Interlayer spin-singlet pairing induced by magnetic interactions in an antiferromagnetic superconductor

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It is shown that interlayer spin-singlet Cooper pairing is induced by magnetic interactions in a metallic antiferromagnet of stacked conductive layers in which each layer is ferromagnetically polarized and they order antiferromagnetically in stacking direction. As a result, the antiferromagnetic long-range order and superconductivity coexist at low temperatures. It is shown that \( T_{AF} > T_c \) except for in a very limited parameter region unless \( T_{AF} = 0 \), where \( T_{AF} \) and \( T_c \) denote the antiferromagnetic and superconducting transition temperatures, respectively. It is found that the exchange field caused by the spontaneous staggered magnetization does not affect superconductivity at all, even if it is very large. The resultant superconducting order parameter has a horizontal line node, and is isotropic in spin space in spite of the anisotropy of the background magnetic order. We discuss the possible relevance of the present mechanism to the antiferromagnetic heavy fermion superconductors UPd$_2$Al$_3$ and CePt$_3$Si.

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In this paper, we show that interlayer spin-singlet Cooper pairing is induced by magnetic interactions in a certain kind of metallic antiferromagnet. We consider a layered system of itinerant electrons in which each layer is ferromagnetically polarized but the majority-spin alternates in stacking direction. Therefore, the magnetic order is characterized by the wave vector \( Q = (0, 0, \pi/c) \), where we have assumed the \( a \) and \( b \) crystal axes to be parallel to the layers, and the \( c \)-axis in the stacking direction, and \( c \) denotes the \( c \)-axis lattice constant. It is also shown that the exchange field caused by spontaneous staggered magnetization does not influence superconductivity, however large it is.

The heavy fermion superconductors, such as UPd$_2$Al$_3$ and CePt$_3$Si, can be candidates of the present mechanism. The antiferromagnetic long-range order is considered to be characterized by the wave vector \( Q = (0, 0, \pi/c) \), both in UPd$_2$Al$_3$ \cite{1} and in CePt$_3$Si \cite{2}. Superconducting transitions have been observed at \( T_c = 2.0 \) K and 0.7 K, below the antiferromagnetic transition temperatures \( T_{AF} = 14.3 \) K and 2.2 K, in UPd$_2$Al$_3$ \cite{3} and CePt$_3$Si \cite{4}, respectively. It has been suggested that the magnetic moment is large, \( i.e., 0.85 \mu_B/U_i \) in UPd$_2$Al$_3$ \cite{2}, but small, \( i.e., 0.16 \mu_B/Ce \) in CePt$_3$Si \cite{2}.

The order parameter of interlayer spin-singlet pairing has a horizontal line node. This also agrees with the experimental results in the compound UPd$_2$Al$_3$. The existence of the line node is suggested by the nuclear magnetic resonance (NMR) measurement \cite{2}, in which the Hebel-Slichter peak was absent, and \( T_1^{-1} \propto T_3^3 \) was observed. The singlet state is supported by the presence of NMR Knight shift \cite{2}, and the Pauli limited upper critical field \cite{2} \cite{2}. In recent angle resolved magnetothermal transport measurements \cite{5}, two-fold oscillation in the rotation perpendicular to the \( ab \) plane was observed, while no oscillation was observed in rotation in the \( ab \) plane. These experimental results are reproduced by the order parameter of the form of \( \Delta(k) = \Delta_0 \cos(k_c c) \).

Coexistence of superconductivity and magnetism has been studied in various models by many authors \cite{6} \cite{7} \cite{8} \cite{9} \cite{10} \cite{11}. In particular, spin singlet superconductivity in the presence of ferromagnetic layers has been studied by many authors \cite{3}. In the models examined in those papers, superconductivity occurs in a subsystem different from the magnetic layers. In contrast, we examine a model in which superconductivity occurs in electrons on magnetic layers in the present model. Kopaev also studied superconductivity when only magnetic electrons are present \cite{10}, although it exists only in the vicinity of the domain wall.

The magnetic structure mentioned above can be modeled most simply by the Hamiltonian

\[
H = H_0 + H_U + H_J
\]

with the kinetic energy term

\[
H_0 = \sum_{k \sigma} \xi(k) c_{k \sigma}^\dagger c_{k \sigma},
\]

the on-site Coulomb interactions

\[
H_U = U \sum_i n_{i \uparrow} n_{i \downarrow},
\]

and the exchange interactions

\[
H_J = \frac{1}{2} \sum_{i,j} J_{ij} (S_i \cdot S_j - \frac{1}{4} n_i n_j).
\]

We have defined \( S_i = \frac{1}{2} \sum_{\sigma \sigma'} c_{i \sigma}^\dagger \sigma \sigma' c_{i \sigma'} \), \( n_i = \sum_{\sigma} n_{i \sigma} \), and \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \), where \( \sigma \) denotes the vector of Pauli matrices, and \( c_{i \sigma} \) and \( c_{i \sigma}^\dagger \) denote the electron operators. We define \( J_{ij} = J > 0 \) for \( R_i = R_j \pm \hat{c} \), \( J_{ij} = -J \) if \( R_i \neq R_j \), and \( J_{ij} = 0 \) for nearest neighbor sites \((i, j)\) on the same layer, and
of interlayer exchange interaction \( J_{ij} \) expresses the effect of the exchange Coulomb interaction, which is usually smaller than \( U \) and \( J \), but necessary to stabilize the present magnetic structure. The ferromagnetic correlation in each layer is due to \( U \) and \( J_{ij} \). However, two-dimensional (2D) long-range order without order in the \( c \)-direction cannot occur due to the thermal fluctuations in the present isotropic model, however large \( U \) is. Transition to the long-range order occurs only in the presence of interlayer exchange interaction \( J \), and the transition to the three dimensional antiferromagnetic long-range order at \( T = T_{AF} \) is the only magnetic transition.

Many examples of compounds which can be modeled by 2D Heisenberg ferromagnetic model with antiferromagnetic interlayer exchange interactions are summarized by a review article by Jough and Miedema [12]. For example, it was obtained from experimental data that \( J_{ij}/J_1 \approx 8 \times 10^{-5}, 3.4 \times 10^{-5} \) and 0.21, \( T_{AF} = 13.8, 16.8 \) and 18K, and \( J_{ij}/k_B = 18.8, 5.25 \) and 3.0K in the compounds \( \text{Rb}_2\text{CuCl}_4, \text{CrCl}_3 \) and \( \text{NaCrS}_2 \), respectively. These compounds have the ferromagnetic short-range order in each layer at temperatures higher than the transition temperature due to the intralayer ferromagnetic exchange interaction \( J_{ij} \), and undergo the long-range order by the weak interlayer exchange interaction \( J \) at the transition temperature \( T_{AF} \). In many examples, the interlayer exchange interactions are antiferromagnetic and much weaker than the intralayer interaction in most cases. In our model, we also take into account the on-site Coulomb repulsion \( U \) in addition to the intralayer exchange interaction \( J_{ij} \) to stabilize the ferromagnetic structure in each layer. Later, we consider a situation in which \( U \gg J_{ij} \) as an example, but it is straightforward to apply the theory to the opposite case \( U \ll J_{ij} \).

It is well-known due to the Mermin-Wagner’s theorem [13] that purely 2D isotropic Heisenberg model cannot exhibit any long-range order at any finite temperature. For the long-range order to be stabilized, an additional Ising type intralayer interaction or a three dimensional (interlayer) interaction is necessary. However, the former does not stabilize the present antiferromagnetic configuration in the stacking direction, as observed in \( \text{UPd}_2\text{Al}_3 \) [14] and \( \text{CePt}_3\text{Si} \) [2]. Therefore, more or less, interlayer antiferromagnetic interaction must exist in the present compounds. The physical origin of the antiferromagnetic interlayer interaction is interlayer kinetic exchange or superexchange process. In the former process, the interlayer exchange interaction \( J \) is written as \( J \sim 4t^2_c/U \), where \( t_c \) denotes interlayer electron hopping energy. Since \( t_c \) is expected to be small from the crystal structure, the perturbation theory to derive the above expression of \( J \) would be justified.

When we apply the Hamiltonian eq. (1) to the compound \( \text{UPd}_2\text{Al}_3 \), we should note that it has been suggested [14,15] by thermodynamic measurements that the magnetic and superconducting transitions occur in nearly disjoint subsystems in this compound. However, even if this is true, the present theory holds if the superconducting subsystem has a \( \delta f \) character and coexist in the same crystal structure. We discuss an application of the present theory taking into account the two-fluid model later.

The interaction terms can be rewritten as

\[
H_U + H_J = \frac{1}{N} \sum_{kk'q} V(k, k', q) \hat{c}^\dagger_{k+q} \hat{c}_{k} \hat{c}^\dagger_{k'q} \hat{c}_{k'q},
\]

with

\[
V(k, k', q) = U - \hat{J}(q) - \hat{j}(k - k' + q) + \hat{j}_{\parallel}(q) + \hat{j}_{\parallel}(k - k' + q),
\]

where \( \hat{J}(q) \equiv J(\cos(q \cdot \hat{c})) \) and \( \hat{j}_{\parallel}(q) \) are the Fourier transforms of the interlayer and intralayer exchange interactions, respectively. Since we have not specified the lattice structure of the layer, the expression of \( \hat{J}_{\parallel}(q) \) is not shown, but it does not depend on \( q_{y} \) and must have a peak around \( q_{y} = 0 \), where \( q_{y} = (q_x, q_y) \). Similarly, the form of \( \hat{J}(k) \) also depends on the lattice structure of the layer. We have simplified it as \( \hat{J}(k) = \hat{J}_{\parallel}(k_{||}) + \hat{J}_{\perp}(k_{\perp}) \) with \( \hat{J}_{\parallel}(k_{||}) = h^2|k_{||}|^2/2m^* - \mu \) and \( \hat{J}_{\perp}(k_{\perp}) = -2t_{\perp} \cos(k_{\perp}c) \) for convenience, where \( k_{||} = (k_x, k_y) \). This simplification does not essentially change the qualitative results. In this paper, we examine the system in which \( t_{\perp} \) and \( J_{\parallel} \) are small. We take units with \( h = k_B = 1 \).

First, we describe the magnetic transition. Let us examine the spin propagator

\[
\chi(R_i - R_j, \tau) = -\langle T_{\tau} S_i^z(\tau) S_j^z(0) \rangle
\]

in the random phase approximation (RPA). We define the Fourier transform \( \chi(q, i\nu_m) \) by

\[
\chi(q, i\nu_m) \equiv \sum_{j} \oint_{0} e^{-i(q \cdot R_j - \nu_m\tau)} \chi(R_j, \tau),
\]

where \( \nu_m = 2\pi m T \) denotes the Matsubara frequency, and \( \beta = 1/T \). If \( \chi(Q, 0) \) diverges, it indicates the phase transition to the magnetic long-range order with \( Q \). If we omit \( t_{\perp} \) and \( J_{\parallel} \), we obtain

\[
\chi(q, i\nu_m) = \frac{1}{2} 1 - [U - \hat{J}(q)] \chi_0(q, i\nu_m),
\]

where

\[
\chi_0(q, i\nu_m) = \frac{1}{N} \sum_{k} T \sum_{n} G^{(0)}_\sigma(k, i\omega_n) \times G^{(0)}_\sigma(k + q, i\omega_n + i\nu_m).
\]
with the bare electron Green’s function $G^{(0)}_{\sigma}$. When $t_{\perp} = 0$, the free susceptibility $\chi_0$ is expressed as

$$\chi_0(q, 0) = \rho_0 \left(1 - \text{Re} \left[ \frac{2k_F}{q_{\parallel}} \right]^2 \right)$$

(11)

at $T = 0$, where $\rho_0 = n^*ab/2\pi h^2$ denotes the density of states of the 2D system. We have defined the effective mass $m^*$, the in-plane Fermi momentum $k_{F\parallel}$, and the lattice constants $a$ and $b$. The maximum $\chi(q, \nu_m)$ occurs at arbitrary $q = (q_{\parallel}, \pi/c)$ with $|q_{\parallel}| < 2k_{F\parallel}$ and $\nu_m = 0$. This degeneracy is removed by $J_{\parallel} \neq 0$, which is small but exists in practice. Hence, $\chi(q, \nu_m)$ reaches its maximum at $q = (0, 0, \pi/c) = Q$. It is easily verified by replacing $U - J$ with $U - \tilde{J} - \tilde{J}_{\parallel}$ in eq. (11). Furthermore, when we take into account $t_{\perp} \neq 0$, $\chi_0$ has a peak around $q = (q_{\parallel}, \pi/c) = Q'$ with $|q_{\parallel}| \approx 2k_{F\parallel}$, but the difference $\chi_0(Q', 0) - \chi_0(0, 0) \approx \pi_{\perp}$ is small. Therefore, when $t_{\perp} \neq 0$, we must assume $J_{\parallel} \neq 0$ which is small but sufficiently large for the maximum of $\chi$ to occur at $q = Q$, so that the magnetic order of $Q$ is stabilized.

When these conditions are satisfied, antiferromagnetic transition occurs at a temperature which satisfies

$$1 = (U + J) \chi_0(Q, 0)$$

(12)

from eq. (11), where $\chi_0(Q, 0) = \chi_0(0, 0) = \rho_0/(e^{-\beta\mu} + 1)$. The chemical potential $\mu$ is determined by the equation for the electron number per site $n = 2\beta^{-1}\rho_0 \ln(1 + e^{-\beta\mu})$. Thus, we obtain $\chi_0(Q, 0) = \rho_0/(1 - e^{-\beta\mu})$. Therefore, we obtain the antiferromagnetic transition temperature

$$T_{AF} = \frac{n}{2\rho_0 \ln \left(\frac{U + J}{U + J - 1}\right)}$$

(13)

to an ordered state with the wave vector $Q = (0, 0, \pi/c)$ when $(U + J)\rho_0 > 1$, while $T_{AF} = 0$ otherwise.

In the antiferromagnetic phase, the electron states are affected by spontaneous staggered magnetization. We define $A$ and $B$ sublattices (sublayers) whose majority spins are up and down, respectively. We write the electron operators as $a_{i\sigma}$ and $b_{j\sigma}$ for $i \in A$ and $j \in B$. Therefore, we have

$$n_{i\sigma}^A = \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle = \frac{n}{2} + \sigma m,$$

$$n_{j\sigma}^B = \langle b_{j\sigma}^\dagger b_{j\sigma} \rangle = \frac{n}{2} - \sigma m,$$

(14)

where $\langle S_{i\sigma}^z \rangle = -\langle S_{j\sigma}^z \rangle = m$ for $i \in A$ and $j \in B$. We have defined $\sigma = \uparrow$ and $\downarrow$ in suffixes, which correspond to $\sigma = \uparrow$ and $\downarrow$ in suffixes, respectively. Corrections to the kinetic energy due to $H_U + H_J$ are taken into account by the mean field approximation as

$$H_{MF} = \sum_{k\sigma} \sigma h_{MF} \left[a_{k\sigma}^\dagger a_{k\sigma} - b_{-k\sigma}^\dagger b_{k\sigma} \right]$$

(15)

with $h_{MF} = (U + J_0 + z_J J_{\parallel}/2) m$, where $z_J$ denotes the number of nearest neighbor sites in the layer, and the summation $\sum_{k}$ is carried out over the half Brillouin zone. Therefore, the total kinetic energy term $\tilde{H}_0 = H_0 + H_{MF}$ is written as

$$\tilde{H}_0 = \sum_{k\sigma} \xi_{\parallel}^A a_{k\sigma}^\dagger a_{k\sigma} + \xi_{\parallel}^B b_{-k\sigma}^\dagger b_{k\sigma}$$

$$+ \xi_{\parallel} (a_{k\sigma}^\dagger b_{k\sigma} + b_{-k\sigma}^\dagger a_{k\sigma})$$

(16)

where $\xi_{\parallel}^A = \xi_{\parallel} - \sigma h_{MF}$ and $\xi_{\parallel}^B = \xi_{\parallel} + \sigma h_{MF}$. The mean field approximation is consistent with the RPA, which we have used to derive $T_{AF}$, although we have neglected $J_{\parallel}$ in eq. (13).

Now, let us examine superconductivity. We will show its formulation in the antiferromagnetic phase, but it is immediately reduced to that in the paramagnetic phase by putting $m = 0$. The exchange interaction $H_J$ contributes to pairing interaction, while it causes the antiferromagnetic transition and creates the exchange field. We rewrite $H_J$ as

$$H_J = -\sum_{i \in A, j \in B} J_{ij} \Psi_{ij}^{(s)} \Psi_{ij}^{(s)}$$

(17)

where $\Psi_{ij}^{(s)} = 2^{-1/2}(a_{i\uparrow} b_{j\downarrow} - a_{i\downarrow} b_{j\uparrow})$. The statistical average $\langle \Psi_{ij}^{(s)} \rangle$ is the order parameter of interlayer spin-singlet pairing. Here, we have neglected $J_{\parallel}$, since it does not have an important effect on superconductivity if it is small. In eq. (17), it is found that $J$ contributes only to spin-singlet pairing as an attractive interaction in its first order. In the BCS approximation, eq. (17) is written as

$$H_J \approx \sum_{k\sigma} \sigma [\Delta(k) a_{k\sigma} b_{-k\sigma} + h.c.]$$

(18)

with the order parameter

$$\Delta(k) = -\frac{1}{2N} \sum_{k'\sigma'} \sigma' J(k - k') (b_{-k'\sigma'}^\dagger a_{k\sigma'})$$

(19)

Therefore, we obtain

$$\Delta(k) = \Delta_0 \cos(k_z c)$$

(20)

with

$$\Delta_0 = -\frac{J}{2N} \sum_{k'\sigma'} \sigma' \cos(k_z c) (b_{-k'\sigma'}^\dagger a_{k\sigma'})$$

(21)

In the same approximation, the on-site Coulomb interaction $H_U$ is ineffective for anisotropic superconductivity. It has been proposed that in the higher order of $J$, the pairing interaction is enhanced by the exchange of magnons [12]. This mechanism has also been examined in the compound UPd$_2$Al$_3$ [17, 18, 19, 20]. However, since the spin fluctuations are weak at temperatures much lower than the antiferromagnetic transition temperature ($T \lesssim T_{AF}/\tau$), the pairing interaction mediated by the magnons is weak [12]. Hence, in this paper, we neglect...
them in comparison to the direct pairing interaction described in eqs. (17) and (18). The present direct pairing interaction is not mediated by the magnons. In a broader sense, however, one may regard the present pairing interaction as mediated by the spin fluctuations, because the superexchange interactions are derived from the virtual process of electrons, with which their spins correlate.

When \( J = 0 \), the present model is reducible to the quasi-2D Hubbard model. In the perturbation theory based on it, it was shown that antiferromagnetic fluctuations induce intralayer singlet pairing near the antiferromagnetic phase [21]. However, the present system is ferromagnetic in each layer. In the absence of \( J \), the propagator of the fluctuations \( \chi(q) \) has a broad peak around \( q || \approx 0 \) as we can see in eq. (12), in contrast to the sharp peak in the antiferromagnetic case, where the Fermi-surface nesting occurs. Therefore, the pairing interaction is not strongly enhanced by the spin fluctuation unless \( U \) is large. Nishikawa and Yamada [22] examined the \( \text{UPd}_2\text{Al}_3 \) on the basis of a 2D Hubbard model taking into account the lattice structure, although they did not examine interlayer pairing. In the presence of interlayer interactions, \( t_{\perp} \) and \( J \), the spin fluctuations will enhance the interlayer singlet pairing interaction.

From eqs. (16) and (18), we obtain

\[
H = \sum_{k} \psi_{k}^{\dagger} \hat{M} \psi_{k},
\]

where we have defined \( \psi_{k}^{\dagger} = (c_{k_{\uparrow}}^{\dagger} b_{k_{\downarrow}}^{\dagger} a_{-k_{\downarrow}} b_{-k_{\uparrow}}) \) and

\[
\hat{M}(k) = \begin{pmatrix}
\xi_{k_{\uparrow}\uparrow} & \xi_{k_{\uparrow}\downarrow} & -\Delta^* & 0 \\
\xi_{k_{\downarrow}\uparrow} & \xi_{k_{\downarrow}\downarrow} & 0 & -\Delta \\
-\Delta & 0 & -\xi_{k_{\uparrow}\uparrow} & -\xi_{k_{\downarrow}\downarrow} \\
0 & -\Delta & -\xi_{k_{\uparrow}\downarrow} & -\xi_{k_{\downarrow}\uparrow}
\end{pmatrix}.
\]

The Green’s function is defined in matrix form by

\[
\hat{G}(k, \tau) = -\langle T \psi_{k}(\tau) \psi_{k}^{\dagger} \rangle.
\]

From the equation of motion, we obtain

\[
\hat{G}(k, i\omega_n) = [i\omega_n I - \hat{M}(k)]^{-1},
\]

where \( I \) denotes the \( 2 \times 2 \) unit matrix. We obtain the quasi-particle energies, \( \pm E_{A}(k) \) and \( \pm E_B(k) \), where \( E_{A} = E^2 + F, E_{B} = E^2 - F, E^2 = \xi_{k_{\uparrow}k_{\uparrow}} + \xi_{k_{\downarrow}k_{\downarrow}} + h_{MF}^2 + |\Delta|^2 \) and \( F = 2[\xi_{k_{\uparrow}k_{\downarrow}}^2 + h_{MF}^2 + |\Delta|^2]/2 \). If we define \( G_{ij} \) as the \( (i, j) \) component of the matrix \( \hat{G} \), we have

\[
\langle b_{k_{\downarrow}k_{\uparrow}} c_{k_{\uparrow}k_{\downarrow}}^{\dagger} \rangle = G_{32}(k', \tau = 0),
\]

\[
\langle b_{-k_{\downarrow}k_{\uparrow}} c_{-k_{\uparrow}k_{\downarrow}}^{\dagger} \rangle = -G_{41}(k', \tau = 0).
\]

Therefore, we obtain the gap equation

\[
\Delta(k) = \frac{1}{4N} \sum_{k'} \langle \hat{j}(k' - k) \sum_{X=A,B} \frac{\tanh \frac{E_X(k')}{2}}{2E_X(k')} \Delta(k') \rangle.
\]
the order of $v_{F\perp}/\Delta_0$, where $v_{F\perp}$ and $\Delta_0$ denote Fermi velocity in the $c$-direction and the scale of magnitude of the order parameter at $T = 0$, respectively. We obtain $\xi_{c\perp} \gg c$, if $t_\perp \gg \Delta_0$.

When $t_\perp$ is negligible, the transition temperature $T_c$ is obtained as follows. Since $\delta_c = |h_{MF}|$, we can integrate $\cos^2(k'_z c)$ with respect to $k'_z$ first in eq. (28). Unless $\delta_c > \mu$, the density of states is constant when $t_\perp \approx 0$. The $k'_z$ integral is approximated by the $\xi_{||} \pm h_{MF}$ integrals with an effective cutoff energy $W_c$, which is on the order of the band width. More explicitly, it is expressed as $W_c = [(W - \mu - h_{MF})(W - \mu + h_{MF})(\mu + h_{MF})(\mu - h_{MF})]^{1/4}$, where $W$ and $\mu$ denote the band width and the chemical potential measured from the bottom of the band, respectively. Carrying out the integral, we obtain

$$T_c = 1.13 W_c e^{-2/J \rho_0}.$$  \hspace{1cm} (29)

Here, it is found that $T_c$ is not influenced by the spontaneous staggered magnetization $g\mu_B m_i$, as expected from the above argument.

Figure 2 depicts the antiferromagnetic transition temperature $T_{AF}$ and the superconducting transition temperature $T_c$, scaled by $n/\rho_0$ and $W_c$, respectively. These scales have the same orders of magnitude, i.e., $\rho_0 \sim 1/\rho_c$. It is found that, as the order of the magnitudes, the experimental results in UPd$_2$Al$_3$, $T_{AF} = 14.3$ K and $T_c = 2.0$ K could be explained within the present mechanism, if the effective band width is on the order of $W = 10 \sim 100$ K, which is realistic for heavy fermion systems.

Figure 3 shows the values of $J \rho_0$ and $U \rho_0$ for a given ratio of $\alpha \equiv (T_{AF} \rho_0/n)/(T_c/W_c) = T_{AF}/T_c \times W_c \rho_0/n$. If we consider $W_c \rho_0/n \sim 1$, the experimental data $T_{AF} = 14.3$ K and $T_c = 2.0$ K give $\alpha \sim 7$. Therefore, the experimental value of ratio $\alpha$ can be reasonably reproduced for moderate values of the coupling constants $J$ and $U$. We will compare the theoretical and experimental results more closely below. We obtain $T_{AF} > T_c$ or $T_{AF} = 0$, except in a very small region of the phase diagram.

We note that the resultant singlet order parameter is invariant under rotation in spin space. The rotational transformation is made by

$$R(\theta) = \exp[i \frac{\theta}{2} \sigma_y] = \cos \frac{\theta}{2} + i \sigma_y \sin \frac{\theta}{2}. \hspace{1cm} (30)$$

The electron operators in the rotated space are defined by

$$\begin{pmatrix}
\tilde{c}_{k \downarrow} \\
\tilde{c}_{k \uparrow}
\end{pmatrix} = R(\theta) \begin{pmatrix}
c_{k \downarrow} \\
c_{k \uparrow}
\end{pmatrix}, \hspace{1cm} (31)$$

where $c_{k\sigma} = a_{k\sigma}$ or $b_{k\sigma}$. It is easily verified that

$$\sum_{\sigma} \sigma \langle \hat{b}_{-k - \sigma} \hat{a}_{k\sigma} \rangle = \sum_{\sigma} \sigma \langle \hat{\tilde{b}}_{-k - \sigma} \hat{\tilde{a}}_{k\sigma} \rangle. \hspace{1cm} (32)$$

In addition, the present pairing interaction is rotationally invariant, i.e., $J(\mathbf{k}, \mathbf{k}')$ does not have spin suffixes.

Therefore, $\Delta(k)$ given by eq. (19) is isotropic in spin space, irrespective of the direction of the magnetic order. In fact, the resultant gap equations 24 and 28 are invariant under spin rotation.

These results may explain the experimental data of the muon spin rotation measurements in UPd$_2$Al$_3$ 22, in which it was observed that the London penetration depth and the magnetic susceptibility reduction below
$T_c$ are essentially isotropic, while the total susceptibility remains strongly anisotropic. In the present mechanism, not only the singlet nature but also the rotational invariance of the pairing interaction play essential roles in the spin isotropy of $\Delta(k)$. In contrast, in the “magnetic exciton” mechanism, the pairing interaction and the order parameter are anisotropic if the magnetic system is anisotropic.

The compound CePt$_3$Si is another candidate for the present pairing mechanism, although the ratio of the transition temperatures $T_{AF}/T_c$ is much smaller than that in UPd$_2$Al$_3$. In contrast to UPd$_2$Al$_3$, the critical field largely exceeds the Pauli paramagnetic limit $H_P$ estimated by the simplified formula $H_P \approx 1.86[T/K] \times T_c[K] \approx 1.4T$ in CePt$_3$Si [4]. If the present mechanism of singlet pairing is realized in CePt$_3$Si, the large critical field cannot be attributed to equal spin pairing. It can be explained by an effect of exchange field created by coexisting antiferromagnetic long-range order, which reduces the Pauli paramagnetic pair-breaking effect [24]. It is still controversial whether dominant pairing in CePt$_3$Si is of singlet or triplet. Recent NMR data suggest that the gap function may have some novel structure [25].

Here, we simply put $\nu = 3$ for order estimations. From the values of $\tilde{J}_m$ and $\tilde{\rho}_s$ estimated above, the values of $\tilde{J}_m$ and $\tilde{\rho}_m$ can be obtained, if the ratio $Z_m/Z_s$ is known. Therefore, we only need the values of $Z_m/Z_s$ and $\tilde{U}_m$ for estimation of $T_{AF}$. However, since they are not known for UPd$_2$Al$_3$ at the present, we need to assume them. In the assumption, we require that $\tilde{W}_m$ is smaller than $T_{AF}$ consistently with the observation of a large local magnetic moment in UPd$_2$Al$_3$ [14]. Physically, it is also plausible that $\tilde{U}_m$ is not much larger than $T_{AF}$ but larger than $\tilde{W}_m$. As an example, let us assume that $Z_m/Z_s = 30$, which gives $\tilde{W}_m \approx 8K < T_{AF}$ and $\tilde{J}_m \approx 0.19K$. In this case, if we assume $\tilde{U}_m = 20K$ and 30K as examples, we obtain $T_{AF} \approx 10K$ and 21K, respectively. As another example, we assume $Z_m/Z_s = 20$, which gives $\tilde{W}_m \approx 12K < T_{AF}$ and $\tilde{J}_m \approx 0.43K$. In this case $\tilde{U}_m = 30K$ and 40K give $T_{AF} \approx 16K$ and 27K, respectively. The values $\tilde{J}_m \approx 0.19K$ and 0.43K obtained in these examples are not outrageous as energy parameters in real materials. In fact, $J \approx 0.15K$ and 0.63K were obtained from experimental data in Rb$_2$CuCl$_4$ and NaCrS$_2$, respectively [12]. Here, $J$ was not estimated as the bare parameter but estimated as the dressed (observed) parameter like $\tilde{J}_m$. Although our estimations are crude, the values of $T_{AF}$ obtained above are on the same order of the experimental result $T_{AF} = 14.3K$. Therefore, we find that the present mechanism reproduces consistent orders of magnitudes of $T_c$ and $T_{AF}$ for appropriate values of $Z_m/Z_s$ and $\tilde{U}_m$.

The result that $T_{AF} > T_c$ except for in a very limited region unless $T_{AF} \neq 0$ can be explained physically as follows. In the present mechanism, both interlayer antiferromagnetic long-range order and interlayer singlet superconductivity are induced by interlayer antiferromagnetic exchange interaction. However, strong on-site repulsion contributes to stabilization of the ferromagnetic structure in each layer, while it does not contribute to interlayer singlet pairing. Therefore, the magnetic transition occurs at a higher temperature than the superconducting transition temperature unless the on-site $U$ is negligibly small.

Interlayer pairing has been studied by many authors [24]. In this paper, we have examined the magnetic mechanism of the pairing interactions for interlayer singlet pairing, when the electrons are on the magnetic layers. However, irrespective of the pairing mechanism, interlayer pairing of the present type seems to be the most favorable, apart from equal spin pairing, when the present type of antiferromagnetic long-range order coexists. Other pairing states, such as intralayer singlet pairing, are strongly suppressed by the splitting of the Fermi-surfaces of the electrons with up and down spins due to the antiferromagnetic moment. Even in the two-fluid model, the exchange field must be induced on the electrons responsible to superconductivity.

In conclusion, in antiferromagnets with the magnetic order of the wave vector $Q = (0, 0, \pi/c)$, magnetic interactions may induce the superconductivity of interlayer spin-singlet pairing, the order parameter of which has a horizontal line node. It was found that superconductivity and an antiferromagnetic long-range order with large localized magnetic moments $m$ can coexist, and that $T_c$
is not influenced by the magnitude of $m$. It was also found that $T_{AF} > T_c$ in most cases, unless $T_{AF} = 0$. The present model may describe an essential aspect of antiferromagnetic heavy fermion superconductors, such as UPd$_2$Al$_3$ and CePt$_3$Si. The orders of the magnitude of $T_{AF}$ and $T_c$ and their ratio $T_{AF}/T_c \approx 3 \sim 7$ can be reproduced by assuming moderate parameter values. The resultant order parameter is consistent with the observations mentioned above.

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