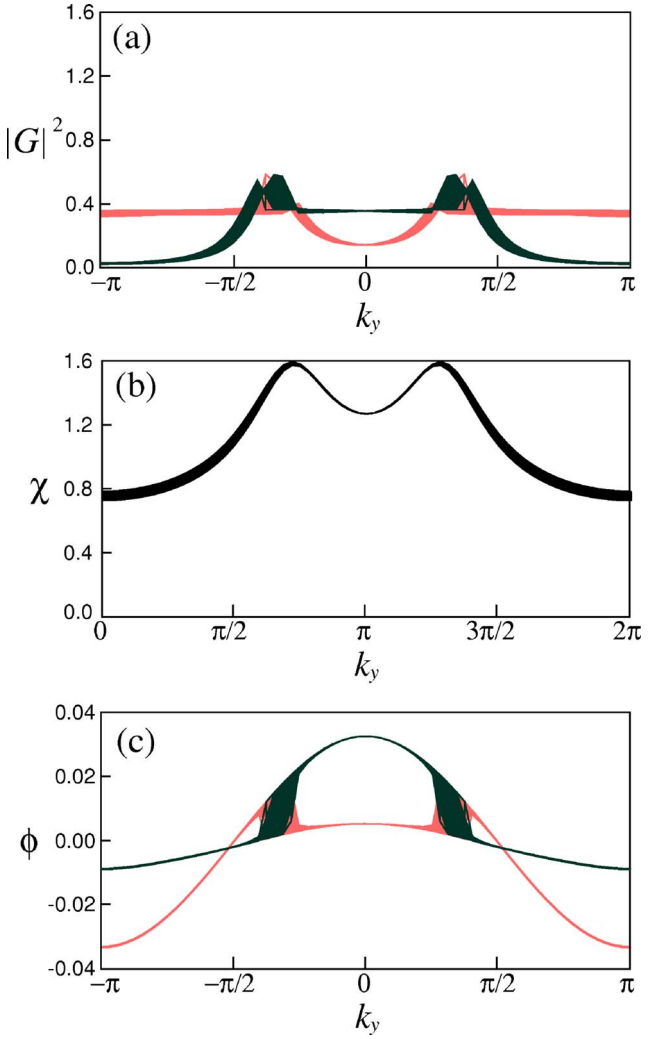

FIG. 5. (Color online) Plots similar to Fig. 4 for $n=0.9$ and $t'=-0.95t_l$.

tions. 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. 3(b), we fix $-t'$ at $0.95t_l$ 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 is within the narrow band B.

In fact, when the Fermi level is *within* the narrow band, we find a t' dependence that is completely the opposite of what is seen in Fig. 3(a). In Fig. 3(c), we plot the eigenvalue λ of the Eliashberg equation for $n=0.9$ at $T=0.05t_l$. In this case, a finite T_c is not obtained for all of the t' values, so we plot λ for a fixed temperature instead of T_c. As seen in the figure, λ takes its *minimum* around $-t'=t_l$. In this case, the Fermi level is within band B as can be seen from the Green's function shown in Fig. 5(a); namely, the length between the two peaks is about 0.7π (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 have to be partially occupied.[11] We can see in Fig. 5(a) that the Green's functions are small (the quasiparticle renormalization is strong) compared to those in Fig. 4(a), so this should suppress T_c. Moreover, the gap function [Fig. 5(c)] changes sign within the wide and the narrow bands near the Fermi surface, and this also should be destructive for 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. 5(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.[12] The condition for the maximum T_c, $-t'\simeq t_l$, 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 $-t'=t_l$, and relatively high T_c

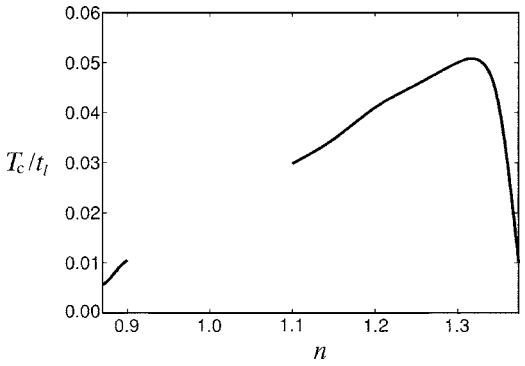

FIG. 6. T_c plotted as a function of n for $t'=-0.4t_l$.

($\sim 0.04t_l$) is obtained even below $-t'=0.5t_l$. Note that t' should be around $t' \simeq -0.4t_l$ in the actual cuprate ladder compounds, assuming that t' has values similar to those for the layered cuprates such as $YBa_2Cu_3O_7$.[10]

To look in more detail into the possibility of high-T_c superconductivity for realistic values of the hopping integrals, we plot in Fig. 6 the band filling dependence of T_c for $-t'=0.4t_l$. 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 $\sim 0.05t_l$, 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 $0.001t_l$, which is of the same order as the T_c ($\simeq 12$ K) for the actual 14-24-41 compound.[4] The origin of the difference between the electron- and 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 $t'=-0.95t_l$ (Fig. 4) still remain to some extent. The details on this point will be published elsewhere.[13]

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.[13] These results seem to suggest that the present mechanism is likely to work on two band lattices having the Hamiltonian of the form

$$H_{\mathrm{kin}} = \sum_{\boldsymbol{k},\sigma} (c^{\dagger}_{\boldsymbol{k},\sigma}, d^{\dagger}_{\boldsymbol{k},\sigma}) \begin{pmatrix} \varepsilon(\boldsymbol{k}) & \alpha\varepsilon(\boldsymbol{k})+\beta \\ \alpha\varepsilon(\boldsymbol{k})+\beta & \varepsilon(\boldsymbol{k}) \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k},\sigma} \\ d_{\boldsymbol{k},\sigma} \end{pmatrix},$$

where α and β are constants. Here, a flat band coexists with a wide band for $\alpha=\pm 1$ [$\varepsilon(k)=-2t_l \cos k$ 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 wider 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. For the 14-24-41 compound, recent NMR experiments have observed a coherence peak and an unchanged Knight shift across T_c.[14] 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 if this is due to spin-triplet pairing originating from effects not included in the present study (e.g., phonons), we have to explain why the T_c of singlet pairing is even lower than 12 K. 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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[10] See, e.g., K. Kuroki, R. Arita, and H. Aoki, Phys. Rev. B **60**, 9850 (1999), and references therein.
[11] Since $n<1$, neither of the bands can be fully filled. On the other hand, if there were completely no electrons in one of the bands, the volume of the Fermi surface of the other would be 0.9π for $n=0.9$.
[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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