

# Spin-triplet superconductivity in repulsive Hubbard models with disconnected Fermi surfaces: A case study on triangular and honeycomb lattices

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We propose that spin-fluctuation-mediated spin-triplet superconductivity may be realized in repulsive Hubbard models with disconnected Fermi surfaces. The idea is confirmed for Hubbard models on triangular (dilute band filling) and honeycomb (near half-filling) lattices using fluctuation exchange approximation, where triplet pairing order parameter with  $f$ -wave symmetry is obtained. Possible relevance to real materials is suggested.

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## I. INTRODUCTION

A fascination toward spin-triplet superconductivity has a long history, but recent experimental suggestions for triplet pairing in a heavy fermion system  $\text{UPt}_3$ ,<sup>1</sup> organic conductors  $(\text{TMTSF})_2\text{X}$  ( $\text{X}=\text{ClO}_4$ ,<sup>2</sup>  $\text{PF}_6$ ),<sup>3</sup> and a ruthenate  $\text{Sr}_2\text{RuO}_4$ ,<sup>4,5</sup> have renewed our interests in mechanisms of triplet superconductivity. In particular, it is fairly intriguing to investigate whether electron-electron repulsive interactions can lead to triplet superconductivity. Ferromagnetic-spin-fluctuation mechanism has been proposed from the early days, but to our knowledge, realization of triplet superconductivity (at sizable temperatures) has yet to be established theoretically for repulsive electron models with renormalization effects of the quasiparticles taken into account. The lifetime of the quasiparticles is important since this is a factor dominating  $T_c$ .

Recently, the present authors with Aoki have investigated the possibility of triplet pairing in the Hubbard model for a variety of lattice structures and band fillings using fluctuation exchange (FLEX) approximation.<sup>6</sup> A naive expectation is that triplet superconductivity may be realized when the band is away from half filled and the density of states (DOS) at the Fermi level is large, since ferromagnetic fluctuations become strong in such a situation. In Ref. 6, however, it has turned out that the transition temperature ( $T_c$ ) of triplet superconductivity, if any, is too low to be detected as far as the cases surveyed there are concerned. A typical case is a square lattice with appreciable next-nearest-neighbor hoppings and dilute band fillings. First let us briefly review this situation as a reference for the results presented later.

## II. FORMULATION

We consider the Hubbard model,  $\mathcal{H} = \sum_{\langle i,j \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$ , on a square lattice shown in Fig. 1, where  $t$  ( $=1$ ) is the nearest and  $t'_1$  ( $=t'_2$  here) is the next-nearest-neighbor hopping. In the FLEX calculation,<sup>7-9</sup> (i) Dyson's equation is solved to obtain the renormalized Green's function  $G(k)$ , where  $k \equiv (\mathbf{k}, i\epsilon_n)$  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  $\chi_{\text{irr}}(q) \equiv -(1/N) \sum_k G(k+q)G(k)$  ( $N$ : number of  $k$ -point meshes), (iii) the self-energy is obtained as  $\Sigma(k) \equiv (1/N) \sum_q G(k-q)V^{(1)}(q)$ , which is substituted into Dyson's equation in (i), and the self-consistent loops are repeated until convergence is attained. Throughout the study, we take  $64 \times 64$   $k$ -point meshes and the Matsubara frequencies  $\epsilon_n$  from  $-(2N_c - 1)\pi T$  to  $(2N_c - 1)\pi T$  with  $N_c$  up to 16384 in order to ensure convergence at low temperatures.

To obtain  $T_c$ , we solve the eigenvalue (Eliashberg) equation for the superconducting order parameter  $\phi(k)$ ,

$$\lambda \phi(k) = -\frac{T}{N} \sum_{k'} \phi(k') |G(k')|^2 V^{(2)}(k-k'), \quad (1)$$

where the pairing interaction  $V^{(2)}$ , which mediates pair scattering from  $(\mathbf{k}, -\mathbf{k})$  to  $(\mathbf{k}', -\mathbf{k}')$  [ $\equiv (\mathbf{k} + \mathbf{q}, -\mathbf{k} - \mathbf{q})$ ], is given as

$$V_s^{(2)}(q) = \frac{3}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 - U \chi_{\text{irr}}(q)} \right] - \frac{1}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 + U \chi_{\text{irr}}(q)} \right] \quad (2)$$

for singlet pairing, and

$$V_t^{(2)}(q) = -\frac{1}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 - U \chi_{\text{irr}}(q)} \right] - \frac{1}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 + U \chi_{\text{irr}}(q)} \right] \quad (3)$$

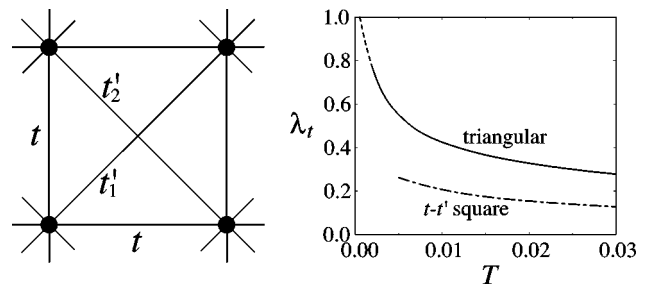


FIG. 1. The left panel shows the hopping integrals for square ( $t'_1 = t'_2$ ) or triangular ( $t'_2 = 0$ ) lattice. In the right panel,  $\lambda_t$  is plotted as a function of temperature for the Hubbard model on a square lattice with  $t'_1 = t'_2 = 0.4$ ,  $U = 6$ , and  $n = 0.3$  (dash-dotted line), or on an isotropic triangular lattice with  $t'_1 = 1$ ,  $U = 8$ , and  $n = 0.15$  (solid line). In the latter case, a spline extrapolation to lower temperatures is also plotted (dashed line).

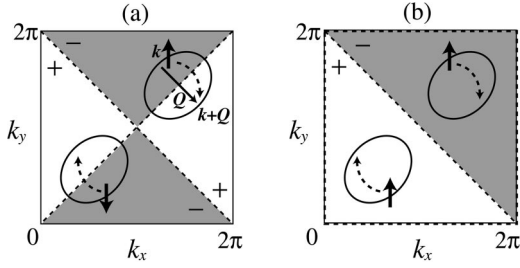


FIG. 2. Basic idea of the present mechanism is presented. Intra-FS pair scattering (dashed curves) is mediated by  $V^{(2)}(\mathbf{Q})$  within each piece of the disconnected FS (closed solid curves). The dashed straight lines represent nodes of the order parameter for singlet (a) and triplet (b) pairing.

for triplet pairing. In either case, the first (second) term represents the contribution from spin (charge) fluctuations.  $T_c$  is the temperature at which the maximum eigenvalue  $\lambda$  reaches unity. We denote the eigenvalue and the order parameter for triplet (singlet) pairing as  $\lambda_t$  ( $\lambda_s$ ) and  $\phi_t$  ( $\phi_s$ ), respectively.

In Ref. 6,  $t'$ ,  $U$ , and the band filling  $n$  (Ref. 10) were varied in search of triplet superconductivity, but  $\lambda_t$  remained below  $\sim 0.2$  in the tractable temperature range as typically displayed in Fig. 1 (dash-dotted line). The main reason why triplet pairing instability is weak is because  $|V_t^{(2)}|$  is only one third of  $|V_s^{(2)}|$  when spin fluctuation is dominant as can be seen from Eqs. (2) and (3).

### III. TRIPLET PAIRING MECHANISM FOR SYSTEMS WITH DISCONNECTED FERMI SURFACES

Here, we propose that the above difficulty for spin-fluctuation-mediated triplet pairing in the Hubbard model can be overcome under certain conditions. Let us first present our idea. We consider a situation (see Fig. 2) where (i) the Fermi surface (FS) is disconnected (preferably well separated) into two pieces which are located point symmetrically about  $\mathbf{k}=\mathbf{0}$ , and (ii) the spin structure is pronounced around a wave vector  $\mathbf{Q}$  in such a way that two electrons with zero total momentum can be scattered *within each piece of the FS* (this process will be called intra-FS pair scattering hereafter) by exchanging spin fluctuations having momentum  $\sim \mathbf{Q}$ . Now, according to the BCS theory, the quantity  $-\left[\sum_{\mathbf{k}, \mathbf{k}' \in FS} V^{(2)}(\mathbf{k}-\mathbf{k}') \phi(\mathbf{k}) \phi(\mathbf{k}')\right] / \left[\sum_{\mathbf{k} \in FS} \phi^2(\mathbf{k})\right]$  [the numerator being  $\sim -\sum_{\mathbf{k} \in FS} V^{(2)}(\mathbf{Q}) \phi(\mathbf{k}) \phi(\mathbf{k}+\mathbf{Q})$ ] has to be positive and large in order to have superconductivity having an order parameter  $\phi$ . Then, pair scatterings from  $(\mathbf{k}, -\mathbf{k})$  to  $(\mathbf{k}+\mathbf{Q}, -\mathbf{k}-\mathbf{Q})$  for *singlet* pairing, mediated by *repulsive*  $V_s^{(2)}(\mathbf{Q})$ , have to accompany a sign change in the order parameter  $\phi_s(\mathbf{k})$  [Fig. 2(a)]. Hence the nodes of  $\phi_s(\mathbf{k})$  must intersect the FS. For *triplet* pairing, by contrast, pairs can be scattered within a region having the same sign in  $\phi_t(\mathbf{k})$  because  $V_t^{(2)}(\mathbf{Q})$  is *attractive*. In this case, since the gap nodes [which exist due to triplet pairing symmetry  $\phi(\mathbf{k}) = -\phi(-\mathbf{k})$ ] do not intersect the FS [Fig. 2(b)], the entire FS can be exploited for pairing, so that triplet pairing may be enhanced. Quite recently, a related proposal has been

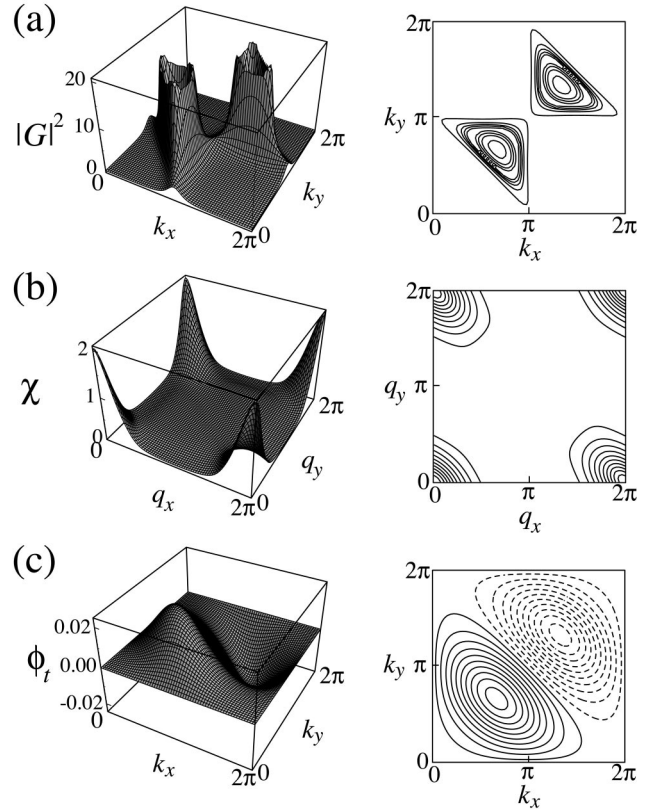


FIG. 3.  $|G(\mathbf{k}, i\pi k_B T)|^2$  (a),  $\chi(\mathbf{k}, 0)$  (b), and  $\phi_t(\mathbf{k}, i\pi k_B T)$  (c) are plotted for the Hubbard model on a triangular lattice with  $t'_1=1$ ,  $U=8$ ,  $n=0.15$ , and  $T=0.01$ . The right panels are contour-plots of the left panels.

raised by Kohmoto and Sato for systems with both phonons and spin fluctuations present,<sup>11</sup> as discussed later.

### IV. ISOTROPIC TRIANGULAR LATTICE

The above conditions are not satisfied for the  $t$ - $t'$  square lattice because it has a connected FS. As an example of a system in which the above conditions are indeed satisfied, we consider the Hubbard model on an isotropic triangular lattice with dilute band fillings. The band dispersion for  $U=0$  is given by  $\varepsilon_{\Delta}(\mathbf{k}) = 2[\cos k_x + \cos k_y + \cos(k_x + k_y)]$  when we represent an isotropic triangular lattice by setting  $t=t'_1=1$ <sup>12</sup> and  $t'_2=0$  in Fig. 1. Superconductivity on an isotropic triangular lattice has been studied by several authors,<sup>13-16</sup> but their interest was mainly focused on  $n \sim 1$ . In Ref. 6, the possibility of triplet superconductivity was studied at quarter filling ( $n=0.5$ ), where ferromagnetic fluctuations become strong because the Fermi level lies right at the position where the DOS diverges. However,  $\lambda_t$  was again found to be small, which, in the present context, is because the FS is connected. If we set  $n < 0.5$ , on the other hand, the FS is disconnected into two pieces, which are centered respectively at  $k=(2\pi/3, 2\pi/3)$  and  $k=(4\pi/3, 4\pi/3)$ . Here we take  $n=0.15$ , where the two pieces of the FS are well separated. In Fig. 3, we plot the FLEX result for  $|G(\mathbf{k}, i\pi k_B T)|^2$  (a) and the spin susceptibility  $\chi(\mathbf{k}, 0) \equiv \chi_{\text{irr}}(\mathbf{k}, 0) / [1$

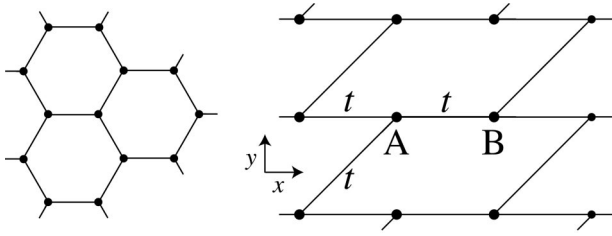


FIG. 4. For the honeycomb lattice shown in the left panel, we employ the topologically equivalent structure shown in the right.

$-U\chi_{\text{irr}}(\mathbf{k},0)$  (b) against  $\mathbf{k}$  for  $U=8$  and  $T=0.01$ . The FS as identified from the ridge in  $|G(\mathbf{k},i\pi k_B T)|^2$  is indeed disconnected into two pieces.  $\chi(\mathbf{k},0)$  is sharply peaked at  $\mathbf{k}=0$  as seen in Fig. 3(b), indicating ferromagnetic fluctuations.<sup>17</sup> This is partially because the FS is small, but it is also because the Fermi level for  $n=0.15$  is still not too far away from the peak position of the DOS. In this case,  $\lambda_s$  is shown to be small, which is because  $V_s^{(2)}(\mathbf{Q})$  can only mediate pair scatterings in the vicinity of the nodes when  $\mathbf{Q}\sim\mathbf{0}$ .

If we turn to triplet pairing, the order parameter  $\phi_t(\mathbf{k},i\pi k_B T)$ , plotted against  $\mathbf{k}$  for  $T=0.01$  in Fig. 3(c), has  $f$ -wave ( $f_{x^3-3xy^2}$ -wave in the notation of the  $C_6$  symmetry group) symmetry with three sets of nodal lines [ $k_x \equiv 0 \pmod{2\pi}$ ,  $k_y \equiv 0$ , and  $k_x + k_y \equiv 0$ ]. Comparing Figs.3(a) and (c), we can see that these nodes do not intersect the FS. Accordingly,  $\lambda_t$  (Fig. 1, solid line) is strongly enhanced compared to the case for the  $t$ - $t'$  square lattice. A spline extrapolation to low temperatures suggests a possible low but finite  $T_c$ .

## V. HONEYCOMB LATTICE

As another example, we next propose that the Hubbard model on a *honeycomb* lattice (Fig. 4) should also be interesting. Since there are two sites (A and B) in a unit cell, this is a two-band system. The noninteracting band dispersion  $\varepsilon_{\text{hc}}(\mathbf{k}) = \pm \sqrt{\varepsilon_{\Delta}(\mathbf{k}) + 3}$  has two pairs of vertex-sharing cones at  $k = (2\pi/3, 2\pi/3)$  and  $k = (4\pi/3, 4\pi/3)$ , so again the FS becomes disconnected, this time for fillings close to  $n=1$ .

In the multiband version of FLEX,<sup>18,19</sup> the quantities  $G$ ,  $\chi$ ,  $\Sigma$ , and  $\phi$  have  $2 \times 2$  matrix forms, e.g.,  $G_{\alpha\beta}(\mathbf{k},i\omega_n)$ , where  $\alpha, \beta$  denote A or B sites. The band representation of the Green's function and the order parameters is obtained by using the relation between the annihilation operators of upper ( $u$ ) and lower ( $l$ ) band electrons ( $c_{\mathbf{k}}^u, c_{\mathbf{k}}^l$ ) and those of A and B site electrons ( $c_{\mathbf{k}}^A, c_{\mathbf{k}}^B$ ). As for  $\chi$ , we diagonalize the  $2 \times 2$  matrix  $\chi_{\alpha\beta}$  to obtain  $\chi_{\pm} = (\chi_{AA} + \chi_{BB})/2 \pm \sqrt{[(\chi_{AA} - \chi_{BB})/2]^2 + |\chi_{AB}|^2}$ .

In Fig. 5, we plot  $|G^l(\mathbf{k},i\pi k_B T)|^2$  (a) and  $\chi_+(\mathbf{k},0)$  (b) for  $n=0.95$ ,  $U=8$  and  $T=0.01$ . Since  $\chi_{AB}(\mathbf{0},0)$  is found to be negative, the peak around  $\mathbf{k}=\mathbf{0}$  in  $\chi_+(\mathbf{k},0)$  is an indication of antiferromagnetic fluctuations, as expected for a nearly half filled bipartite lattice system. Note that  $\chi_+(\mathbf{k},0)$  has a broad structure compared to the case for the triangular lattice [Fig. 3(b)].

If we turn to  $\lambda_s$  and  $\lambda_t$  as functions of  $T$  in Fig. 6(a),  $\lambda_t$  is again large, but this time  $\lambda_s$  is in fact larger. We can

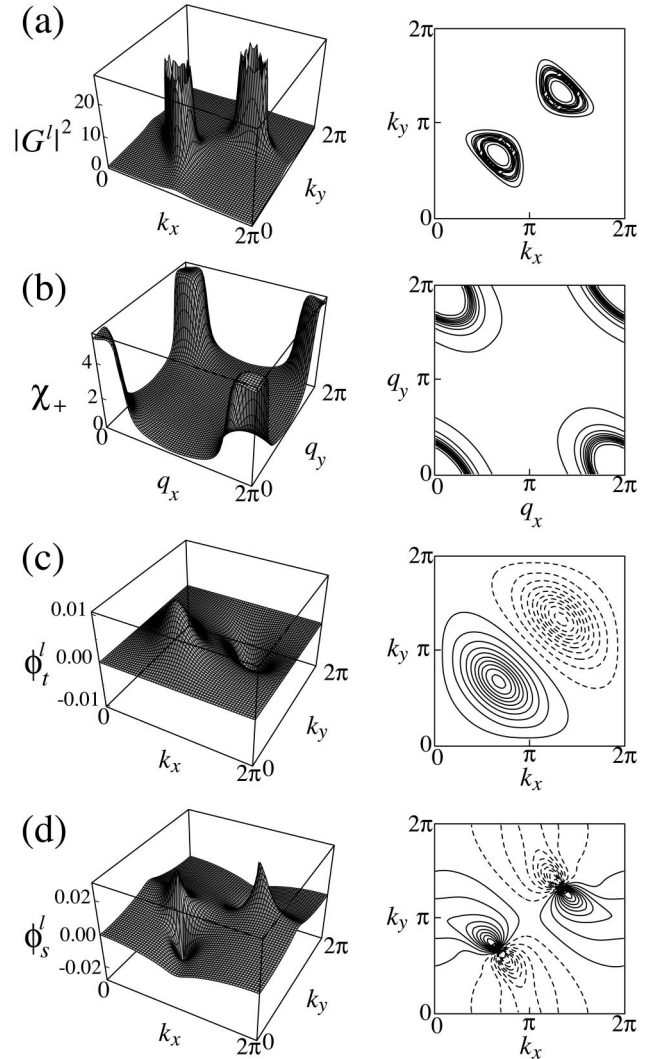


FIG. 5.  $|G^l(\mathbf{k},i\pi k_B T)|^2$  (a),  $\chi_+(\mathbf{k},0)$  (b),  $\phi_t^l(\mathbf{k},i\pi k_B T)$  (c), and  $\phi_s^l(\mathbf{k},i\pi k_B T)$  (d) are plotted for the Hubbard model on a honeycomb lattice with  $U=8$ ,  $n=0.95$ ,  $\Delta_{AB}=0$  and  $T=0.01$ .

trace this to the broad spin structure, for which spin fluctuations with relatively large momentum can be exchanged to mediate singlet pairing at wave vectors away from the nodes. Nevertheless, we can still observe that  $\lambda_t$  is enhanced above  $\lambda_s/3$  (recall that  $|V_t^{(2)}| \sim |V_s^{(2)}|/3$ ), which should be due to the fact that the nodes in  $\phi_s^l$  intersect the FS, while those in  $\phi_t^l$  do not as seen by comparing Figs. 5(a) and (c)/(d).

We have found that  $|\phi_{AB}| > (<) |\phi_{AA}|$  for singlet (triplet) pairing, meaning that singlet (triplet) pairing mainly takes place on different (same) sublattices. This is in fact consistent with the antiferromagnetic alignment of the spins. Then, we can intuitively expect that triplet can dominate over singlet if we introduce a level offset,  $\Delta_{AB}$ , between A and B sites. In Fig. 6(b), we plot  $\lambda_s$  and  $\lambda_t$  for the same parameter values as in Fig. 6(a), except for a finite  $\Delta_{AB}=5$ . Triplet pairing indeed dominates over singlet pairing at low temperatures, and here again a possible finite  $T_c$  for triplet superconductivity is suggested. The intuitive picture can be



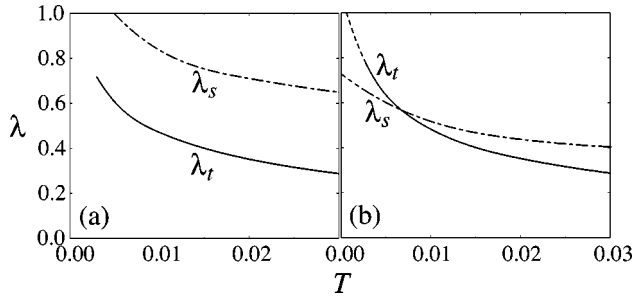


FIG. 6.  $\lambda_t$  (solid line) and  $\lambda_s$  (dash-dotted line) are plotted as functions of temperature for the Hubbard model on a honeycomb lattice with  $U=8$ ,  $n=0.95$ , and  $\Delta_{AB}=0$  (a) or  $\Delta_{AB}=5$  (b). In (b), spline extrapolations to lower temperatures are indicated by dashed lines.

paraphrased in the momentum space that the peak structure of  $\chi$  (not shown) becomes sharper when  $\Delta_{AB} \neq 0$ .

## VI. DISCUSSION

At this point, let us stress that the present study should not be regarded as a simple confirmation of the earlier proposals that anisotropic pairing interactions may lead to spin-triplet superconductivity.<sup>20</sup> As opposed to this expectation, we have found in Ref. 6 that anisotropic pairing interaction (driven by ferromagnetic spin fluctuations) *alone do not lead to triplet superconductivity* (with an appreciable  $T_c$ ) in the Hubbard model, as already mentioned.

In fact, the pairing interaction (or the spin susceptibility) in the triangular lattice for  $n=0.5$ , a case with a connected Fermi surface, is more sharply peaked around  $\mathbf{k}=(0,0)$  (thus being more anisotropic and more favorable for triplet pairing) than for  $n=0.15$ , but the triplet pairing is much more enhanced in the latter case. This means that here, the absence of the gap nodes on the Fermi surface plays a more important role than the anisotropy of the pairing interaction. Thus the present study opens a *renewed* possibility of realizing triplet pairing in systems having a disconnected Fermi surface.

## VII. RELEVANCE TO SUPERCONDUCTIVITY IN REAL MATERIALS

Finally, let us make some remarks concerning possible relevance to real materials. As for a possible triplet superconductor  $\text{UPt}_3$ , if we examine the FS calculated by full-potential linearized augmented plane wave (FLAPW) method,<sup>21</sup> we notice that there are two disconnected pockets (band 37 in Ref. 21),<sup>22</sup> which, in our view, is favorable for triplet pairing. It would be an interesting future problem to investigate in detail the applicability of the present mechanism.

Disconnected FS can arise similarly in graphite intercalation compounds (GIC), except that the FS is cylindrical (quasi-2D).<sup>23</sup> This is because graphite is a system where honeycomb sheets of carbon atoms are stacked. Although spin fluctuations in GIC may not be strong enough to induce superconductivity purely electronically, the discon-

nectivity of the FS itself should be favorable for triplet pairing, so a cooperation between certain phonon modes and (weak) spin fluctuations might lead to triplet superconductivity (even in the absence of  $\Delta_{AB}$  considered above). Namely, if attractive intra-FS pair scatterings mediated by phonons are present, antiferromagnetic spin fluctuations as considered here would work constructively with phonons to enhance intra-FS pair scatterings for triplet pairing, while the converse is true for singlet pairing. Experimentally, although triplet pairing has not been claimed to our knowledge, a large value of  $H_{c2}$  (extrapolated to  $T=0$ ) observed in  $\text{C}_4\text{KTl}_{1.5}$ <sup>24</sup> is in fact reminiscent of a large  $H_{c2}$  in  $(\text{TMTSF})_2\text{X}$ .<sup>2,3</sup>

Application to solid-state surfaces may also be of interest. For example, it is known that  $\text{Si}(111)-(\sqrt{3} \times \sqrt{3})\text{-B}$  surface takes a triangular lattice structure,<sup>25</sup> while  $\text{Si}(111)-(\sqrt{3} \times \sqrt{3})\text{-Ag}$  has a honeycomb lattice structure with inequivalent A and B sites.<sup>26</sup> Moreover, it has been proposed experimentally,<sup>27</sup> and in fact been reinforced theoretically,<sup>28</sup> that  $\text{K/Si}(111)-(\sqrt{3} \times \sqrt{3})\text{-B}$  is a Mott insulator, meaning that electron correlation is strong in this system. In fact, electron correlation is expected to be strong on  $\text{Si}(111)-(\sqrt{3} \times \sqrt{3})$  surface because the bandwidth of the surface states is rather narrow due to large interorbital spacings. Then, if we can adjust the Fermi level so as to make the FS disconnected,<sup>29</sup> an occurrence of triplet superconductivity might be expected according to the present theory.

As for  $(\text{TMTSF})_2\text{X}$  and  $\text{Sr}_2\text{RuO}_4$ , Kohmoto and Sato have recently proposed that disconnectivity (quasi-one dimensionality) of the FS, along with the presence of spin fluctuations originating from the nesting of the FS, plays an essential role in stabilizing *phonon-mediated* triplet *p*-wave pairing.<sup>11</sup> Our study is related to this proposal in that disconnectivity is important, but in these systems, as seen in Kohmoto and Sato's argument, the dominant spin fluctuations have wave vectors that *bridge* the two pieces of the FS, so that they mediate *inter-FS* pair scatterings<sup>30</sup> rather than *intra-FS* ones. Thus our *purely* spin-fluctuation-mediated pairing mechanism does not directly apply to these materials, although we do believe that the disconnectivity of the FS may be playing a certain role in realizing triplet superconductivity.

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  - <sup>30</sup>In inter-FS pair scatterings, electrons are scattered from one piece of the FS to the other. Such scatterings mediated by spin fluctuations suppress  $p$ -wave pairing, but they also suppress  $s$ -wave pairing even more strongly, which is the reason why  $p$  wave dominates over  $s$  wave in the presence of phonons in Kohmoto-Sato's mechanism.