Fully gapped $s$-wave superconductivity enhanced by magnetic criticality in heavy fermion system

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In heavy fermion systems, higher-rank multipole operators are active thanks to the strong spin-orbit interaction (SOI), and the role of diverse multipole fluctuations on the pairing mechanism attracts a lot of attention. Here, we study a mechanism of superconductivity in heavy fermion systems, by focusing on the impact of vertex corrections (VCs) for the pairing interaction going beyond the Migdal approximation. In heavy fermion systems, strong interference between multipole fluctuations cause significant VCs, that represent many-body effects beyond mean-field-type approximations. Especially, the coupling constants between electrons and charged-bosons, including the electron-phonon coupling constant, are strongly magnified by the VCs. For this reason, moderate even-rank (=electric) multipole fluctuations give large attractive interaction, and therefore $s$-wave superconductivity can emerge in heavy-fermion systems. In particular, phonon-mediated superconductivity is expected to be realized near the magnetic criticality, thanks to the VCs due to magnetic multipole fluctuations. The present mechanism may be responsible for the fully gapped $s$-wave superconducting state realized in CeCu$_2$Si$_2$.

I. INTRODUCTION

Heavy fermion systems are very interesting platform of exotic electronic states induced by strong Coulomb interaction and spin-orbit interaction (SOI) on $f$-electrons. In Ce-based compounds, $4f^1$ configuration is realized in Ce$^{3+}$ ion. Due to strong SOI, the total angular momentum $J = L + S$ becomes good quantum number. Since the energy of $J = 5/2$ multiplet is about 0.3eV lower than that of $J = 7/2$ multiplet, the latter can be safely dropped in the theoretical model. In tetragonal crystals, the degeneracy of $J = 5/2$ multiplet is separated into three Kramers doublets due to the crystalline electric field (CEF). Usually, the CEF splitting energy is of order 1 meV $\sim$ 10 meV.

In many $f$-electron systems, magnetic fluctuations cause interesting quantum critical phenomena and unconventional superconductivity [1–7]. In addition, higher-rank multipole operators are also active thanks to the strong SOI of $f$-electrons. For this reason, various interesting multipole order and fluctuations are caused by strong $f$-electron interaction. As an example of higher-rank order, CeB$_6$ exhibits quadrupole (rank 2) order and field-induced octupole (rank 3) order [8, 9]. Also, emergence of hexadecapole (rank 4) in PrRu$_4$P$_{12}$ [10] and hexadecapole or dotriacontapole (rank 5) in URu$_2$Si$_2$ [11–13] have been discussed. The fluctuations of these multipole operators mediate interesting unconventional superconductivity. For example, $d$-wave superconductivity appears next to the the magnetic order phase in CeMIn$_5$ ($M$=Rh,Co,Ir) [14]. In addition, superconductivity appears next to the quadrupole order in Pr$_2$Zn$_{20}$ ($T$ = Rh and Ir) [15] and Pr$_2$T$_2$Al$_{20}$ ($T$=V,Ti) [16]. These Pr-based superconductors indicate that the higher-rank ($\geq$ 2) multipole fluctuations inherent in $f$-electron systems mediate exotic superconducting states.

CeCu$_2$Si$_2$ is the first discovered heavy-fermion superconductor [17, 18], and its discovery triggered huge amount of research on unconventional superconductivity in various compounds [19]. At ambient pressure, CeCu$_2$Si$_2$ shows superconducting transition at $T_c \approx 0.6$K near the magnetic instability [20]. Under pressure, $T_c$ suddenly increases to 1.5K at $P_c \approx 4.5$GPa. For long time, CeCu$_2$Si$_2$ has been considered as a typical $d$-wave superconductor mediated by magnetic fluctuations. However, $d$-wave nodal gap structure contradicts with exponentially small specific heat at $T \ll T_c$ as reported in Refs.[21, 22]. Later, the fully gapped state is confirmed by the measurements of thermal conductivity and penetration depth at very low temperatures [23, 24]. In addition, the robustness of $T_c$ against randomness indicates that plain $s$-wave superconductivity without sign-reversal is realized in CeCu$_2$Si$_2$ [23].

It is a significant challenge for theorists to establish a realistic microscopic theory of fully gapped $s$-wave superconductivity in heavy-fermion systems, against large Coulomb repulsion. It is believed that fluctuations of even-rank multipole operators, such as charge, quadrupole and hexadecapole operators, mediate attractive pairing interaction. To realize large even-rank multipole fluctuations, at least two Kramers doublets should contribute to the Fermi surface, if the charge (rank 0) fluctuations are suppressed by Coulomb interaction. In fact, in CeCu$_2$Si$_2$ at ambient pressure, two Kramers doublets form the Kondo resonance below 10K according to the first-principles study based on the LDA+DMFT [25]. Pressure-induced change in multiorbital nature may be a key to understand the $P$-$T$ phase diagram in CeCu$_2$Si$_2$ [25–27].

In the random-phase-approximation (RPA), even-rank multipole fluctuations are always smaller than odd-rank ones. Therefore the obtained gap structure inevitably possesses sign reversal within the Migdal approximation [28]. This discrepancy indicates the significance of higher-order many-body effects called the vertex corrections (VCs). In fact, the VC for the electron-boson cou-
pling, which we call U-VC, has been studied in Refs. [2, 3, 5, 29−33]. The violation of Migdal theorem [34] due to the Maki-Thompson (MT) and Aslamazov-Larkin (AL) VCs, which are respectively the first-order and second-order corrections with respect to the susceptibility, have been studied in Refs. [5, 29, 33, 35]. In multiorbital systems, moderate orbital fluctuations induce strong attractive pairing interaction thanks to the AL-type U-VC [35, 36]. However, strong SOI in f-electron systems has prevented the detailed analysis of the VCs. Thus, it is highly required to construct the theoretical formalism to analyze the VCs in systems with strong SOI. We stress that the DMFT has been successfully applied to f-electron systems [11, 25, 37−41], while strong k-dependence of VCs near the magnetic quantum-critical point (QCP) is not fully taken into consideration.

In this paper, we propose a mechanism of s-wave superconductivity in multi-orbital heavy fermion systems by focusing on the VCs beyond Migdal approximation. Near the magnetic QCP, various types of multipole fluctuations develop simultaneously, due to the combination of strong SOI and Coulomb interaction. The developed multipole fluctuations give significant VCs in heavy fermion systems. Especially, the VCs significantly magnify the attractive pairing interaction due to even-rank multipole fluctuations, so the Migdal theorem is no more valid. Due to this mechanism, s-wave superconductivity can be realized in heavy fermion systems, once moderate (phonon-induced) quadrupole or hexadecapole fluctuations exist. The s-wave superconductivity is strongly enhanced near the magnetic criticality. The present mechanism may be responsible for the fully gapped superconducting state realized in CeCu$_2$Si$_2$.

In 3$d$-electron systems, the AL-type VCs are efficiently calculated by using the SU(2) symmetry in the spin-space. Thus, the same formalism cannot be applied to 5$d$ or f-electron systems because of the violation of SU(2) symmetry. To overcome this difficulty, we introduce a natural 2-orbital periodic Anderson model, in which the pseudo-spin of f-electron satisfies the axial rotational symmetry. By virtue of this fact, we can analyze complicated VCs efficiently. In the present model, 16 type multiple operators (rank 0−5) are active, so we can discuss rich physics associated with higher-rank multipole operators.

II. MODEL

In this section, we derive an useful simplified PAM for CeCu$_2$Si$_2$ from Eq.(1). According to the LDA+DMFT study for CeCu$_2$Si$_2$[25], the following two Kramers doublets give dominant DoS around the Fermi energy at ambient pressure. They are expressed in the $J_z$ basis as,

$$
\begin{align}
\{ |f_1 \uparrow \rangle \} &= |a| | \frac{5}{2} \rangle + |b| | \frac{3}{2} \rangle, \\
\{ |f_1 \downarrow \rangle \} &= |a| | \frac{3}{2} \rangle + |b| | \frac{5}{2} \rangle, \\
\{ |f_2 \uparrow \rangle \} &= -|a| | \frac{3}{2} \rangle + |b| | \frac{5}{2} \rangle, \\
\{ |f_2 \downarrow \rangle \} &= -|a| | \frac{5}{2} \rangle + |b| | \frac{3}{2} \rangle,
\end{align}
$$

where $| \uparrow \rangle$ denotes pseudo-spin up (down) of $f_1$-electron ($l = 1, 2$), We drop the third Kramers doublet $|f_3 \rangle = \pm | \frac{1}{2} \rangle$ , since it gives negligibly small weight near the Fermi level. We study 2D square lattice model as shown in Fig.1(a). Both f- and s-orbital are on Ce-ion. For simplicity, we consider only the above-mentioned 2-orbitals. We introduce only the nearest neighbor s-f and s-s hopping integrals. In this case, f-electron with pseudo-spin $\uparrow$ ($\downarrow$) hybridizes with only s-electron with $\uparrow$ ($\downarrow$) as we confirm in Appendix A. Thus, the pseudo-spin is conserved, and we can put $\Sigma = \sigma$. In the present 2-orbital model, the kinetic term is given by

$$
\hat{H}_0 = \sum_{k \sigma} \epsilon_k c_{k \sigma}^{\dagger} c_{k \sigma} + \sum_{kl \Sigma} E_{l} f_{kl \Sigma}^{\dagger} f_{kl \Sigma} + \sum_{k \sigma} \sum_{kl \Sigma} \left( V_{kl \Sigma \Sigma}^{n} f_{kl \Sigma}^{\dagger} c_{k \sigma} + V_{kl \Sigma \sigma}^{n} c_{k \sigma} f_{kl \Sigma} \right),
$$

where $c_{k \sigma}^{\dagger}$ ($c_{k \sigma}$) is a creation (annihilation) operator for f-electron with momentum $k$, spin $\sigma$, and energy $\epsilon_k$. $f_{kl \Sigma}^{\dagger}$ ($f_{kl \Sigma}$) is a creation (annihilation) operator for f-electron with $k$, orbital $l$ ($l = 1, 2, 3$), pseudo-spin $\Sigma$, and energy $E_l$. $V_{kl \Sigma \Sigma}$ is the hybridization term between f-electron and s-electron.

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case, we obtain $|V_{k_f f_1}/V_{k_f f_2}| = \sqrt{5}$. Thus, $f_1$-orbital is more itinerant than $f_2$-orbital. This feature is consistent with the results of previous DMFT calculation for CeCu$_2$Si$_2$ in Ref.[25], which shows $V_{k_f f_2} \approx 2V_{k_f f_1}$. The schematic picture of the $s$-s and $s$-$f$ hopping integrals are shown in Fig.1(a). We fix the parameters $\epsilon_k = 2t_{ss}(\cos k_x + \cos k_y) + \epsilon_0$, $t_{ss} = -1.0$, $\epsilon_0 = 3.0$, $t_{sf} = 0.7$, and $f$-electron energy $E_{f_1} = 0.2$ and $E_{f_2} = 0.1$. We set the temperature $T = 0.02$ and the chemical potential $\mu = -5.52 \times 10^{-3}$ in the following numerical study. Then, $f$-electron number is $n_f = 0.9$, and $s$-electron number is $n_s = 0.3$.

In Fig.1(b), we show the obtained band structure. $\epsilon = 0$ corresponds to the chemical potential. In the present 3 band model, the lowest band crosses the Fermi level. The total band width is $W_D \sim 10$ (in unit $|t_{ss}| = 1$). $|t_{ss}|$ is of order 1eV since $W_D \sim 10eV$ in CeCu$_2$Si$_2$ [28]. The width of quasi-particle band (=the lowest band) is $W_D^{qp} \sim 1$. Density of states (DoS) for $f_1$-orbital; $D_f^j(\epsilon)$ is given in Fig.1(c). Here, the relation $D_f^j(0) \sim D_f^j(0)$ is satisfied. In the present study, we neglect self energy. Figure 1(d) shows the obtained Fermi surface. In Fig.1(e), we plot the $\theta$-dependence of the $f_1$-orbital weight, where $\theta$ is angle of the Fermi momentum defined in Fig.1(d). We stress that the weights of $f_1$- and $f_2$-orbital are comparable regardless of $\theta$, which originates from the isotropic $s$-$f$ hybridization given in Eq.(4) due to the strong SOI. (In contrast, in 3d-electron system such as Fe-based compounds, the $d$-orbital weight shows strong $\theta$-dependence.) This fact is favorable for the development of multiple higher-rank multipole susceptibilities, as we will show in Sec. IV.

If we consider the $f$-$f$ hopping, the $f_i$-orbital weight comes to have $\theta$-dependence. Even in this case, the multiple higher-rank multipole susceptibilities can develop when $t_{ff} \ll t_{sf}$, which is naturally expected in heavy fermion compounds. We will discuss in more detail in Appendix D and in the future publication [45].

We introduce on-site Coulomb interaction in $f$-electrons,

$$\hat{H}_U = u \cdot \frac{1}{4} \sum_i \sum_{\sigma, \rho} U^0_{i \sigma \rho} \hat{n}_i^{\sigma} \hat{n}_{i \rho} = \frac{1}{4} \sum_i \sum_{\sigma, \rho} U^0_{i \sigma \rho} \hat{n}_i^{\sigma} \hat{n}_{i \rho},$$

where $i$ is site index, and $u$ is the value of Coulomb interaction. $U^0$ is the interaction matrix normalized on the condition that $U^0_{i \sigma \rho} \hat{n}_i^{\sigma} \hat{n}_i^{\rho} = U^0_{i \sigma \rho} \hat{n}_i^{\sigma} \hat{n}_i^{\rho} = 1$. Note that $U^0$ in Eq.(5) is antisymmetrized.

Here, we derive $U^0$ in Eq.(5) from the following $L_z$-basis Coulomb interaction:

$$U^0_{l_z, l_z', t_x, t_x'} = \sum_{\alpha \beta} \sum_{\sigma \rho} \frac{\epsilon^2}{4 \pi e_0} \int dr dr' \left| \frac{\Theta_{l_z}(r) \Theta_{l_z'}(r')}{|r - r'|} \right| u_{l_z}(r) u_{l_z'}(r') u_{t_x}(r) u_{t_x'}(r'),$$

where $u_{l_z}(r) = (R(r) \Theta_{l_z}(\phi)) e^{i l_z \phi}$ is the wave function of the $f$-electron with $l_z$ in the absence of the SOI. $F^p$ is Slater integral introduced in Ref.[46], which is defined as

$$F^p = \frac{\epsilon^2}{4 \pi e_0} \int dr dr' R^2(r) R^2(r') \int d\phi d\phi' \left[ \Theta_{l_z}(\phi) \Theta_{l_z'}(\phi') \right] e^{i l_z \phi} e^{-i l_z' \phi'} |r - r'|^{-p+1} r^{2-p} r'^{2-p},$$

where $r_{min} = \min\{r, r'\}$ and $r_{max} = \max\{r, r'\}$. In this paper, we put $(F^0, F^2, F^4, F^6) = (5.3, 9.09, 6.927, 4.756)$ in unit eV by referring Ref.[47]. Finally, we determine $U^0$ in Eq.(5) by performing the unitary transformation of Eq.(6) and normalizing it on condition that $U^0 \sum_i \hat{n}_i^{\sigma} \hat{n}_i^{\rho} = 1.$
The present Coulomb interaction in Eq.(5) does not satisfy SU(2) symmetry in the pseudo-spin space. Nonetheless, the pseudo-spin is conserved in Eq.(5) for any value of $a$ in Eq.(2). Equivalently, $\hat{U}^0$ satisfies the axial rotational symmetry along $z$-axis. Then, $\hat{U}^0$ is uniquely decomposed into in-plane spin (= $s$), out-of-plane spin (= $s \perp$) and charge (= $c$) channels as follows:

$$
\hat{U}_{mm'}^{0:s} = \frac{1}{2} \hat{U}_{mm'}^{0:s}(s^x, s^y, s^z) + \frac{1}{2} \hat{U}_{mm'}^{0:0}(0^x, 0^y, 0^z),
$$

where $\sigma = (s^x, s^y, s^z)$ is Pauli matrix vector in the pseudo-spin space, and $\sigma^0$ is identity matrix. $\hat{U}^{0:ch}(ch = s, s \perp, c)$ is defined as

$$
\begin{cases}
\hat{U}^{0:s}_c = \hat{U}^{0:τ:τ:τ} - \hat{U}^{0:τ:τ:τ};
\hat{U}^{0:s}_c = \hat{U}^{0:τ:τ};
\hat{U}^{0:s}_c = \hat{U}^{0:τ:τ:τ} + \hat{U}^{0:τ:τ:τ};
\end{cases}
$$

The matrix elements of $\hat{U}^{0:ch}(ch = s, s \perp, c)$ are summarized in TABLE I. Each elements are composed of the intra-orbital Coulomb interaction $U$, inter-orbital one $U'$, exchange interactions $J, J^\perp, J', J^x$, and $J^2$. The definition and numerical value of each component are given in Appendix B. In the case of $a = 1$ and $b = 0$, the other elements not listed in the TABLE I become zero. Although some of these elements (e.g., $r_0^{0:ch}$) come to be finite for $a \leq 1$, they remain very small and negligible. Therefore, TABLE I is still useful, practically. Note that $a = \sqrt{5}/6$ and $b = \sqrt{1/6}$ are satisfied in cubic symmetry.

| $s \perp$ | $s$ | $s \perp$ | $s$ | \hline
| $U_{11:13}^{0:s}$ | $U^1$ | $1.0$ | $U_{11:13}^{0:s}$ | $U^1$ | $1.0$ | \\
| $U_{22:22}^{0:s}$ | $U^2$ | $0.90$ | $U_{22:22}^{0:s}$ | $U^2$ | $0.90$ | \\
| $U_{11:13}^{0:s}$ | $U' - J + J^\perp$ | $0.80$ | $U_{11:13}^{0:s}$ | $U' - J + J^\perp$ | $0.80$ | \\
| $U_{11:13}^{0:s}$ | $J - J^x$ | $-0.12$ | $U_{11:13}^{0:s}$ | $J - J^x$ | $0.0$ | \\
| $U_{11:13}^{0:s}$ | $J' - J^2$ | $0.20$ | $U_{11:13}^{0:s}$ | $J' - J^2$ | $0.20$ | \\
| $J$ | $U^1$ | $-U^1$ | $-1.0$ | \\
| $U'$ | $-U^2$ | $-0.90$ | \\
| $U' - J - J^\perp$ | $0.80$ | \\
| $J - 2J' + J^x$ | $-1.5$ | \\
| $-J' + J^2$ | $-0.20$ | \\

TABLE I: Matrix elements of Coulomb interaction for in-plane spin channel (top left), out-of-plane spin channel (top right), and charge channel (bottom) for $l \neq m$. $J = J'$, $J^\perp = 0$ and $J^x = -J^2x$ are satisfied in the present 2-orbital model.

In the present two-orbital model in Eq.(2), there are 16-type active multipole operators up to rank 5; monopole (rank 0), dipole (rank 1), quadrupole (rank 2), octupole (rank 3), hexadecapole (rank 4) and dotriacontapole (rank 5) moment as shown in TABLE II [13]. Some operators belong to the same irreducible representation (IR). Since the system is inversion symmetric, an even-rank (odd-rank) operator corresponds to an electric (magnetic) multipole operator. Each multipole operator of rank $k$ are composed of $4 \times 4$ tensor $J_q^{(k)} (q = -k \sim k)$ [8,48] which is given by

$$
[J_q^{(k)} , J_{q}^{(k)}] = \sqrt{(k + q)(k + q + 1)} J_q^{(k)}_{q+1}^{(k)}
$$

$$
J_q^{(k)} = (-1)^k \sqrt{(2k - 1)!!} J_{2q}^{(k)}. \tag{10}
$$

By using $J_q^{(k)}$, we obtain $4 \times 4$ multipole operators $\hat{\mathcal{O}}\hat{Q}$.

| \hline
| \hline
| $\hat{\mathcal{O}}\hat{Q}$ | $\Gamma$ | $rank (k)$ | Operator (Q) | $N_T$ | $ch\mathcal{F}$ | \\
| $A_{1+}$ | $0$ | $0$ | $\hat{1}$ | $3$ | $c$ | \\
| $A_{2+}$ | $4$ | $H_0$ | $1$ | $s$ | \\
| $E_{+}$ | $2$ | $\hat{O}_{2x}, \hat{O}_{2y}$ | $2$ | $s_l$ | \\
| $A_{1-}$ | $5$ | $D_x$ | $1$ | $c$ | \\
| $A_{2-}$ | $3$ | $T_x$ | $3$ | $s_l$ | \\
| $E^{-}$ | $1$ | $J_xJ_y$ | $6$ | $s_l$ | \\

TABLE II: Irreducible representation and 16-type active multipole operators in the present 2-orbital model. Operator with rank $k$ corresponds to $2^k$-pole. $N_T$ is the number of operators in symmetry $\Gamma$. Each operator is classified into the pseudo-spin or charge channel, $ch\mathcal{F}$.

Here, we introduce the effective on-site electric multipole-multipole interaction $V^{ph}$ that belongs to $A_1^+$ symmetry (= identical representation),

$$
\begin{align*}
V^{ph}_{l'm'm'} &= 2gW_{l'm'm'} \\
&= 2g(\hat{C}A_1^+)_{l'm'}(\hat{C}A_1^+)_{mm'},
\end{align*}
$$

where $\hat{C}A_1^+$ is the dimensionless matrix given by a linear combination of multipole operators belong to $\Gamma = A_1^+$ in TABLE II. It is expressed as

$$
\hat{C}A_1^+ \equiv \alpha \hat{r}^0 + \beta \hat{r}^2 + \gamma \hat{r}^x,
$$

(12)
where $\hat{r}^\mu(\mu = x, y, z)$ is Pauli matrix in the orbital basis $(\ell_1, \ell_2)$, and $\hat{r}^0$ is identity matrix. In the presence of $g$, the Coulomb interaction $u\hat{U}^{0c}$ is replaced with $u\hat{U}^{0c} + 2g\hat{W}$. In the present numerical study, we put $(\alpha, \beta, \gamma) = (0, 1, -1)$. We verified that the main results are qualitatively same as those of $(\alpha, \beta, \gamma) = (0, 1, 1)$. The numerical results are not sensitive to the ratio of $(\alpha, \beta, \gamma)$.

This effective interaction can be induced by (for instance) the electron-phonon interaction due to $A_1^+$ mode, such as the oscillation of $c$-axis length [49]. In this case, $g$ is expressed as $g = \hat{g}\frac{\omega_D}{\omega_D + \omega_j}$, where $\hat{g} = \frac{2g^2}{\omega_D} (> 0)$: $\omega_D$ is the phonon frequency, $\eta$ is the coupling constant between electrons and phonon, and $\omega_j = 2j\pi T$ is the Boson Matsubara frequency. In the present study, we drop $\omega_j$-dependence of $g$ for simplicity. That is, we neglect the retardation effect, which leads to underestimation of the $s$-wave superconducting $T_c$ as discussed in Ref.[35]. The $A_1^+$ effective interaction in Eq.(11) is classified into even-rank multipole interaction. Therefore, strong electric (=even-rank) multipole fluctuations are induced by the interaction $g$. On the other hand, the magnetic (=odd-rank) multipole susceptibilities are independent of $g$.

### III. GREEN FUNCTION

Here, we introduce the Green functions in the present model. The $3 \times 3$ matrix form of the Green function is given by

$$G^\sigma(k, \epsilon_n) = \left((\epsilon_n - \mu)\hat{1} - \hat{h}_k^\sigma\right)^{-1}, \quad (13)$$

where $\hat{h}_k^\sigma$ is introduced in Eq.(3). The first two rows and columns of Eq.(13) give the $f$-orbital Green functions. They are expressed as

$$G_{lm}^{\sigma\sigma'}(k) = G_{l}^{0\sigma'}(k)\delta_{lm} + G_{l}^{0\sigma'}(k)V_{kl}\sigma\sigma'G_{kl}^{0\sigma'}(k)$$

where $l, m = 1, 2, k = (k, \epsilon_n) = (k, (2n + 1)\pi T)$, and

$$G_{l}^{0\sigma}(k) = (i\epsilon_n - \mu - E_l)^{-1}. \quad (15)$$

$G_{\sigma}(k)$ is the $s$-electron Green function given by the $(3, 3)$ component of Eq.(13). It is expressed as

$$G_{\sigma}(k) = \left(i\epsilon_n - \mu - \epsilon_k - \sum_l V_{kl}\sigma G_{l}^{0\sigma}(k)V_{kl}\sigma\right)^{-1}. \quad (16)$$

In the present 2-orbital model, the relation $V_{kl}\sigma V_{km}\sigma' = V_{kl}\sigma V_{km}\sigma'$ is satisfied, as we can verify from Eq.(4). For this reason, the Green functions become independent of spin index:

$$G_{lm}^{\sigma}(k) = G_{lm}^{\sigma\sigma'}(k) = G_{lm}^{\sigma\sigma'}(k),$$

$$G_{\sigma}(k) = G_{\sigma}^{\sigma\sigma}(k) = G_{\sigma}^{\sigma\sigma}(k). \quad (17)$$

In the present model, diagonal $(l = m)$ components of $G_{lm}^{\sigma}(k)$ and off-diagonal $(l \neq m)$ ones are comparable since each $s-f$ hybridization in Eq.(4) is isotropic in magnitude. It is a characteristic feature of the multiorbital $f$-electron systems.

### IV. SUSCEPTIBILITY

![FIG. 2](a) $q$ dependence of the magnetic dipole susceptibility. $\chi_{z^2-r^2}^{J_{z^2}-J_{z^2}}(q, 0) \gg \chi_{z^2-r^2}^{J_{z^2}-J_{z^2}}(q, 0)$ is satisfied at $q = (0, 0)$. (b) $\alpha_S$ dependence of magnetic multipole susceptibility. Higher-rank magnetic multipole susceptibilities are strongly enlarged.

First, we perform the random phase approximation (RPA) in order to obtain the $f$-electron susceptibility. In this calculation, we use $32 \times 32 \times$-meshes and 128 Matsubara frequencies. The irreducible susceptibility of $f$-electron is given by

$$\chi_{lm\sigma\sigma'}^0(q) = -T\sum_k G_{lm\sigma}(k + q)G_{lm\sigma'}^F(k), \quad (18)$$

where $q = (q, \omega_j) = (q, 2j\pi T)$. In the RPA, the susceptibility for each channel $(\sigma, \sigma')$ is given as

$$\hat{\chi}_c^c(q) = \hat{\chi}_c^0(q)(\hat{1} - u\hat{U}^{0\sigma\sigma'}\hat{\chi}_c^0(q))^{-1}. \quad (19)$$
where $\chi^{ch}(q)$ is $2^2 \times 2^2$ matrix. Using $\chi^{ch} (ch = s, s\perp, c)$, the $f$-electron susceptibility in the $L = (l, \sigma)$ basis is expressed as

$$\chi^{\sigma \prime \lambda \prime} = \frac{1}{2} \chi^{s-}(\sigma_{\sigma \prime} \sigma_{\lambda \prime} + \sigma_{\sigma}^{\prime \prime} \sigma_{\lambda}^{\prime \prime}) + \frac{1}{2} \chi^{s-}_{\sigma \sigma} \sigma_{\lambda \lambda}^{\prime \prime} + \frac{1}{2} \chi^{s-}_{\sigma \sigma} \sigma_{\lambda \lambda}^{\prime \prime} \chi^{s-}_{\sigma \sigma} \sigma_{\lambda \lambda}^{\prime \prime}. \quad (20)$$

Here, we define the pseudo-spin Stoner factor $\alpha_S(\alpha_S \perp)$ as the largest eigenvalue of $u \hat{U}^{\alpha \alpha}(\alpha \perp) \chi^{(q)}(q)$. In the present model, each matrix element of $\hat{U}^{\alpha \alpha}$ and that of $\hat{U}^{\alpha \alpha}$ in TABLE I are the same except for $(lmm)$ and $(llmm)$ elements. For this reason, $\chi^{s} = \chi^{s-}$ and $\alpha_S = \alpha_S \perp$ are satisfied.

Now, we define the multipole susceptibility for $Q = (\Gamma, \phi)$;

$$\chi^{Q\cdot Q'}(q) = \int_0^\beta d\tau \left\langle O^Q(q, \tau) O^{Q'}(-q, \tau) \right\rangle e^{i\omega_\tau}, \quad (21)$$

where $O^Q(q, \tau) = \sum_{L, M, k} O^Q_{L, M} f^\dagger_{k, \sigma}(\tau) f_{k+q, \sigma}(\tau)$. In 3D models, $\chi^{(\Gamma, \phi)}(\Gamma, \phi)(q)$ can be finite even in the case of $\Gamma \neq \Gamma'$. In contrast, in the present 2D model, $\chi^{(\Gamma, \phi)}(\Gamma, \phi)(q)$ for $\Gamma = A_2^+, A_2^-, E^+$ is classified into electric susceptibility, and that for $\Gamma = A_2^+, A_2^-, E^-$ is classified into magnetic susceptibility. In the present model, $\alpha_S$ corresponds to the $A_2^-$ magnetic (=odd-rank) susceptibility, so that, $\alpha_S = \alpha_{A_2^-}$ in the RPA. We obtain the relation $1 \geq \alpha_{A_2^-} \geq \alpha_{E^\perp}$.

In Fig.2(a), we show obtained susceptibilities at $u = 0.31$ for the magnetic dipole $J_z = (A_2^+, 1)$, $\chi^{J_{z1}, J_{z2}}(q, 0)$, and $J_z = (E^-, 1)$, $\chi^{J_{z1}, J_{z2}}(q, 0)$. In this case, $\alpha_S = 0.90$. Note that $\chi^{J_{z1}, J_{z2}}(q, 0)$ is much larger than $\chi^{J_{z1}, J_{z2}}(q, 0)$ while they are almost the same around the peak at $q \approx (\pi/2, \pi/2)$. Thus, the uniform magnetic susceptibility shows strong Ising anisotropy, which is actually observed in CeCu$_2$Si$_2$.

Hereafter, to compare among different-rank of multipole susceptibilities, we define normalized multipole operator $\hat{\chi}^{Q}$ as $Tr(\hat{\chi}^{Q})/1$, that is,

$$\hat{\chi}^{Q} = \hat{\chi}^{Q} / \sqrt{Tr(\hat{\chi}^{Q})}. \quad (22)$$

The normalized susceptibility $\chi^{Q\cdot Q'}(q)$ is given by replacing $\hat{\chi}^{Q}$ in Eq.(21) with $\hat{\chi}^{Q}$. In Fig.2(b), we show $\alpha_S$ dependences of the maximum of magnetic multipole susceptibilities $\chi^{Q}_{\max} = \max_q \chi^{Q\cdot Q'}(q)$. $\alpha_S$ linearly increases in proportion to $u$. The obtained $\chi^{Q}_{\max}$ is the most divergent for $Q = T_x$. This fact is consistent with the RPA result based on the first-principles model in Ref[28]. Secondly, $\chi^{Q}_{\max}$ for $Q = D_2, J_x, T_x, D_4$ is also strongly enlarged. Therefore, various magnetic multipole (including higher-rank) susceptibilities are simultaneously enlarged in the RPA. This is a characteristic feature of $f$-electron systems with strong SOI [13]. We find that the inter-rank magnetic multipole susceptibilities, such as $\chi^{J_z, T_z}$, are also enlarged.

Now, we explain the reason why higher-rank magnetic multipole susceptibilities are enlarged. Our result means that orbital-off-diagonal components of $\chi^{Q}_{\perp\perp}$ are comparable to orbital-diagonal ones. In fact, $\chi^{\perp\perp}_{ll\pm\pm} \approx \chi^{\perp\perp}_{ll\pm\pm}$ is satisfied in the present model. It originates from the fact that each $s-f$ hybridization in Eq.(4) is isotropic in the $x$- and $y$-directions due to the strong SOI, and therefore each $f_i$-orbital weight is independent of $\theta$ as shown in Fig.1(e). This is the origin of the large orbital-off-diagonal components of $G_{\perp\perp}$ and those of $\chi^{Q}_{\perp\perp}$.

Finally, we comment on electric (=even-rank) susceptibilities obtained by the RPA. In the absence of electric multipole-multipole (phonon-induced) interaction: $g = 0$, the obtained electric susceptibilities are much smaller than magnetic ones. That is, charge Stoner factor $\alpha_C$, which is defined as the largest eigenvalue of $(u \hat{U}^{\alpha\alpha} + 2g\hat{W}) \chi^{Q\cdot Q'}(q)$, satisfies $\alpha_C \ll \alpha_S$. In the present model, $(\alpha_C, \alpha_S) = (0.55, 0.90)$. On the other hand, the hexadecapole $\chi_{Q^3}^{Q^3}$ and quadrupole $\chi_{Q^2}^{Q^2}$ susceptibility are enlarged at $q \approx (\pi, \pi)$ when we consider the small $g \gg 0$. In this case, $\alpha_C$ increases to 0.84 at $g = 0.04$. Note that the obtained electric susceptibilities work as attractive interaction for $s$-wave superconductivity, as we will explain in the following section.

In principle, some experimental signatures due to the electric multipole susceptibility can be observed. The enhancement of $\chi^{Q\cdot Q'}(q) \neq 0$ obtained in the present model may cause the softening of phonon dispersion, which is observable by using (for instance) neutron scattering experiment.

V. GAP EQUATION

Now, we solve the linearized gap equation by focusing on the important roles of the vertex corrections, which we call $U$-$VC$. The bare electron-boson couplings are dressed by the $U$-$VC$, which is totally dropped in conventional Migdal approximation. The gap equation for spin-singlet paring in the band basis is given as

$$\lambda \Delta(k, \epsilon_n) = -\frac{\pi T}{(2\pi)^2} \sum_{\epsilon_m} \int_{FS} \frac{dk'}{2\pi} \frac{\Delta(k', \epsilon_m)}{\epsilon_m} V_k^\text{sing}, \quad (23)$$

where $\Delta(k, \epsilon_n)$ is the gap function on Fermi surface, $\lambda$ is the eigenvalue, and $v_k$ is the Fermi velocity on Fermi surface. $V_k^\text{sing}$ is the spin singlet paring interaction including $U$-$VC$. The diagrammatic expression of the gap equation is shown in Fig.3(a). The black triangle shows the three-point vertex correction due to many body effects. We consider the AL-type diagram for $U$-$VC$ given
in Fig. 3(b), which is explained in more detail in the Section VI. The paring interaction in Eq. (23) is obtained by

$$V_{k,k'}^{\text{sing}} = V_{k,k'}^{udud} - V_{k,k'}^{uudd}$$

$$= \frac{1}{2} \sum_{\Sigma, \Lambda} V^{\Sigma \Lambda \Sigma \Sigma}_{k,k'} (1 - 2\delta_{\Sigma \Lambda}),$$  

(24)

where $\Sigma, \Lambda = u (d)$ is pseudo-spins up (down) that denotes the Kramers doublet of the Bloch function, and $\Sigma \equiv -\Sigma$. $V^{\Sigma \Lambda \Sigma \Sigma}_{k,k'}$ is given as

$$V^{\Sigma \Lambda \Sigma \Sigma}_{k,k'} = \sum_{l^\prime m^\prime} \sum_{\sigma' \sigma \lambda} U^{\Sigma \sigma}_{l^\prime \sigma l}(k) U^{\Sigma \sigma}_{m^\prime \lambda}(k')$$

$$\times V^{\sigma \sigma' \lambda \lambda'}_{ll^\prime mm'}(k,k') U^{\lambda}_{m^\prime \lambda}(-k') U^{\lambda}_{m^\prime \lambda}(k') ,$$

(25)

where $U^{\Sigma \sigma}_{l \sigma l}(k)$ is the unitary matrix connecting between $f_{k \sigma}^l$ and the quasi-particle creation operator $f_{k \sigma}^{\dagger}$. In the presence of the time reversal symmetry, $U^{\Sigma \sigma}_{l \sigma l}(k)$ is related to $U^{\Sigma \sigma}_{l \sigma l}(-k) = (-1)^{\delta_{\sigma \sigma'} + 1} U^{\Sigma \sigma}_{l \sigma l}(k)^* \ [50]$. $V^{\sigma \sigma' \lambda \lambda'}_{ll^\prime mm'}(k,k')$ is the paring interaction in the orbital basis.

VI. IMPORTANT ROLES OF U-VC

Here, we discuss the important roles of U-VC in the paring interaction. Until now, U-VC in $d$-electron systems has been studied intensively by some theoretical methods, such as the functional renormalization group (fRG) theory and perturbation theory. Both theoretical frameworks reveal that U-VC makes significant contributions to the superconductivity, especially in multi-orbital systems, so Migdal approximation fails. In more detail, AL-type U-VC becomes more important than MT-type one near the magnetic QCP. However, U-VC in $f$-electron systems with strong SOI has not been understood at all. In the present study, we show that U-VC in $f$-electron systems is more important than that in $d$-electron systems due to large SOI.

Now, we discuss the paring interaction with U-VC. In the present model, the electric multipole paring interaction corresponds to attraction, while the magnetic one corresponds to repulsion. To understand this fact, we consider the paring interaction in the absence of SOI, like in 3$d$-electron systems. In this case, we can put $U^{\Sigma \sigma}_{l \sigma l}(k) = U^{\sigma}_{l \sigma l}(k) \delta_{\sigma \sigma'}$ and

$$\left\{ \begin{array}{l} A^{udud}_{\ll^\prime mm'} = A^{uudd}_{\ll^\prime mm'} \\
A^{uudd}_{\ll^\prime mm'} = A^{udud}_{\ll^\prime mm'} = A^{uudd}_{\ll^\prime mm'} = 0 \end{array} \right. \]$$

Then, we obtain the following simple expression:

$$V^{\Sigma \Lambda}_{k,k'} = \sum_{ll^\prime mm^\prime} \left( \hat{V}^{\Sigma \Lambda}_{ll^\prime mm^\prime}(k,k') \right) U^{\Sigma \Lambda}_{ll^\prime mm^\prime}(k,k') ,$$

where $V^{\Sigma \Lambda}_{ll^\prime mm^\prime}$ is satisfied when SOI is dropped. Thus, $V^{\Sigma \Lambda}_{k,k'}$ in Eq. (27) is reduced to the well-known expression $V^{\Sigma \Lambda}_{k,k'} \propto \frac{1}{2} V^{\Sigma \Lambda}_{l \sigma l} V^{\Sigma \Lambda}_{l \sigma l}$. In conclusion, the charge- or electric-channel paring interaction works as attraction, while the spin- or magnetic-channel one works as repulsion.

FIG. 3: (a) Linearized gap equation in the present study. The black triangle shows three-point vertex correction (U-VC). (b) U-VC due to the AL process.

(b)
where \( \hat{L}^{ch}_{k,k'} \) is AL-type U-VC, whose diagrammatic expression is given in Fig.3(b). In Eq.(28), \((\hat{L}^{ch}_{k,k'})_{l'mm'} = (\hat{\Lambda}^{ch}_{k,k'})_{l'mm'}\). In the present model, the MT-type U-VC is negligible compared to AL-type one. For this reason, we calculate only AL-type U-VC. Note that \( V^{ch} = \hat{v}^{ch} \) in the Migdal approximation (\( \hat{\Lambda}^{ch} = 1 \)).

Hereafter, we discuss only the charge-channel U-VC \( \hat{\Lambda}^{ch}_{k,k'} \) since it becomes much larger than unity near the magnetic QCP, whereas spin-channel one remains order of unity. Hence, the charge-channel pairing interaction is enlarged by \( \hat{\Lambda}^{ch}_{k,k'} \). Here, \( \hat{L}^{ch}_{k,k'} \) is derived from the U-VC in the \((l, \sigma)\) basis.

\[
\hat{L}^{ch}_{k,k'} = \hat{L}^{\uparrow\downarrow\uparrow\downarrow}_{k,k'} + \hat{L}^{\uparrow\downarrow\downarrow\uparrow}_{k,k'} = \hat{L}^{\downarrow\uparrow\uparrow\downarrow}_{k,k'} + \hat{L}^{\downarrow\uparrow\downarrow\uparrow}_{k,k'}, \tag{31}
\]

whose Feynman diagram is shown in Fig.4(a). The analytic expression of \( \hat{L}^{ch}_{k,k'} \) is given as

\[
(\hat{L}^{ch}_{k,k'})_{l'mm'} = \frac{T}{2} \sum_{p,abcdef} B^{mm'}_{abcdef}(k - k', p) \times \sum_{dch} a^{ch}_{l} I^{ch}_{laced}(k - k' + p) I^{ch}_{d}(p). \tag{32}
\]

where \((a^*, a^\dagger a^c) = (1, 2, 1)\), and

\[
B^{mm'}_{abcdef}(q, p) = \frac{1}{4} G^{l}_{ab}(k - k' - p) \{ C^{mm'}_{efcd}(q, p) + C^{mm'}_{efcd}(q, q + p) \}. \tag{33}
\]

\[
C^{ab}_{efcd}(q, p) = -T \sum_{k'} G^{l}_{ca}(k' + q) G^{l}_{bf}(k') G^{l}_{de}(k' - p). \tag{34}
\]

Here, \( a \sim f \) are orbital indices. In the present numerical study, we put \( q = 0 \) in the \( \hat{L}^{ch}_{k,k'} \), since the contribution from \( \chi^c \) is negligibly smaller than that from \( \chi^s \) and \( \chi^{s\dagger} \) [35].

Next, we show numerical results of \( \hat{\Lambda}^{ch}_{k,k'} \). Here, we use 16 \( \times \) 16 \( k \)-meshes and 128 Matsubara frequencies. In Figs.4(b) and (c), we show the \( \alpha_S \) dependence of maximum value of \( \hat{\Lambda}^{ch}_{k,k'} \) on the Fermi surface,

\[
\hat{\Lambda}^{ch}_{l'mm'}_{\text{max}} = \max_{k,k' \in FS} |(\hat{\Lambda}^{ch}_{k,k'})_{l'mm'}|. \tag{35}
\]

at \( \epsilon_n = \epsilon_{n'} = \pi T \). We plot various orbital components of U-VC. Note that the other elements are obtained by using the symmetry relation of orbital indices, that is, \( \hat{\Lambda}^{ch}_{l'mm'} = \hat{\Lambda}^{ch}_{l'mm'} \). We find that they work as large enhancement factors for the coupling constant between electrons and charged-bosons (\( |\hat{\Lambda}^{c} | \gg 1 \)) near the magnetic QCP (\( \alpha_S \leq 1 \)). Note that all magnetic multipole susceptibilities except for \( D_4, Q = (A_1^+) \), are included in either \( \chi^s \) or \( \chi^{s\dagger} \). This behavior originates from the relation \( \hat{\Lambda}^{ch}_{k,k} \propto \sum_{p} \hat{\chi}^s(k - k' + p) \hat{\chi}^s(p) + 2 \hat{\chi}^{s\dagger}(k - k' + p) \hat{\chi}^{s\dagger}(p) \). This is qualitatively similar to \( d \)-electron systems without SOI as shown in Fig.2(c) in Ref.[35]. In conclusion, U-VC in \( f \)-electron systems give significant contribution as well as in \( d \)-electron systems.

We stress that there are some significant differences from \( d \)-electron systems. In fact, in the present \( f \)-electron system, (i) various orbital components of U-VC are equally enlarged, and (ii) the magnitude of U-VC are even larger than in \( d \)-electron systems at the same \( \alpha_S \). These results originate from multiple (higher-rank) magnetic multipole fluctuations as shown in Fig.2(b). To clarify this fact, we are going to elucidate what types of multipole fluctuations are significant for U-VC below. We recall that the \( f \)-electron susceptibility in Eq.(20) is uniquely expanded on the basis of \( 4 \times 4 \) matrix expression of multipole operator \( \hat{O}^Q = \hat{O}^{(1,\sigma)} \) given in Appendix.
C as follows,
\[ \chi_{LL'M'M'}(q) = \sum_{\Gamma,\phi,\phi'} a^{\Gamma,\phi,\phi'}(q)O_{LL'}^{(\Gamma,\phi)}O_{MM'}^{(\Gamma,\phi')*}. \] (36)

Note that \( \sum_{LL'} O_{LL'}^{(\Gamma,\phi)} O_{LL'}^{(\Gamma,\phi')*} = 0 \) for \( \Gamma \neq \Gamma' \). The derivation of the coefficient \( a^{\Gamma,\phi,\phi'}(q) \) is explained in Appendix D. In the same way, the interaction \( \hat{I}(=u^2\hat{U}^0\hat{\chi}\hat{U}^0+u\hat{U}^0) \) in the \( L=(l,\sigma) \) basis is expanded as
\[ \hat{I}_{LL'M'M'} = \sum_{\Gamma,\phi,\phi'} b^{\Gamma,\phi,\phi'}(q)O_{LL'}^{(\Gamma,\phi)}O_{MM'}^{(\Gamma,\phi')*}. \] (37)

By utilizing the pseudo-spin conservation law, each term in the right-hand-side of Eq.(37) is expressed in the \( l \)-basis as \( \hat{I}_{Llmm'}^{\Gamma,\phi,\phi'} \). Note that \( \hat{I}_{Llmm'}^{\Gamma,\phi,\phi'} = 0 \) for \( ch \neq ch' \). By replacing \( \hat{I}_{Llmm'}^{\Gamma,\phi,\phi'} \) in Eq.(32) with \( \hat{I}_{Llmm'}^{\Gamma,\phi,\phi'} \), we obtain multipole-decomposed \( U-VC \) symbolically expressed as
\[ \hat{L}_{c,QQ'}^{ch} = \frac{T}{2} \sum_{ch} \hat{B}^{ch,Q} \hat{L}_{c,QQ'}^{ch,Q}, \] (38)
\[ \hat{L}_{c,QQ'}^{ch} = \frac{T}{2} \sum_{ch} \hat{B} = (\hat{L}_{c,QQ'}^{ch,Q} + \hat{L}_{c,QQ'}^{ch,Q'} \hat{J}_{c,QQ'}^{ch}), \] (39)
where \( Q \neq Q' \). The diagrammatic expression of Eq.(39) is given in Fig.5(a). Note that the relation \( \hat{L}_{c,QQ'}^{ch} = \sum_{(Q,Q')} \hat{L}_{c,QQ'}^{ch} \) is satisfied. \( \hat{L}_{c,QQ'}^{ch} \) is given by
\[ \frac{\hat{L}_{c,QQ'}^{ch}}{\hat{L}_{c,QQ'}^{ch}} \delta_{l,m} \delta_{l,m'} + (\hat{L}_{c,QQ'}^{ch})_{llmm'}^{llmm'} \] (40)

In Figs.5(b)-(e), we show the maximum of multipole-decomposed \( U-VC \) defined as
\[ \Lambda_{c,QQ'}^{llmm'} = \max_{k,k'} \left| (\hat{L}_{c,QQ'}^{ch})_{llmm'} \right| \] (41)

at \( \epsilon_n = \epsilon_{n'} = \pi T \). We consider only odd-rank (=magnetic) multipole operators for \( Q \) and \( Q' \) since the contributions from even-rank multipole operators are negligibly small in EPA. In addition, \( \Lambda_{c,QQ'}^{llmm'} \) with \( Q=(\Gamma,\phi) \) and \( Q'=(\Gamma',\phi') \) becomes zero except for \( \Gamma = \Gamma' \) in the present model. Figures 5(b) and (c) show the orbital-diagonal component of \( U-VC \) given by \( \Lambda_{c,QQ'}^{llmm'} \). It becomes the largest for \( (Q,Q') = (T_x, T_x) \). Subsequently, \( (Q,Q') = (T_z, T_z), (T_z, T_z), (D_z, D_z) \) are also enlarged. In Figs.5(d) and (e), we show orbital-off-diagonal component given by \( \Lambda_{c,QQ'}^{llmm'} \). It takes the largest value for \( (Q,Q') = (T_x, D_z) \). Its value for \( (Q,Q') = (T_z, D_z), (D_z, D_z), (T_x, T_x), (J_z, D_z) \) are also enlarged.

In summary, in heavy fermion systems, multiple multipole fluctuations lead to the strong enhancement of \( U-VC \), \( \Lambda^c \). In Figs.4(b) and (c), both orbital-diagonal and off-diagonal components of \( \Lambda^c \) are enlarged. In Figs.5(b)-(e), many pairs of multipole fluctuations \((Q,Q')\) contribute to the enhancement of \( \Lambda^c \). These facts lead to above-mentioned differences (i) and (ii), which are not seen in 3d-electron system. Thus, we conclude that the \( U-VC \) in f-electron system plays more significant roles due to the strong SOI compared to 3d-electron systems.

FIG. 5: (a) Multipole-decomposed \( U-VC \) given by \( \Lambda_{c,QQ'}^{llmm'} \). \( Q \) and \( Q' \) are magnetic multipole operators. Obtained \( \Lambda_{c,QQ'}^{llmm'} \) for (b) \( Q = Q' \) and (c) \( Q \neq Q' \), and \( \Lambda_{c,QQ'}^{llmm'} \) for (d) \( Q = Q' \) and (e) \( Q \neq Q' \). Many pairs of multipole fluctuations \((Q,Q')\) contribute to the enhancement of \( U-VC \).
VII. SUPERCONDUCTIVITY

Now, we discuss obtained superconducting states by solving the gap equation in Eq.(23). The paring interaction is given by Eqs.(27)-(29). We solve the gap equation in the presence of both $u$ and $g$, by the following replacement,

$$u\hat{U}^{0;c} \rightarrow u\hat{U}^{0;c} + 2g\hat{W}$$ (42)

in $\hat{I}^{c}(k-k')$ in the paring interaction (28). For finite $g$, $\hat{I}^{c}(\chi^{c})$ develops as large as $\hat{I}^{s}$ and $\hat{I}^{s+1}$. We put $g = 0$ for $\hat{\Lambda}^{ch}$ approximately since the contribution from $\chi^{c}$ remains small even for $g > 0$ [35].

Figures 6(a)-(b) are obtained phase diagrams, which show the largest eigenvalue and its symmetry of the gap function. In the presence of $U$-$VC$, fully gapped $s$-wave state without any sign reversal emerges when $\alpha_{S} \lesssim 1$ and $\alpha_{C} \lesssim 1$ as shown in Fig.6(a). The region of $s$-wave phase gets wider as the magnetic fluctuations develop. These results originate from the fact that the charge-channel attractive interaction $-\frac{1}{2}V^{c}$ are strongly enhanced by the charge-channel $U$-VC, which is enlarged due to the magnetic (odd-rank) multipole fluctuations when $\alpha_{S} \lesssim 1$. In fact, $-\frac{1}{2}V^{c}$ is expressed as $-\frac{1}{2}V^{c} \propto -\frac{1}{4}\hat{\Lambda}^{ch}((u-2g)^{2}\chi^{c} - (u-2g))$, which takes large negative (=attractive) value when $\alpha_{C} \lesssim 1$ [35]. In addition, we find that quite small $g$ is enough for realizing the $s$-wave superconductivity. For instance, $s$-wave state emerges even at $g = 0.025$. This is much smaller than Coulomb interaction $u = 0.31$.

In contrast, the $s$-wave region in Fig.6(a) is drastically reduced if we neglect $U$-$VC$ ($\hat{\Lambda}^{ch} = \hat{1}$) as shown in Fig.6(b). In this case, $d_{x^{2}-y^{2}}$-wave state appears in wide parameter region. Furthermore, the eigenvalue $\lambda$ for $d_{x^{2}-y^{2}}$-wave state in Fig.6(b) is much smaller than that for $s$-wave state in Fig.6(a), so $T_{c}$ of $d_{x^{2}-y^{2}}$-wave state should be very low if realized. Therefore, we clearly confirmed that $U$-$VC$ is important for realizing the $s$-wave superconductivity. Obtained gap functions on Fermi surface for $s$- and $d_{x^{2}-y^{2}}$-wave states are expressed in Fig.6(c) and (d), respectively. The obtained $s$-wave gap function is almost isotropic while the $d_{x^{2}-y^{2}}$-wave gap function has accidental nodes in addition to the symmetry nodes.

In conclusion, once the small electron-phonon interaction exist, fully gapped $s$-wave superconducting state can appears in $f$-electron system near the magnetic QCP. This counter-intuitive result is given by the large $U$-$VC$ caused by multiple (higher-rank) multipole fluctuations. We comment that the obtained large eigenvalues $\lambda$ in Fig.6 are overestimated since the self-energy effects (such as the mass-renormalization and the quasi particle damping) are dropped in the gap equation.

Finally, we show that multi-orbital nature is a necessary condition for realizing the $s$-wave superconductivity. In the present model, $f$-orbitals $|f_{1}\rangle$ and $|f_{2}\rangle$ have different itinerancy: $|f_{1}\rangle$ is relatively itinerant and $|f_{2}\rangle$ is relatively localized. We also introduce the CEF splitting $\Delta E$ between $|f_{1}\rangle$ and $|f_{2}\rangle$: $E_{1} = E_{2} + \Delta E$ as shown in Fig.7(a). In this model, the ratio between the $f$-orbital DoS at the Fermi level, $D^{f_{1}}(0)/D^{f_{2}}(0)$, is much larger than unity at $\Delta E = 0$, and the ratio decreases with $\Delta E$ as shown in Fig.7(b). The ratio reaches unity at $\Delta E \simeq 0.12$. In Fig.7(c) and (d), we show the obtained phase diagram at $\Delta E = 0.06$ and $\Delta E = 0.12$, respectively. The region of $s$-wave state at $\Delta E = 0.12$ is much wider than that at $\Delta E = 0.06$, which means that $s$-wave state is favored as $\Delta E$ increases. As a result, the condition $D^{f_{1}}(0) \approx D^{f_{2}}(0)$ is significant for realizing the $s$-wave superconducting state. In other words, the multi-orbital nature on Fermi surface is important for realizing $s$-wave states. Therefore, the $s$-wave state emerges in the presence of finite CEF splitting of $f$-levels when the $s$-$f$ hybridization has strong orbital dependence. This situation is expected to be realized in CeCu$_{2}$Si$_{2}$ at $P = 0$[25].

FIG. 6: (a) Phase diagram in the presence of $U$-$VC$. The $s$-wave state emerges due to the significant contribution from $U$-$VC$. The white region corresponds to $\alpha_{C} > 1$. (b) Phase diagram in the absence of $U$-$VC$. Anisotropic $d_{x^{2}-y^{2}}$-wave state appears in wide parameter region. The gap function on Fermi surface for (c) $s$-wave and (d) $d_{x^{2}-y^{2}}$-wave.
rem. (iii) Thanks to $U$-VC, electric-multipole fluctuation mediated $s$-wave superconductivity is realized when $D^{f1}(0) \approx D^{f2}(0)$, which is a necessary condition for realizing moderate quadrupole or hexadecapole fluctuations.

In this study, we introduced a phenomenological interaction term in Eq.(11) in order to realize the moderate $A^{\uparrow\downarrow}$-channel multipole fluctuations. This term can originate from moderate electron-phonon interaction, as we discussed in the main text. In fact, strong coupling between $f$-electrons and phonons via the $s$-$f$ hybridization and $f$-orbital level is expected in heavy fermion systems, as discussed in Refs.[51–53]. For example, large Gruneisen parameter in heavy fermion systems ($\eta \equiv -d\log T_K/d\log \Omega \sim 30 - 80$) indicates the significance of electron-phonon interaction [51]. The phonon-mediated $s$-wave superconductivity in heavy fermion systems discussed in Refs.[51–53] becomes a realistic scenario by considering the significant role of $U$-VC revealed in the present study. Another promising microscopic origin of Eq.(11) is the AL-type VCs for the susceptibility. In fact, in 3$d$-electron systems without SOI, the AL-type VCs cause large orbital fluctuations [29]. Recently, the present authors found that the AL-type VCs give large even-rank multipole fluctuations in heavy-fermion systems with strong SOI, which we will discuss in future publication [45].

There are many important future issues. For example, it is interesting to apply the present theory to more realistic three-dimensional model for CeCu$_2$Si$_2$. Also, study of self-energy correction, which gives strong mass-enhancement whereas neglected in the present study, is an important future issue. In addition, the present theory may be applicable for spin-triplet superconductor UPt$_3$. In fact, we analyzed the multiorbital Hubbard model for Sr$_2$RuO$_4$, and found that the triplet state is realized under the coexistence of spin and orbital fluctuations [54, 55].

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Appendix A: $s$-$f$ Hybridization

Here, we derive the expression of $s$-$f$ hybridization given in Eq.(4). In the LS basis, the wave function of $f$-electrons in Eq.(2) are given by

$$|f_1 \uparrow \rangle = a \left\{ \sqrt{\frac{6}{7}} |-3, \uparrow \rangle - \sqrt{\frac{1}{7}} |-2, \downarrow \rangle \right\}$$
Then, we obtain in Eq.(43)-(46) and $s$

Now, we consider the hybridization between $f$

where $\uparrow (\downarrow)$ is the real spin. Note that the wave functions for $L_z = \pm 2$ are proportional to $z$ as follows,

$$\langle \vec{r} \mid \pm 2, \sigma \rangle \propto z.$$  

Now, we consider the hybridization between $f$-electrons in Eq.(43)-(46) and $s$-electron. In 2D system, the hybridization between $s$-orbital at $\vec{R}_i$ site and $\mid \pm 2, \sigma \rangle$ at $\vec{R}_j$ site goes to zero, that is, $\langle s, \sigma, \vec{R}_i \mid \pm 2, \sigma, \vec{R}_j \rangle = 0$. Then, we obtain

$$\langle s \uparrow \mid f_1 \uparrow \rangle = \frac{\sqrt{6}}{7} \langle s \uparrow \mid -3, \uparrow \rangle,$$
$$\langle s \downarrow \mid f_1 \uparrow \rangle = -\frac{\sqrt{6}}{7} \langle s \downarrow \mid 3, \downarrow \rangle,$$
$$\langle s \uparrow \mid f_2 \uparrow \rangle = -\frac{\sqrt{2}}{7} \langle s \uparrow \mid 1, \uparrow \rangle,$$
$$\langle s \downarrow \mid f_2 \uparrow \rangle = \frac{\sqrt{2}}{7} \langle s \downarrow \mid -1, \downarrow \rangle,$$

where $a = 1$ and $b = 0$. Therefore, we obtain the relation $\langle s \uparrow \mid f_1 \downarrow \rangle = \langle s \downarrow \mid f_1 \uparrow \rangle = 0$. As a results, we confirm that the pseudo-spin is conserved in the $s$-$f$ hybridization in the present 2-orbital model. Therefore, we can use the pseudo-spin channel $(s, s \downarrow, \sigma)$ in the present study, which is a great merit for performing detailed analysis.

**Appendix B: Coulomb interaction**

Here, we explain about the Coulomb interaction in TABLE I in more detail. The Coulomb interaction is obtained by the following steps. Firsts, we calculate the Lz-basis-Coulomb interaction $\bar{U}_{1, l^l', l^l''}$ by using Eq.(6). The obtained Coulomb interaction is written by using the Slater integral parameters $(F_0, F_2, F_4, F_6)$. Note that $\bar{U}_{1, l^l', l^l''} = 0$ for $l_z + l_z'' \neq l_z' + l_z''$. Next, we transfer it from the Lz-basis into the $L = (l, \sigma)$ basis, which is given by the unitary transformation from the right hands to the left hands in Eqs.(43)-(46). The obtained Coulomb interaction satisfies the axial rotational symmetry expressed as Eq.(7) after antisymmetrization. In the case of $a = 1$ and $b = 0$, the obtained Coulomb interaction is written by using the $U^1, U^2, J^\perp, J, J^z1, J^z2$ and $J^z2$. The definition of each elements are given in Fig.8(a), and the obtained value are shown in Fig.8(b). Although the other elements not listed in Fig.8 (e.g., $U^6_{3d;6d}$) are zero at $a = 1$, they become finite for $a \lesssim 1$. Note that, in 3$d$-electron systems without SOI, the relations $J = J^\perp$ and $J^z1 = J^z2 = 0$ in TABLE I. We stress that the pseudo-spin is conserved even for $a \neq 1$.

**Appendix C: Multipole operator**

Here, we explain about the multipole operators in TABLE II. We numerically obtain each operators by using $4 \times 4$ tensor $J^{(k)}_q$ in Eq.(10). As a result, electric (even-rank) multipole operators in $D_{4h}$ symmetry are expressed.

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**TABLE I**

| type | value |
|------|-------|
| $U^1$ | 1.0   |
| $U^2$ | 0.90  |
| $U^\perp$ | 0.84 |
| $J$ | 0.036 |
| $J^\perp$ | 0.0   |
| $J^z1$ | 0.16  |
| $J^z2$ | -0.16 |

**FIG. 8:** (a) Definition of multi-orbital Coulomb interaction in the pseudo-spin representation; $U^1, U^2, J^\perp, J, J^z1, J^z2$. (b) Obtained value for the Coulomb interaction when $a = 1$ and $(F_0, F_2, F_4, F_6) = (5.3, 9.09, 6.927, 4.756)$ in unit eV. These values are normalized as $U^1 = 1.0$. (Before the normalization, $U^1 = 6.1$ eV.)
as
\[ \begin{align*}
A_1^+ & \{ \begin{cases} 
\hat{i} = \sigma_0 \hat{t}^0 \\
\hat{O}_{20} = \sigma_0 (2.00 \hat{t}^0 + 3.00 \hat{t}^z) \\
\hat{H}_0 = \sigma_0 (-5.73 \hat{t}^0 + 11.5 \hat{t}^z - 12.8 \hat{t}^z) 
\end{cases} \}, \\
A_2^+ & \{ \begin{cases} 
\hat{H}^z = -19.8 \hat{t}^z \\
\hat{O}_{yz} = -3.87 \sigma^z \hat{t}^y \\
\hat{O}_{xz} = +3.87 \sigma^y \hat{t}^x 
\end{cases} \}, \\
E^+ & \{ \begin{cases} 
\hat{O}_{yz} = -3.87 \sigma^z \hat{t}^y \\
\hat{O}_{xz} = +3.87 \sigma^y \hat{t}^x 
\end{cases} \}, \\
\end{align*} \]

Magnetic (odd-rank) multipole operators are given by
\[ \begin{align*}
A_1^- & \{ \begin{cases} 
\hat{D}_y = +29.8 \hat{t}^y \\
\hat{D}_2^x = \hat{D}_2^z = \hat{D}_2^y = 0 \\
\hat{D}_{42} = -1.12 \hat{t}^y \\
\hat{J}^x = -1.12 \hat{t}^z \\
\hat{J}^y = -1.12 \hat{t}^x \\
\hat{J}^z = \hat{D}_2^{x2} (3.75 \hat{t}^z - 3.75 \hat{t}^z + 5.03 \hat{t}^z) \\
\hat{D}_2^x = \hat{D}_2^z = \hat{D}_2^y = 0 \\
\end{cases} \}, \\
A_2^- & \{ \begin{cases} 
\hat{J}^x = -1.12 \hat{t}^z \\
\hat{J}^y = -1.12 \hat{t}^x \\
\hat{D}_2^x = \hat{D}_2^z = \hat{D}_2^y = 0 \\
\hat{D}_2^y = \hat{D}_2^z = \hat{D}_2^x = 0 \\
\end{cases} \}, \\
E^- & \{ \begin{cases} 
\hat{D}_y = \hat{D}_2^y = \hat{D}_2^z = \hat{D}_2^x = 0 \\
\hat{J}^y = \hat{J}^x = \hat{J}^z = 0 \\
\hat{D}_2^x = \hat{D}_2^z = \hat{D}_2^y = 0 \\
\hat{D}_2^x = \hat{D}_2^z = \hat{D}_2^y = 0 \\
\end{cases} \}, \\
\end{align*} \]

where $\sigma^\mu$ and $\hat{t}^\nu (\mu = x, y, z)$ are Pauli matrices for the pseudo-spin and orbital basis, respectively. $\sigma_0$ and $\hat{t}_0$ are identity matrices. We express the obtained 16 matrix expressions in Eq.(51) and (51) as $O^\mu(Q = (\Gamma, \phi))$. Note that $\sum_{XX'} O^{(\Gamma, \phi)}_{LL'} O^{(\Gamma', \phi')*}_{LL'} = 0$ for $\Gamma \neq \Gamma'$, whereas $\sum_{XX'} O^{(\Gamma, \phi)}_{LL'} O^{(\Gamma', \phi')*}_{LL'} = 0$ $A_1^2 (E^+)$ electric multipole operators belong to pseudo-spin s (l) channel since it is proportional to $\sigma^z (\sigma^x, \sigma^y)$. Also, $A_1^2$ magnetic multipole operators belong to the charge channel since it is proportional to $\sigma^0$. The In summary, some electric (magnetic) multipole operators belong to pseudo-spin (charge) channels as summarized in TABLE II. The relation between multipole and pseudo-spin (charge) channels We have to take care of this fact in analysis.

Appendix D: Effects of f-f hopping

In this section, we discuss the effects of f-f hopping. In the main text, we neglected f-f hopping, and therefore the f orbital weight is quite isotropic on Fermi surface as shown in Fig.1(e). However, this orbital-isotropy can be broken if we introduce finite f-f hopping. Now, we introduce the orbital-dependent f-f hopping. In this case, f-electron energy $E_f$ have $k$-dependence. As a result, the f orbital weight comes to have $\theta$-dependence on the Fermi surface. The f-f hopping is expressed as
\[ \hat{H}_{ff} = \sum_{kl\sigma} E_{kk'f, fkl\sigma} \hat{f}_{kl\sigma}. \]

Here, we set $E_{kk',1} = E_1 + \delta E_k$ and $E_{kk',2} = E_2 - \delta E_k$, where the $k$-dependence of $\delta E_k$ is shown in Fig.9(a). Technically, to realize the $\delta E_k$, we introduce the intra-orbital $f-f$ hopping up to the fifth nearest neighbor hopping integrals according to Ref.[36], In Fig.9(b), we show the obtained $f$-orbital weight along $\theta$-axis on Fermi surface. It shows strong $\theta$-dependence irrespective of the fact that $|\delta E_k| (\sim 0.2)$ is much smaller than $|t_{\sigma f}| (\sim 0.7)$.

One may suspect that higher rank multipole susceptibilities may be suppressed when the $f$-orbital weight is $\theta$-dependent, since the orbital off-diagonal components of $\chi_{ll\mu
u}$ may be suppressed. To answer this question, we perform the RPA analysis. Figure 9(c) shows the obtained magnetic multipole susceptibilities. We find that multiple higher-rank magnetic multipole susceptibilities develop, which is quite similar to our result without $f-f$ hopping in Fig.2(b). This unexpected results originate from the fact that many body effects away from Fermi surface also contribute to the multipole susceptibility. This result strongly indicates that U-VC is still important even in the presence of small f-f hopping. We study this issue in more detail in the future publication [45].

![FIG. 9: (a) The Fermi surface with f-f hopping. Each number at k shows intra-orbital energy shift $\delta E_k$. (b) Obtained $\theta$-dependence of the f orbital weight on Fermi surface. The red (green) line corresponds to $f_1, (f_2)$-orbital. (c) $\alpha S$ dependence of magnetic multipole susceptibilities, which are almost equal to those in Fig.2(b).](image-url)
Appendix E: Multipole expansion

In this section, we explain about the derivation of the coefficient $a^\Gamma_{\phi,\phi'}$ in Eq.(36). First, we solve the characteristic equation for the $f$-electron susceptibility in the $L = (l, \sigma)$ basis,

$$\sum_{MM'} \chi_{LL'M'M'}(q)v_{MM'}^{i}(q) = \lambda^{i}(q)v_{LL'}^{i}(q), \quad (54)$$

where $\lambda^{i}(q)$ is $i$-th real eigen value ($i = 1 \sim 16$), $v_{LL'}^{i}(q)$ is 16-dimensional eigen vector. In the present model, $\chi^{(\Gamma,\phi),(\Gamma,\phi')} = 0$ for $\Gamma \neq \Gamma'$. Thus, for each $i, v_{LL'}^{i}(q)$ is classified into the corresponding IR ($\Gamma$). If we normalize $\vec{v}$ as $\sum_{\Gamma} v_{LL'}^{i}(q)^{\ast} = \delta_{i,j}$, the $f$-electron susceptibility is expressed as

$$\chi_{LL'M'M'}(q) = \sum_{i} v_{LL'}^{i}(q)\lambda^{i}(q)v_{MM'}^{i}(q)^{\ast} \quad (55)$$

Then, we expand $\vec{v}(q)$ for $i \in \Gamma$ on the basis of the multipole matrices $\hat{O}^{(\Gamma,\phi)}$ for $\phi = 1 \sim N_{\Gamma}$ listed in Eqs.(51) and (52) as follows:

$$v_{LL'}^{i}(q) = \sum_{\phi = 1}^{N_{\Gamma}} b^{i,\phi}(q)O_{LL'}^{(\Gamma,\phi)} \quad (56)$$

where the coefficient $b^{i,\phi}(q)$ is uniquely determined. Note that the basis $\{ \hat{O}^{(\Gamma,\phi)} \}$ is complete but not orthogonal within the same $\Gamma$. By inserting Eq.(56) into Eq.(55), we obtain

$$\chi_{LL'M'M'}(q) = \sum_{\Gamma,\phi,\phi'} a^{\Gamma,\phi,\phi'}(q)O_{LL'}^{(\Gamma,\phi)}O_{MM'}^{(\Gamma,\phi')}, \quad (57)$$

where

$$a^{\Gamma,\phi,\phi'}(q) = \sum_{i \in \Gamma} b^{i,\phi}(q)\lambda^{i}(q)b^{i,\phi'}(q)^{\ast}. \quad (58)$$

As a result, the decomposition of $\chi_{LL'M'M'}(q)$ in Eq.(36) is obtained. In the same way, the paring interaction $I$ in Eq.(37) can be decomposed. Using $a^{\Gamma,\phi,\phi'}$, the multipole susceptibility $\chi^{(\Gamma,\phi),(\Gamma,\phi')}$ defined in Eq.(21) is expressed as

$$\chi^{(\Gamma,\phi),(\Gamma,\phi')} = \sum_{\phi'' \phi'''} a^{\Gamma,\phi,\phi'''}(T_{\phi,\phi''})^{\ast}T_{\phi',\phi''''}(\Gamma,\phi'), \quad (59)$$

where

$$T_{\phi,\phi'}^{\Gamma} = \sum_{MM'} O_{MM'}^{\Gamma,(\phi)}O_{MM'}^{(\phi')}, \quad (60)$$

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In the present model, we introduce $t_{sf}$ between the nearest Ce sites in the (001) plane. Then, the relation $|V_{k_1,\sigma}| \approx 2|V_{k_2,\sigma}|$ holds according to Slater-Koster tight-binding method [42]. In contrast, Pourovskii [25] consider the hybridization between Ce site at $\vec{r} = 0$ and the nearest neighbor Si sites at $(\pm 1/2, \pm 1/2, \pm c)$, and then the relation $|V_{k_2,\sigma}| \approx 2|V_{k_1,\sigma}|$ holds. In both cases, electric multipole fluctuation mediated superconductivity proposed in this paper is realized when $D^{(1)}(0) \approx D^{(2)}(0)$ at finite $\Delta E$. 

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