Possible high-T_c superconductivity mediated by antiferromagnetic spin fluctuations in systems with Fermi surface pockets

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(Received 22 January 2001; published 7 June 2001)

We propose that if there are two small pocketlike Fermi surfaces, and the spin susceptibility is pronounced around a wave vector **Q** that bridges the two pockets, the spin-singlet superconductivity mediated by spin fluctuations may have a high transition temperature. Using the fluctuation exchange approximation, this idea is confirmed for the Hubbard on a lattice with alternating hopping integrals, for which T_c is estimated to be almost an order of magnitude larger than those for systems with a large connected Fermi surface.

DOI: 10.1103/PhysRevB.64.024501 PACS number(s): 74.20.Mn

Fascination for electronic mechanisms of superconductivity has a long history. Given the large energy scale of the electrons itself, there has been an expectation from the early days that purely electronic mechanisms of superconductivity may lead to high transition temperature (T_c). The discovery of high-T_c superconductivity in the cuprates[1] has raised renewed interest in this possibility. In fact, the repulsive Hubbard model, one of the simplest purely electronic models for the cuprates, has been studied extensively to investigate whether the model can account for $T_c \sim 100$ K. In particular, the fluctuation exchange (FLEX) studies have shown that the Hubbard model near half-filling on a two-dimensional (2D) square lattice exhibits spin-singlet *d*-wave superconductivity, mediated by antiferromagnetic spin fluctuations, having $T_c \sim O(0.01t)$.[2] Here t is the hopping integral in the Hubbard model, which is estimated to be $\sim O(1$ eV) for the cuprates, so that $T_c \sim 100$ K, namely, a ''high T_c.'' Studies along this line have been performed on various lattices near half filling, where T_c of the *d*-wave superconductivity has always turned out to be $\sim O(0.01t)$ on two-dimensional (2D)[3–6] and quasi-1D lattices,[7–9] and even lower on 3D lattices.[10]

On the other hand, the present authors have recently studied the Hubbard model for various cases (i.e., combinations of 2D or 3D lattice structures and band filling) having *ferromagnetic* spin fluctuations to find that *spin-triplet* superconductivity mediated by ferromagnetic spin fluctuations, if any, has very low T_c in general.[10] In fact, the possibility of finite T_c has been suggested only in systems having two *disconnected* pieces of Fermi surface lying point symmetrically about the Γ point.[11] There, superconductivity is enhanced because the nodal lines of the gap function do not intersect the Fermi surface.

Conversely, we may say that a reason why the singlet *d*-wave superconductivity mediated by antiferromagnetic spin fluctuations has such ''low T_c'' [$\sim O(0.01t)$] compared to the original electron energy scale t is because *the gap function has nodes on the Fermi surface*. Let us first see why this is the case. Superconductivity arises due to pair scattering processes near the Fermi surface mediated by a pairing interaction. Within the BCS theory, contributions to superconductivity from pair scattering processes $[\mathbf{k},-\mathbf{k}] \in \mathrm{FS} \rightarrow [\mathbf{k}',-\mathbf{k}'] \in \mathrm{FS}$ (FS stands for Fermi surface) are summed up in the form

$$V_{\mathrm{eff}} = -\frac{\sum_{\mathbf{k},\mathbf{k}' \in \mathrm{FS}} V^{(2)}(\mathbf{k}-\mathbf{k}')\,\phi(\mathbf{k})\,\phi(\mathbf{k}')}{\sum_{\mathbf{k} \in \mathrm{FS}} \phi^2(\mathbf{k})},$$

where $V^{(2)}(\mathbf{k}-\mathbf{k}')$ is the pairing interaction and $\phi(\mathbf{k})$ is the superconducting gap function. In order to have superconductivity with an order parameter ϕ, V_{eff} has to be positive and large. When the pairing is mediated by spin fluctuations that are pronounced around a certain wave vector **Q**, the pairing interaction $V^{(2)}$ is positive and roughly proportional to the spin susceptibility, so only the pair scattering processes $[\mathbf{k}, -\mathbf{k}] \in \mathrm{FS} \rightarrow [\mathbf{k}',-\mathbf{k}'] \in \mathrm{FS}$ that accompany a momentum transfer $\sim \mathbf{Q}$ and a sign change in ϕ give significant positive contributions to V_{eff}. This is the origin of the nodes in the *d*-wave gap function. The nodes intersect the Fermi surface for a connected Fermi surface, so that some pair scatterings give *negative* contributions to V_{eff} as far as the spin susceptibility has a finite spread $\Delta\mathbf{Q}$ [see Fig.1(a)]. In order to reduce negative contributions, the spin susceptibility has to have a sharp structure around **Q**, but in that case, pair scattering processes giving positive contributions will be strictly restricted to certain combinations of **k** and **k**′, so in any case, V_{eff} should be rather limited when the nodes of the gap function intersect the Fermi surface.

Due to the above considerations, we propose that if (i) there are two small pocketlike Fermi surfaces A and B and (ii) the spin susceptibility is pronounced around a wave vector **Q** with a spread $\Delta\mathbf{Q}$, where **Q** *bridges* the Fermi surfaces A and B, and $\Delta\mathbf{Q}$ is about the size of the pockets [see Fig. 1(b)], the resulting *spin-singlet* superconductivity may have a T_c much larger than $0.01t$. Namely, with different signs of the gap function assigned on A and B (with no nodes on the Fermi surface), *interpocket* pair scattering processes $\forall[\mathbf{k},$

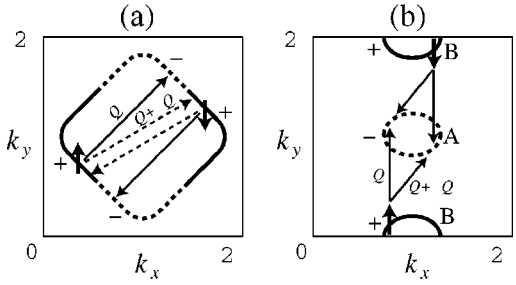

FIG. 1. The *d*-wave gap function for a system with a large connected Fermi surface (a) or a gap function for systems with two pocketlike Fermi surfaces A and B (b). The solid (dashed) curves represent positive (negative) values of the gap function on the Fermi surface. The solid (dashed) arrows represent spin-fluctuation-mediated pair scattering processes which give positive (negative) contribution to $V_{\rm eff}$. **Q** is the wave vector at which the spin susceptibility peaks, while $\Delta\mathbf{Q}$ is the spread of the peak structure.

$-\mathbf{k}]\in \mathrm{A}\rightarrow\forall[\mathbf{k}',-\mathbf{k}']\in \mathrm{B}$ (and vice versa) all have significant positive contribution to $V_{\rm eff}$, resulting in a high T_c. This idea can be applied either to single band systems having disconnected pieces of Fermi surface or to systems with multiple Fermi surfaces corresponding to different bands.

In order to provide an example in which such a scenario is realized, we start with a 2D rectangular lattice with different hopping integrals between the x and y directions ($t_{x2}=t_{x1}\equiv t_x$ in Fig. 2). For $t_x/t_y>1$, the Fermi surface becomes open in the y direction (Fig. 3, left panel). When the band filling is close to half filling, i.e., $n\sim 1$, the Fermi surface intersects the lines $k_x=\pi,3\pi/2$ for values of t_x/t_y not too large.[12] The nesting vector **Q** in this case bridges the parts of the Fermi surface that lie inside and outside of the region $\pi/2<k_x<3\pi/2$. If we now introduce an alternation in the hopping integrals in the x direction ($t_{x1}\neq t_{x2}$ in Fig. 2), the band will be folded at $k_x=\pi,3\pi/2$, resulting in two pocketlike Fermi surfaces, each in different bands (Fig. 3, right panel). The important point here is that the nesting vector **Q** should not change, at least when t_{x1}/t_{x2} is not too far from unity, so that **Q** *bridges the two Fermi surfaces*.

We have performed FLEX calculation for the Hubbard model $\mathcal{H}=-\Sigma_{\langle i,j\rangle\sigma=\uparrow,\downarrow}t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma}+c^{\dagger}_{j\sigma}c_{i\sigma})+U\Sigma_i n_{i\uparrow}n_{i\downarrow}$, on

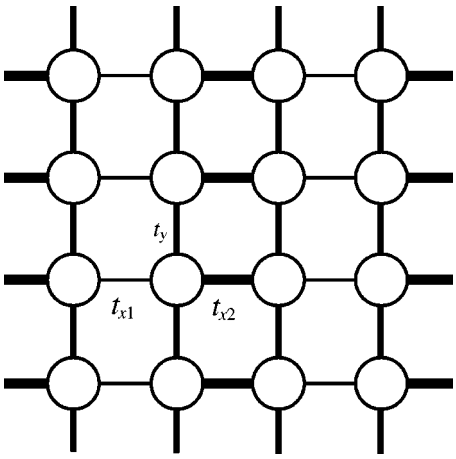

FIG. 2. The lattice considered in the present study.

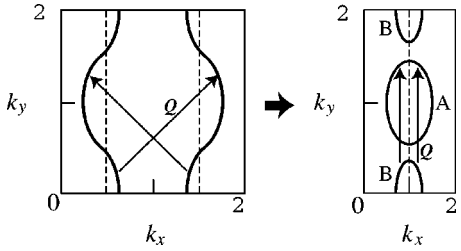

FIG. 3. The Brillouin zone and the Fermi surface(s) for $t_{x1}=t_{x2}$ (right panel) and for $t_{x1}\neq t_{x2}$ (left panel).

the above lattice. In the two band version of FLEX,[7] 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., $G_{lm}(\mathbf{k},i\varepsilon_n)$, 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 (denoted as α and β) indexed ones with a unitary transformation. As for the spin susceptibility, we diagonalize the 2×2 matrix $\chi_{\rm sp}$ and concentrate on the larger eigenvalue, denoted as χ.

The actual calculation proceeds as (i) Dyson's equation is solved to obtain the renormalized Green's function $G(k)$, where k is a shorthand for the wave vector **k** and the Matsubara frequency $i\epsilon_n$. (ii) The effective interaction $V^{(1)}(q)$ is given as $V^{(1)}(q)=\frac{3}{2}V_{\rm sp}(q)+\frac{1}{2}V_{\rm ch}(q)-U^2\chi_{\rm irr}(q)$. Here, the effective interactions due to spin (sp) fluctuations and those due to charge (ch) fluctuations have the forms $V_{\rm sp}=U^2\chi_{\rm sp}$ and $V_{\rm ch}=U^2\chi_{\rm ch}$, respectively, where the spin and the charge susceptibilities are $\chi_{\rm sp(ch)}(q)=\chi_{\rm irr}(q)[1-(+)U\chi_{\rm irr}(q)]^{-1}$ in terms of the irreducible susceptibility matrix $\chi_{\rm irr}(q)=-(1/N)\Sigma_k G(k+q)G(k)$ (N number of k-point meshes). (iii) $V^{(1)}$ then brings about the self-energy, $\Sigma(k)=(1/N)\Sigma_q G(k-q)V^{(1)}(q)$, which is fed back to Dyson's equation, and the self-consistent iterations are repeated until convergence is attained. We take 64×64 k-point meshes and up to 4096 Matsubara frequencies.

We determine T_c as the temperature at which the eigenvalue λ of the Eliashberg equation

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

reaches unity. Here the pairing interaction $V^{(2)}$ for singlet pairing is given by $V^{(2)}(q)=\frac{3}{2}V_{\rm sp}(q)-\frac{1}{2}V_{\rm ch}(q)$.

We take t_y as the unit of the energy ($t_y=1$). We present the results in the multiband scheme even for the single band case of $t_{x1}=t_{x2}$. Throughout the study, the band filling (number of electrons/number of sites) and the on-site repulsion are fixed at $n=0.95$ and $U=7$, respectively.

Let us now proceed to the calculation results. We first vary t_{x1} fixing $t_{x2}=1.3$ [solid arrow in the inset of Fig. 6(a)]. In Fig. 4, we plot $|G_\alpha|^2$, $|G_\beta|^2$, and χ for the lowest Matsubara frequency for $t_{x1}=1.3$ (a) and 0.8 (b). The ridges of

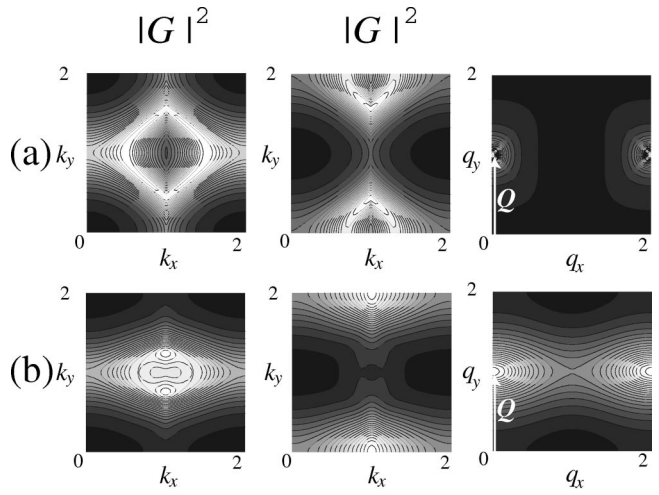

FIG. 4. Contour plots of $|G_\alpha(\mathbf{k})|^2$, $|G_\beta(\mathbf{k})|^2$, and $\chi(\mathbf{q})$ for $t_{x1}=1.3$ (a) and 0.8 (b) with $t_{x2}=1.3$ and $T=0.14$. The lighter the color, the larger the value. Note that $|G_\alpha|^2$ in (b) is a contour plot of Fig. 7(c).

$|G|^2$ represent the Fermi surfaces. For $t_{x1}=1.3(=t_{x2})$, this is a single band system, so the Fermi surfaces in the α and β bands are connected at around $k=(\pi,\pi/2)$ and $(\pi,3\pi/2)$ to result in a single, large (open) Fermi surface. The spin susceptibility peaks at the nesting vector of the Fermi surface, namely at $\mathbf{Q}=(0,\pi)$ in the folded Brillouin zone [or $\mathbf{Q}=(\pi,\pi)$ in the unfolded Brillouin zone]. The corresponding gap function for the lowest Matsubara frequency shown in Fig. 5(a) has a node along $k_x\sim\pi$ in order to satisfy the condition $\phi(\mathbf{k})=-\phi(\mathbf{k}+\mathbf{Q})$ on the Fermi surface.

For $t_{x1}=0.8$ by contrast, there is a small pocketlike Fermi surface in each band, namely, around $\mathbf{k}=(\pi,\pi)$ in the α band and around $(\pi,0)$ in the β band. The spin structure becomes broader having a spread $\Delta\mathbf{Q}$ of the size of the pockets, and it still peaks around $\mathbf{Q}=(0,\pi)$, so that $\mathbf{Q}$ *bridges* the two Fermi surfaces. As seen in Fig. 5(b), the corresponding gap functions have fixed signs in each band, and their variation is small. Thus, interpocket pair scatterings $\forall[\mathbf{k},-\mathbf{k}]\in \mathrm{A}\rightarrow\forall[\mathbf{k}',-\mathbf{k}']\in \mathrm{B}$ (and vice versa) all have significant positive contributions to V_{eff}.

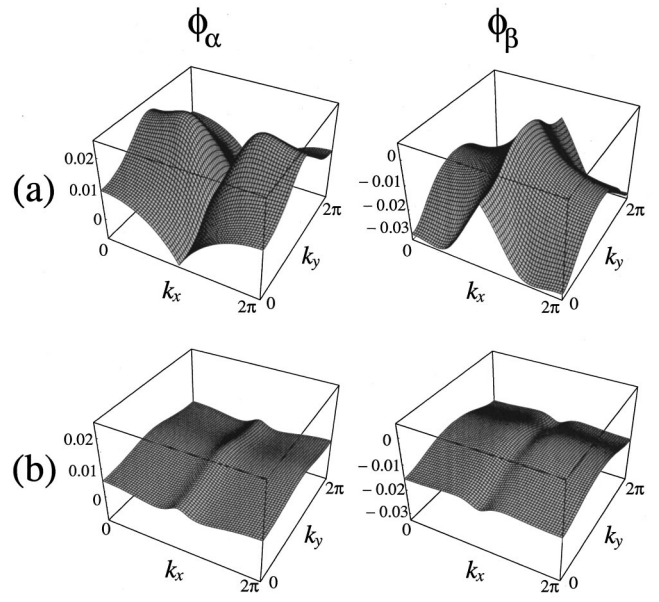

FIG. 5. Plots of $\phi_\alpha(\mathbf{k})$ and $\phi_\beta(\mathbf{k})$ for the same sets of parameter values as in Fig. 4.

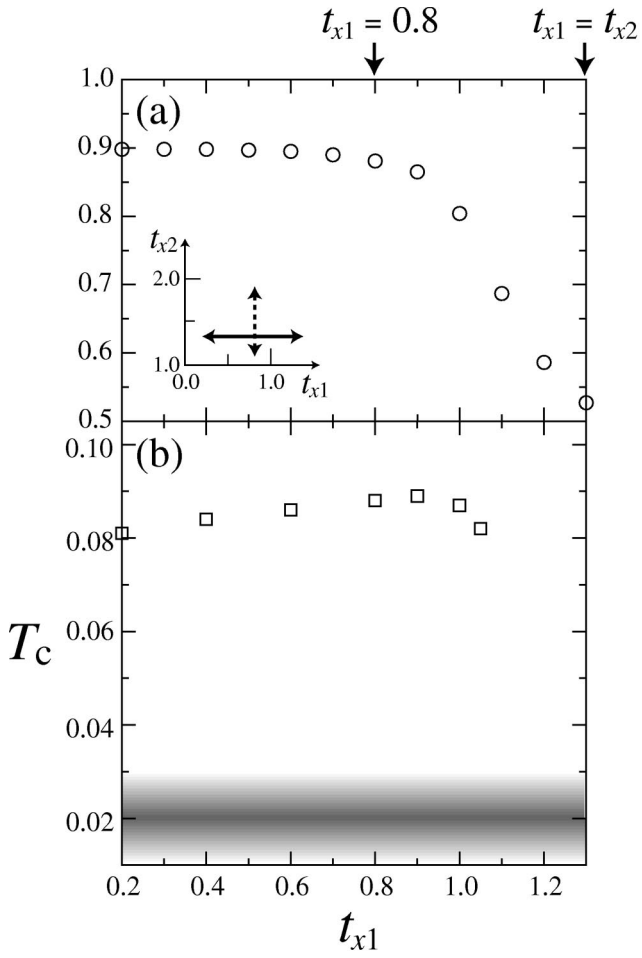

FIG. 6. λ (a) and T_c (b) plotted as functions of t_{x1} with $T=0.14$ in (a) and t_{x2} fixed at 1.3. T_c is not obtained for $t_{x1}>1.1$, where the system comes very close to antiferromagnetic ordering $[U\chi_{\mathrm{irr}}(\mathbf{Q})\sim 1]$ before λ reaches unity upon lowering the temperature. The hatched region in (b) represent the range of T_c for systems having a large connected Fermi surface. The solid (dashed) arrow in the inset of (a) shows the range of the parameter values taken in Fig. 6 (Fig. 8).

Correspondingly, as shown in Fig. 6(a), the maximum eigenvalue λ for $T=0.14$ starts out around ~ 0.5 for the single-band case of $t_{x1}=t_{x2}=1.3$, but it increases up to ~ 0.9 upon decreasing t_{x1}. T_c, plotted in Fig. 6(b), comes close to ~ 0.1 for $t_{x1}<1$, which is almost an order of magnitude larger compared to typical values for the cases with a large connected Fermi surface.

In order to show that the topology and the size of the Fermi surfaces are crucial, we now show results for various values of t_{x2}, fixing $t_{x1}=0.8$ [dashed arrow in the inset of Fig. 6(a)]. When $t_{x2}\simeq t_{x1}$ or smaller, the Fermi surfaces in both bands are open in the x direction. This can be under-

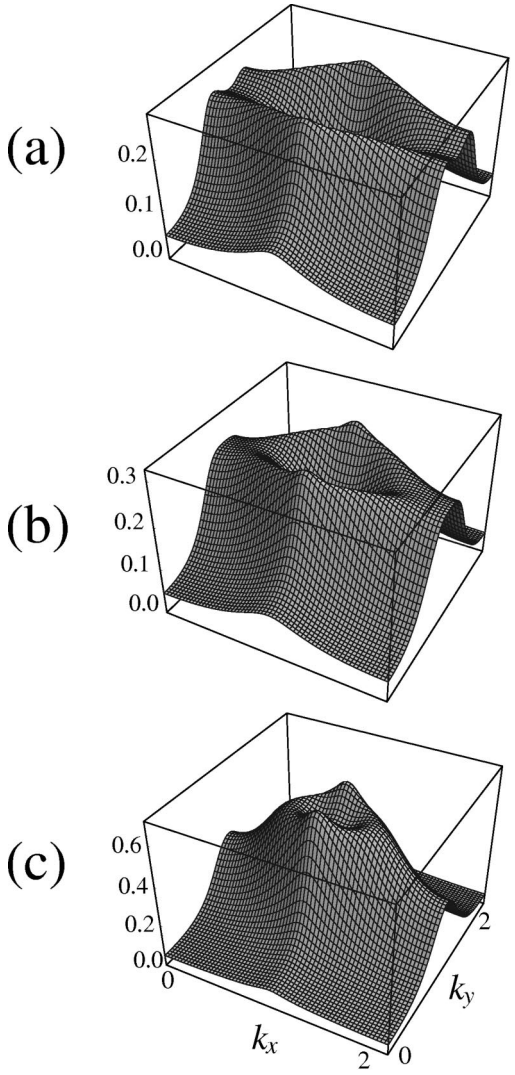

FIG. 7. Plots of $|G_\alpha(\mathbf{k})|^2$ for $t_{x2}=1.1$ (a), 1.2 (b), and 1.3 (c), with $t_{x1}=0.8$ and $T=0.14$.

stood by considering the single band situation $t_{x2}=t_{x1}<t_y$, where the unfolded Fermi surface for $n\sim 1$ is open in the x direction. On the other hand, we have seen that there are two small pocketlike Fermi surfaces for $t_{x2}=1.3$, so each Fermi surface has to change its topology between $t_{x2}\sim 0.8$ and 1.3. In fact, it can be seen from Fig. 7 that the topology of the Fermi surface in the α band changes from a large Fermi surface to a small pocketlike Fermi surface at around $t_{x2}\sim 1.2$. λ rapidly increases corresponding to this change of the topology of the Fermi surface, as can be seen from Fig. 8. On the other hand, λ decreases for too large t_{x2} because the β band lies above the Fermi level in this case.[14]

The Fermi level passes through a van Hove singularity (VHS) when the topology of the Fermi surface changes, namely, at around $t_{x2}\sim 1.2$. The fact that λ takes large values *after* the Fermi level passes VHS suggests that the density of states is not playing a crucial role in giving rise to the high T_c.

Finally, let us discuss the relation between the present study and previous ones. The Hubbard model on coupled-ladder lattices[7,9] has been studied using FLEX approximation. In those studies, $T_c\sim O(0.01t)$ has been obtained, which, in light of the present results, is because the parameter values adopted there do not result in small, pocketlike Fermi surfaces.

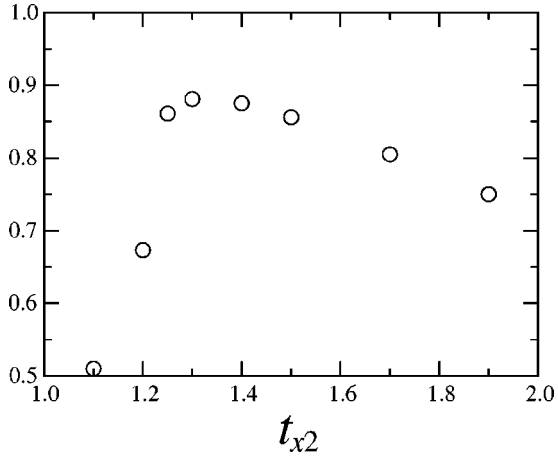

FIG. 8. λ plotted as a function of t_{x2} with $t_{x1}=0.8$ and $T=0.14$.

In the large U limit, the present Hubbard model should tend to the t-J model with alternating t and J. The t-J model with alternating J (dimerized t-J model) has been studied as a *spin-gapped* system.[15] There, however, the correlation between superconductivity and the topology or size of the Fermi surfaces was not discussed. It is not clear at present whether the t-J model with alternation only in J has properties similar to those presented here. The Hubbard and t-J models on *purely* 1D ladder lattices have also been studied extensively as spin gapped systems. In particular, large enhancement of the pairing correlation has been obtained when the Fermi level lies near the bottom of the upper band.[16–18] These results seem to be related to the present study, although we cannot make a definite conclusion because the FLEX approximation cannot be applied to purely 1D systems, which are not Fermi liquid but Luttinger liquid.

At present, it is not clear whether the presence of a spin gap is a sufficient or a necessary condition for a superconducting state without nodes of the gap on the Fermi surface. Intuitively, however, a gapfull superconductivity and a finite spin gap do seem to be consistent with each other. This point remains as an appealing future problem.

To summarize, we have proposed that superconductivity mediated by spin fluctuations in systems having Fermi surface pockets may have rather high T_c. T_c should be restricted by the energy scale of the spin fluctuations, so that there should be an optimal set of parameter values. In fact, for the model considered in the present study, the parameter values adopted here gave roughly the highest T_c in the parameter range we studied.[13]

Our proposal is general and can be applied to systems having higher symmetry,[19] but particularly for anisotropic systems such as the one considered in the present study,

there may be strong electron-phonon coupling due to its low-symmetry of the lattice structure. It would then be an interesting future problem to investigate how the presence of phonons would affect the present conclusion.[20]

Discussions with Hideo Aoki and Takashi Kimura are gratefully acknowledged. This work was in part funded by the Grant-in-Aid for Scientific Research from the Ministry of Education of Japan.

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[12] In the purely 1D limit, that is, when $t_x/t_y \to \infty$, the Fermi surface becomes a straight line parallel to the y axis, so it does not intersect the lines $k_x = \pi, 3\pi/2$ for $n \neq 1$.
[13] To be more precise, we can obtain higher T_c at half-filling, but since the system comes close to antiferromagnetic ordering, T_c might be overestimated there due to an underestimation of the fluctuation in the particle-hole channel. By taking $n = 0.95$ as in the present study, this problem is circumvented since the system stays far away from antiferromagnetic ordering ($U\chi_0 < 0.95$ for $t_{x1} < 1$ and $t_{x2} = 1.3$ at T_c).
[14] For t_{x2} as large as ~ 2, the band width is larger than the case for $t_{x1} = t_{x2} = t_y = 1$, so that we are actually dealing with an effectively lower temperature. For $t_{x2} \sim 1.3$ and $t_{x1} \sim 0.8$, however, the band width is similar to that for $t_{x1} = t_{x2} = t_y = 1$, so our conclusion that T_c is almost an order of magnitude larger in the former compared to the latter holds.
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[19] For example, a system having two round (or square) Fermi surface pockets with about the same size, one centered at (0,0) and the other centered at (π, π), would be a candidate.
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