Generalized Spin Fluctuation Feedback in Heavy Fermion Superconductors

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Experiments reveal that the superconductors UPT\(_3\), PrOs\(_4\)Sb\(_{12}\) and U\(_{1-x}\)Th\(_x\)Be\(_{13}\) undergo two superconducting transitions in the absence of an applied magnetic field. The prevalence of these multiple transitions suggests a common underlying mechanism. A natural candidate theory which accounts for these two transitions is the existence of a small symmetry breaking field, however such a field has not been observed in PrOs\(_4\)Sb\(_{12}\) or U\(_{1-x}\)Th\(_x\)Be\(_{13}\) and has been called into question for UPT\(_3\). Motivated by arguments originally developed for superfluid \(^3\)He we propose that a generalized spin fluctuation feedback effect is responsible for these two transitions. We first develop a phenomenological theory for \(^3\)He that couples spin fluctuations to superfluidity, which correctly predicts that a high temperature broken time-reversal superfluid \(^3\)He phase can emerge as a consequence. The transition at lower temperatures into a time-reversal invariant superfluid phase must then be first order by symmetry arguments. We then apply this phenomenological approach to the three superconductors UPT\(_3\), PrOs\(_4\)Sb\(_{12}\) and U\(_{1-x}\)Th\(_x\)Be\(_{13}\) revealing that this naturally leads to a high-temperature time-reversal invariant nematic superconducting phase, which can be followed by a second order phase transition into a broken time-reversal symmetry phase, as observed.

There has been renewed interest in unconventional superconductors, as they provide a natural platform for topological states\(^1\)\(^4\). Heavy fermion superconductors, such as UPT\(_3\), PrOs\(_4\)Sb\(_{12}\), U\(_{1-x}\)Th\(_x\)Be\(_{13}\), URu\(_2\)Si\(_2\), have been intensely studied as they show time-reversal symmetry-breaking (TRS\(_B\))\(^2\)\(^3\), and are argued to be Weyl superconductors which may host Majorana modes as well as Bogoliubov Fermi surfaces\(^10\)\(^{13}\). Of these, UPT\(_3\), PrOs\(_4\)Sb\(_{12}\), U\(_{1-x}\)Th\(_x\)Be\(_{13}\) show a rich phase diagram, with two superconducting transitions under zero field. The high temperature A phase is time-reversal symmetric (TRS) and the low temperature B phase is TRSB\(^9\)\(^{14}\)\(^{19}\).

The presence of two transitions in three materials raises a question about the underlying mechanism. UPT\(_3\) has been the most studied of these materials and has the phase diagram shown in Fig.\(^2\)\(^{15}\). The most common explanation for this phase diagram relies on coupling the superconducting order parameter to a weak symmetry breaking field (SBF), which splits the degeneracy between the different order parameter components\(^20\)\(^{21}\). The SBF is associated with an antiferromagnetic (AFM) order seen in early neutron scattering measurements\(^22\). However, recent experiments show that there is no static order near \(T_c\), though AFM fluctuations are present\(^23\)\(^{24}\), which casts serious doubts about the use of a SBF to generate two transitions. Meanwhile, there is no accepted model which accounts for the double transition in U\(_{1-x}\)Th\(_x\)Be\(_{13}\) or PrOs\(_4\)Sb\(_{12}\), though there are signatures of antiferroquadrupolar (AFQ) fluctuations in PrOs\(_4\)Sb\(_{12}\) and AFM fluctuations in U\(_{1-x}\)Th\(_x\)Be\(_{13}\) as seen in inelastic neutron scattering (INS)\(^25\)\(^{26}\). It is natural to ask if these fluctuations can account for the generic observation of two transitions.

To gain insight into this question, it is reasonable to consider superfluid \(^3\)He, which is also a topological material with multiple phases. In this case, here there is a high temperature, high pressure TRSB A phase and a low temperature low pressure TRS B phase as shown in Fig.\(^1\)\(^{24}\)\(^{28}\). Originally, the stability of the A phase was a puzzle, as weak coupling theory predicted that the B state is stable for all temperatures\(^29\). This paradox was resolved by Anderson and Brinkmann, who showed that coupling superfluidity to paramagnetic fluctuations, can stabilize the A state, through a mechanism called the spin fluctuation feedback effect (SFFE)\(^30\)\(^{32}\).

In this paper, we propose a mechanism for multiple transitions in heavy fermions by coupling superconductivity to fluctuations (both AFM and AFQ), analogous to superfluid \(^3\)He. We initially formulate a simple phenomenological method to capture the essential physics, and show that it reproduces the microscopic SFFE theory developed by Anderson-Brinkman. We then apply this to UPT\(_3\), U\(_{1-x}\)Th\(_x\)Be\(_{13}\) and PrOs\(_4\)Sb\(_{12}\) and show that fluctuations change the coefficients of the Ginzburg-Landau theory to stabilize a high temperature TRS A phase, instead of the TRSB B weak coupling phase. We then consider the transition into the broken TRS state, implementing the symmetry constraints associated with observing a polar Kerr effect.

These considerations strongly constrain the possible order parameters, for example we show that except for the 3D \(T_{g/u}\) representations (reps) of PrOs\(_4\)Sb\(_{12}\), the only possibility for having two successive transitions requires the B state to be TRSB. We also find that the Kerr effect measurement rules out the 2D \(E_{g/u}\) rep scenario for PrOs\(_4\)Sb\(_{12}\), while for U\(_{1-x}\)Th\(_x\)Be\(_{13}\) in the case of it’s 3D \(T_{g/u}\) reps, the form of the SFFE allows only one A state symmetry, while eliminating the other possible symmetry. These results are tabulated in Table\(^3\).

\(^3\)He. \(^3\)He is a strongly correlated Landau-Fermi liquid, whose quasiparticle excitations pair to form a spin-triplet p-wave superfluid\(^27\)\(^{28}\). The gap function is \(\Delta(\mathbf{k}) = i(d_i(\mathbf{k})\sigma_j)\sigma_y\), with \(d_i = d_{g/u}k_i\), here we use the Einstein
and displays the symmetry properties of the components. The

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an overall TABLE I. Table summarizing our results. The fluctuations of the high temperature high pressure A phase. Anderson-Brinkman [30] used SFFE to stabilize the A phase, which Kerr inactive.

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\text{FIG. 1. Pressure (P)- Temperature (T) Phase Diagram}
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\text{FIG. 2. Magnetic Field (H)-Temperature (T) Phase Diagram of UPt}_{3}\text{ with B field }\perp z \text{ axis}
\]

| Material   | Fluctuations Reps | Order Parameter | A | B          |
|------------|--------------------|----------------|---|------------|
| UPt\textsubscript{3} | AFM             | E $k_xk_z, k_yk_y$ | (1,0) | (0,i)     |
| PrOs\textsubscript{4}Sb\textsubscript{12} | AFQ             | T $k_yk_z, k_xk_y$ | (1,0,0) | (0,i) or (0,0,i) |
| U\textsubscript{1-x}Th\textsubscript{x}Be\textsubscript{13} | AFM             | E $2k_x^2 - k_y^2 - k_z^2$ | (1,0) | (i,0) or (0,i) |

The (i)\textsuperscript{+} is for A–B transitions which are Kerr inactive.

summation convention. The order parameter $d_{i\alpha}$ is a 3 x 3 matrix with complex entries, where $i$ is the spin index and $\alpha$ is the orbital index and both run over $x$, $y$, and $z$. By comparing to experiments, the $^3$He-A phase was identified with the Anderson-Brinkman-Morel (ABM) state with $d_{xx} = \frac{j\Delta}{\sqrt{n}}$ and all other $d_{ij} = 0$, while B state was associated with Balian-Wethamer (BW) which has $d_{ij} = \frac{j\Delta}{\sqrt{n}}\delta_{ij}$ [27, 28]. Weak coupling theory shows that the BW state is stable for all temperatures [29], implying that a strong coupling approach is needed to explain the existence of the high temperature high pressure A phase. Anderson-Brinkman [30] used SFFE to stabilize the A phase, which relies on the pairing glue in $^3$He being paramagnetic fluctuations. This implies that the formation of the superfluid alters the pairing interaction, where the type of modification depends on which state is formed [27]. Thus the A state can be stabilized despite being unstable under weak coupling theory. The A–B transition in this case is first order as the B state is not a subgroup of the A state.

Here SFFE shall be recaptured in a phenomenological manner, by coupling the superfluid order parameter to paramagnetic fluctuations, and calculating the change to the bare free energy. The coupling is constructed to be invariant under independent rotations in orbital and spin space, and is $f_{sff} = A_1m_m i + A_2m_m i d_{ja}^*d_{ja} + K_1m_m i d_{ja}^*d_{ja}$, where $m_i$ is the magnetic order parameter. We assume $A_1$ is parametrically small and positive (i.e. $A_1 \rightarrow 0$) to indicate that we have large fluctuations close to a magnetic transition. The magnetic partition function is given as $Z_m = \int Dm_i e^{-\int d^4x f_{sff}} = \int Dm_i e^{-\int d^4x A_1 m_i m_j}$, where $A_{ij}$ contains couplings between magnetic and superconducting orders, and gives corrections the bare superconducting free energy density. Integrating out the quadratic magnetic fluctuations, gives an effective free energy density

\[
f_{sff} = \left(\alpha + \frac{A_2}{A_1} + \frac{K_1}{A_1}\right)(i\alpha d_{i\alpha}^*d_{i\alpha} + \beta_1 d_{j\alpha} d_{j\alpha} d_{j\alpha}^*d_{j\alpha}^* + \beta_2 d_{i\alpha} d_{j\alpha} d_{i\alpha}^*d_{j\alpha}^* + \left(\beta_3 - \frac{K_1^2}{4A_1^2}\right)d_{j\alpha} d_{j\beta} d_{i\alpha}^*d_{i\beta}^* + \left(\beta_4 - \frac{K_1^2}{4A_1^2} + \frac{12A_2^2}{2A_1^2} + 8K_1A_3\right)d_{i\alpha} d_{j\alpha} d_{j\beta}^*d_{i\beta} + \left(\beta_5 - \frac{K_1^2}{4A_1^2}\right)d_{i\alpha} d_{j\alpha} d_{i\beta}^*d_{j\beta}^* - \frac{K_2^2}{A_1} \left(\vec{d} \times \vec{d}\right)^2, (1)
\]

where the $\beta_i$ are associated with the free energy density without coupling to fluctuations, here assumed to be derived from weak-coupling theory and the terms with the $K$’s originate from SFFE. Close to the paramagnetic instability,
for which $A_1$ is small, the terms that dominate are those that are proportional to $A_1^{-2}$ and we ignore terms of order $A_1^{-1}$. The $K_2$ term in (1) shows that paramagnetic fluctuations can favor non-unitary states [32, 33], but are neglected here due to their weaker $A_1^{-1}$ dependence.

Weak coupling theory gives $\beta_2 = \beta_3 = \beta_4 = -\beta_5 - 2\beta_1 = \frac{5}{4}s$, where $s$ is a positive valued constant [27, 28]. When the SFFE is turned off (i.e. $K_1 = 0$), we see that the BW state is energetically favorable with $f_{eff} = \frac{5}{4}s$, while the A state has a slightly larger free energy density of $f_{eff} = 2s$. The SFFE coupling lowers the energy of the A state by $K_2^2/3A_1^2$ compared to the B state and thus for large fluctuations (i.e. $K_2^2/3A_1^2 > 1/3s$) can stabilize the A state.

The second A–B transition stems from the different temperature dependence of the weak coupling terms versus the SFFE terms. It can be shown using a microscopic theory that the terms originating from the SFFE have a $\frac{1}{T}$ dependence while weak coupling terms scale as $\frac{1}{T^2}$ [27, 31, 37]. This implies that at high temperatures, strong fluctuations may stabilize the A phase, while at lower temperature the weak coupling terms will dominate and the system will undergo a first order transition into the state preferred by weak coupling theory i.e. the B phase. Analogous arguments will be applied to the heavy fermions, where as the temperature is lowered there will be a sign change the coefficients in the free energy density, though the A–B transition will be second order.

$\text{UPt}_3$ - The $\text{UPt}_3$ is a hexagonal crystal with $D_{6h}$ point group symmetry and has two distinct phases under zero field, a high temperature A phase and a low temperature B phase [17, 35]. However, unlike $^4\text{He}$, the A phase is TRS while the B phase is TRSB as seen in muon spin relaxation ($\mu$SR) and polar Kerr measurements [3, 14]. $\text{UPt}_3$ has four 2D reps labeled $E_{1u/g}$ and $E_{2u/g}$, where the order parameter transforms like $\eta_1 \sim k_x k_y$, $\eta_2 \sim k_x k_z$, and $\eta_i \sim k^2 - k_y^2$, $\eta_2 \sim 2k_x k_y$ respectively. The free energy density is the same for all the $E$ reps and is given as $f_{sc} = \alpha (\eta_i \eta_i^*) + \beta_1 (\eta_i \eta_i^*)^2 + \beta_2 |\eta_i|^2$ [39]. The coefficient of $|\eta_i|^2$ determines the behavior below $T_c$, with $\beta_2 > 0$ favoring the $(1, i)$ state, and $\beta_2 < 0$ stabilizing the $(1, 0)$ state. To explain the existence of multiple phases, the currently accepted model involves coupling superconductivity to AFM order [20, 21]. However experiments raise questions over the existence of true AFM order. The Bragg peaks in INS are not resolution limited near the superconducting transition of 550mK and order truly appears around 20mK [23] far away from $T_c$, which is further confirmed by SQUID measurements [40]. We interpret these experiments to imply the presence of AFM fluctuations, instead of AFM order, where a generalized SFFE may stabilize a TRS A state. We shall proceed analogously to [41, 42], thereby allowing a second transition to a TRSB state.

$$f_{sc-m} = A_1 m_2^2 + K_1 (m_2^2)(\eta_i \eta_i^*) + K_2 (2m_1^2 - m_2^2 - m_3^2) |\eta_1|^2 = |\eta_2|^2 + \sqrt{3} (m_3^2 - m_2^2) (\eta_1 \eta_2^* + \eta_2 \eta_1^*) \right].$$

Integrating out the fluctuations as before gives the following free energy density:

$$f_{eff} = \left( \alpha + \frac{3K_1}{2A_1} \right) (\eta_i \eta_i^*) + \left( \beta_1 - \frac{3K_1^2}{4A_1^2} \right) (\eta_i \eta_i^*)^2 + \left( \beta_2 - \frac{6K_0^2}{4A_1^2} \right) |\eta_i|^2.$$

Importantly, the generalized SFFE changes the $|\eta_i|^2$ coefficient, and for large fluctuations can stabilize the A state, instead of the TRSB B by making this coefficient negative. This also implies that two transitions will occur only if the B state is a TRSB state. In particular, if the B state was TRS then the SFFE terms would simply further stabilize the A state by $K_2^2/3A_1^2$ compared to the B state and thus for large fluctuations (i.e. $K_2^2/3A_1^2 > 1/3s$) can stabilize the A state.

To gain further insight, we model the A–B transition as an effective phenomenological theory, by assuming that the SFFE stabilizes the TRS A $(1, 0)$ state, and the TRSB B continuously state grows out of this i.e. $(1 + \tilde{\eta}_1, 0 + \tilde{\eta}_2)$, where $\tilde{\eta}_i$ is small near the transition. Time-reversal symmetry allows us to classify the order parameter $\tilde{\eta}_i$ for the A–B transition into a real part $\tilde{\eta}_R$ which is invariant under $\mathcal{T}$, and an imaginary part $\tilde{\eta}_I$ which changes sign under $\mathcal{T}$. The condition that the second transition break TRS, allows us to consider only the imaginary order parameter. The $(1, 0)$ state has $D_2(C_2) \times \mathcal{T}$ and $D_2 \times \mathcal{T}$ [33] symmetry for the $E_{1u/g}$ and $E_{2u/g}$ reps respectively. The order parameter $\tilde{\eta}_I$ belongs to the $A_1$ rep of $D_2$, while $\tilde{\eta}_R$ belongs to the $B_1$ rep.

The observation of a polar Kerr signal for the A–B transitions [3] further constrains the possible order parameters, as only those order parameters which belong to the same representation as the magnetic moments ($m_x$, $m_y$, $m_z$) will show a Kerr effect and shall be referred to as Kerr active (also labeled as belonging to a ferromagnetic class [43]). This rules out the $A_1$ order parameter as it is Kerr inactive. Thus the A–B transition can be modeled by the effective
order parameter $\eta_{2l}$ with the following free energy $f_{A\rightarrow B} = \alpha_1 \eta_1^2 + \beta_1 \eta_{2l}^4$. We shall use this approach later to shed insight into the possible order parameters.

$PrOs_4Sb_{12}$-$PrOs_4Sb_{12}$ (POS) is a Pr based tetrahedral heavy fermion skutterudite superconductor with a $T_h$ point group, and like UPt$_3$ has two distinct phases [14]. Polar Kerr and $\mu$SR measurements show a TRSB B phase [17,18], while the A phase is TRS. POS has been studied by phenomenological methods [15], however there is no satisfactory mechanism for the double transition. INS experiments indicate the presence of AFQ fluctuations with a $Q = (1, 0, 0)$ [23,16], which is a single $Q$ order, invariant under the point group operations. The order parameter of these AFQ fluctuations is 3D with components that transform as $m_1 \sim k_x k_z$, $m_2 \sim k_x k_y$ and $m_3 \sim k_y k_z$ [17,18]. The AFQ fluctuations can stabilize a time-reversal symmetric A phase for both the $E$ and $T$ reps as shown below.

For the $E$ reps, where the order parameter transforms as $\eta_1 \sim 2k_x^2 - k_y^2 - k_z^2$, $\eta_2 \sim k_x^2 - k_y^2$, the coupling is

$$f_{sc-m} = A_1 (m_1^2) + K_1 (m_1^2)(\eta_1 \eta_1^*) + K_2 \left[ (2m_3^2 - m_1^2 - m_2^2)(|\eta_1|^2 - |\eta_2|^2) - \sqrt{3} (m_1^2 - m_2^2)(\eta_1 \eta_2^* + \eta_2 \eta_1^*) \right]$$

$$+ K_3 \left[ \sqrt{3} (m_1^2 - m_2^2)(|\eta_1|^2 - |\eta_2|^2) + (\eta_1 \eta_2^* + \eta_2 \eta_1^*) (2m_3^2 - m_1^2 - m_2^2) \right]. \quad (4)$$

Integrating out the AFQ fluctuations, we obtain the effective free energy density

$$f_{eff} = \left( \alpha + \frac{3K_1}{A_1} \right) (\eta_1 \eta_1^*) + \left( \beta_1 - \frac{3K_1^2}{4A_1^2} + \frac{3K_2^2}{2A_1^2} - \frac{3K_3^2}{2A_1^2} \right) (\eta_1 \eta_1^*)^2 + \left( \beta_2 - \frac{3K_2^2}{4A_1^2} - \frac{3K_3^2}{2A_1^2} \right) (\eta_1 \eta_2^* + \eta_2 \eta_1^*)^2. \quad (5)$$

This generalized SFSE may again stabilize a TRS A state ($\phi_1, \phi_2$) with $D_2 \times \mathcal{T}$ symmetry [45,49], instead of the TRSB B phase (1, i) with $T(D_2)$ symmetry by changing the sign of the $(\eta_1 \eta_2^* - \eta_2 \eta_1^*)^2$ term, form positive to negative. The A phase has the two components with the same magnitude but an arbitrary phase [45]. Similar to UPt$_3$ two transitions are possible only when the B state is TRSB. The A-B transition is modeled similar to UPt$_3$, however both $\eta_1,1/2$ have $A_1$ Kerr inactive symmetry and are ruled out due to presence of Kerr effect, thereby eliminating the 2D E reps scenario for $PrOs_4Sb_{12}$.

For the 3D $T$ reps, with order parameter which transforms for example as $\eta_1 \sim k_y k_z$, $\eta_2 \sim k_x k_z$ and $\eta_3 \sim k_x k_y$, the coupling is

$$f_{sc-m} = A_1 (m_1^2) + K_1 (m_1^2)(\eta_1 \eta_1^*) + K_2 \left[ (2m_3^2 - m_1^2 - m_2^2)(|\eta_1|^2 - |\eta_2|^2) - \sqrt{3} (m_1^2 - m_2^2)(\eta_1 \eta_2^* + \eta_2 \eta_1^*) \right]$$

$$\times (2m_1^2 - m_2^2 - m_3^2) + K_3 \left[ (|\eta_2|^2 - |\eta_3|^2) (2m_1^2 - m_2^2 - m_3^2) - (2|\eta_1|^2 - |\eta_2|^2 - |\eta_3|^2) (m_1^2 - m_2^2) \right]$$

$$+ K_4 [(\eta_1 \eta_2^* + \eta_2 \eta_3^*) m_2 m_3 + (\eta_3 \eta_1^* + \eta_1 \eta_3^*) m_3 m_1 + (\eta_1 \eta_2^* + \eta_2 \eta_1^*) m_1 m_2]. \quad (6)$$

Integrating out the Gaussian AFQ fluctuations gives the following effective free energy density:

$$f_{eff} = \left( \alpha + \frac{3K_1}{A_1} \right) (\eta_1 \eta_1^*) + \left( \beta_1 - \frac{6K_1^2}{A_1^2} + \frac{6K_2^2}{A_1^2} + \frac{2K_3^2}{A_1^2} - \frac{K_4^2}{4A_1^2} \right) (\eta_1 \eta_1^*)^2 + \left( \beta_2 - \frac{K_2^2}{4A_1^2} \right) |\eta_1|^2$$

$$+ \left( \beta_3 - \frac{18K_3^2}{4A_1^2} - \frac{6K_2^2}{A_1^2} + \frac{K_4^2}{2A_1^2} \right) (|\eta_1|^4 + |\eta_2|^4 + |\eta_3|^4). \quad (7)$$

Again the SFSE has changed the coefficient of the bare free energy density and hence allows for the possibility of a TRS A state. Interestingly, here we may have two transition even if the A state is TRSB, due the indeterminant sign of the correction to the $\beta_3$ coefficient. However since this does not agree with the experimental identification of the B state being TRSB, so we don’t consider this possibility. This rep has two states which are TRS, the (1, 0, 0) state with $D_2(C_2) \times \mathcal{T}$ symmetry and the (1,1,1) state with $C_3 \times \mathcal{T}$ symmetry. Both of these allow for a transition to a TRSB B state which is Kerr active and hence provide two viable channels for the transition. The physics of this is similar to the 2D case for UPt$_3$ and $PrOs_4Sb_{12}$, and is worked out in the supplementary material [50], the results of which are collected in Table I This model assumes that AFQ fluctuations act as the pairing glue, and we suggest INS scattering and tunneling spectra as done in UPd$_2$Au$_3$ to confirm this unconventional glue [51,52].

$U_{1-x}Th_xBe_{13}$-$U_{1-x}Th_xBe_{13}$ is a cubic material with $O_h$ point group, which also has two transitions [3,17], but only for a doping range of 2% $< x < 4%$. The B phase is again a TRSB state [9]. AFM fluctuations are seen in INS with a wave vector of $Q_3 = (1/2, 1/2, 0)$ [20]. We consider both the $E$ and $T$ reps and model the system with $O_h$ symmetry, having AFM fluctuations with wave vector $Q_3$. The star of $Q_3$ gives two additional wave vectors $Q_2 = (1/2, 0, 1/2)$ and $Q_1 = (0, 1/2, 1/2)$, each of which correspond to a 1D order parameter $m_1, m_2, m_3$. Here $\eta_1$ and $\eta_2$ transform exactly as $E$ reps of $PrOs_4Sb_{12}$ is

$$f_{sc-m} = A_1 (m_1^2) + K_1 (m_1^2)(\eta_1 \eta_1^*) + K_2 \left[ (2m_3^2 - m_1^2 - m_2^2)(|\eta_1|^2 - |\eta_2|^2) - \sqrt{3} (m_1^2 - m_2^2)(\eta_1 \eta_2^* + \eta_2 \eta_1^*) \right]. \quad (8)$$
The $K_4$ term present in Eq. 3 is absent above, due to additional symmetry elements present in the $O_h$ as compared to $T_h$ point group. The correction to the free energy density from these fluctuations is

$$f_{\text{eff}} = \left( \alpha + \frac{3K_1}{2A_1} \right) \langle \eta_i \eta_j^* \rangle + \left( \beta_1 - \frac{3K_2}{4A_1^2} + \frac{3K_3}{2A_1^3} \right) \langle \eta_i \eta_j^* \rangle^2 + \left( \beta_2 - \frac{3K_2}{2A_1^3} \right) \langle \eta_i \eta_2^* - \eta_2 \eta_i^* \rangle^2. \quad (9)$$

There are two possible TRS A states. The details of the A–B effective theory follows that of UPt$_3$ and is in the supplementary material [50], with the possible A state being $(1,0)$ with $D_4 \times \mathcal{T}$ symmetry and $(0,1)$ with $D_d^{(1)}(D_2) \times \mathcal{T}$ symmetry [42]. These states are Kerr inactive, and the 2D order parameter can be ruled out if a polar Kerr signal is seen.

For the 3D order parameter case, we note that, U$_{1-x}$Th$_x$Be$_{13}$ has four $T$ reps, one which transforms exactly like $T$ reps of PrOs$_4$Sb$_{12}$ which we call $T_{2g/u}$ and the other $T_{1g/u}$ which transforms as $\eta_1 \sim k_x k_z (k_x^2 - k_y^2)$, $\eta_2 \sim k_x k_y (k_x^2 - k_z^2)$ and $\eta_3 \sim k_x k_y (k_y^2 - k_z^2)$. The coupling for these $T$ reps is

$$f_{\text{sc-m}} = A_1 \left( m_1^2 \right) + K_1 \left( m_1^2 \right) \langle \eta_i \eta_i^* \rangle + K_2 \left[ 3 \left( |\eta_2|^2 - |\eta_3|^2 \right) (m_2^2 - m_3^2) + \left( 2|\eta_1|^2 - |\eta_2|^2 - |\eta_3|^2 \right) (2m_1^2 - m_2^2 - m_3^2) \right]. \quad (10)$$

The $K_4$ term found in Eq. 6 is absent because of higher $O_h$ symmetry compared to the $T_h$ symmetry, while the $K_4$ term is forbidden as $m_i m_j$ is not translationally invariant for this $Q$ vector. The effective free energy density obtained is

$$f_{\text{eff}} = \left( \alpha + \frac{3K_1}{A_1} \right) \langle \eta_i \eta_j^* \rangle + \left( \beta_1 - \frac{3K_2}{4A_1^2} + \frac{3K_3}{A_1^2} \right) \langle \eta_i \eta_j^* \rangle^2 + \left( \beta_2 - \frac{3K_2}{A_1^2} \right) \langle \eta_i \eta_2^* - \eta_2 \eta_i^* \rangle^2. \quad (11)$$

Interestingly, here unlike PrOs$_4$Sb$_{12}$ there is no change to $\beta_2$, which is result of the $K_4$ coupling being absent for Eq. 11 in contrast to Eq. 6. There are four possible TRS A state, two for each $T$ reps, i.e. $(1,0,0)$ and $(1,1,1)$. However due to there being no change to coefficient of the $|\eta_i|^2$ term, $(1,0,0)$ is the only TRS A state which allows for a viable transition to a TRSB B state [33]. This state has $D_4(C_4) \times \mathcal{T} \times D_4^{(2)}(D_2) \times \mathcal{T}$ symmetry for the $T_1$ and $T_2$ reps respectively [43]. The A–B transition, follows similar to UPt$_3$, and is modeled in the supplementary information [50]. Polar Kerr measurements may be useful as they can rule out the $E$ reps scenario, and can eliminate other 3D $T$ order parameters.

Conclusions.- In summary, we have argued that the mechanism for two transitions in heavy fermions needs to be revisited. In analogy to superfluid $^3$He we have argued that a generalized SFFE may stabilize a TRS high temperature A phase. We provide a simple phenomenological model to capture this effect, and show that generalized SFFE provides a unifying mechanism for two transitions in UPt$_3$, PrOs$_4$Sb$_{12}$ and U$_{1-x}$Th$_x$Be$_{13}$.

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See Supplementary Material at....for the effective free energy for A-B transitions.

NK Sato, N Aso, K Miyake, R Shiina, P Thalmeier, G Varellogianmis, C Geibel, F Steglich, P Fulde, and T Komatsubara, “Strong coupling between local moments and superconducting heavyelectrons in UPd$_2$Al$_3$,” Nature 410, 340 (2001).

Martin Jourdan, Michael Huth, and Hermann Adrian, “Superconductivity mediated by spin fluctuations in the heavy-fermion compound UPd$_2$Al$_3$,” Nature 398, 47 (1999).
Effective Phenomenological Theory for A–B Transition

We model the A–B second order transition in terms of an effective theory by assuming that for large fluctuations the SFSE stabilizes the TRS A state and we grow the B state continuously out of the A state, while demanding that the A–B transition break time-reversal symmetry. The condition of time-reversal symmetry breaking for the second transition constrains the possible order parameters for each material. For example, for UPt$_3$ the A state is (1,0) with $D_2(C_2) \times T$ and $D_2 \times T$ symmetry for the $E_{1a/2g}$ and $E_{2u/9}$ reps respectively. The B state grows out as $(1 + \tilde{\eta}_1, 0 + \tilde{\eta}_2)$ continuously. The difference in behavior of the order parameter $\tilde{\eta}_1$ under the action of $\mathcal{T}$ allows us to separate out the real and imaginary part of the order parameter. They transform as follows

$$\tilde{\eta}_R \xrightarrow{\mathcal{T}} \tilde{\eta}_R \quad \tilde{\eta}_I \xrightarrow{\mathcal{T}} -\tilde{\eta}_I. \quad (1)$$

Since we want the A–B transition to break TRS we consider only the imaginary components of the order parameter. For the materials with a polar Kerr signal, the possible order parameters are further restricted depending on whether they are Kerr active or not, as demonstrated for UPt$_3$ in the text.

For the 3D $T_{1g/u}$ reps, we have two possible TRS A states the (1, 0, 0) state with $D_2(C_2) \times T$ symmetry and the (1, 1, 1) state with $C_3 \times T$ symmetry. Both of these allow for a transition to a TRSB B state which is Kerr active and hence provide two viable channels for the transition. In the case of $(1 + \tilde{\eta}_1, 0 + \tilde{\eta}_2, 0 + \tilde{\eta}_3)$, $\tilde{\eta}_1$ belongs to the $A_1$ Kerr inactive reps and hence is not considered, while $\tilde{\eta}_2$ and $\tilde{\eta}_3$ belong to the Kerr active $B_1$ and $B_2$ reps respectively. The form of the free energy will look similar to the 1D A–B transition in UPt$_3$, and the exact transition would depend on which rep has a higher $T_c$. The free energy will be

$$f_{A \rightarrow B} = \alpha_I \eta_2^2 + \beta_I \eta_3^4. \quad (2)$$

For the $(1 + \tilde{\eta}_1, 1 + \tilde{\eta}_2, 1 + \tilde{\eta}_3)$ state we have a 1D $A_1$ Kerr inactive order parameter defined as $\eta_A = \tilde{\eta}_1 + \tilde{\eta}_2 + \tilde{\eta}_3$ and which is ignored, and a 2D Kerr active $E$ order parameter, defined as

$$\eta_x = \frac{1}{\sqrt{6}}(2\tilde{\eta}_3 - \tilde{\eta}_2 - \tilde{\eta}_1), \quad \eta_y = \frac{1}{\sqrt{2}}(\tilde{\eta}_1 - \tilde{\eta}_2), \quad (3)$$

where $\eta_x, \eta_y$ belong to the 2D Kerr active $E$ reps of $C_3$. The free energy for this $E$ rep is

$$f_{A \rightarrow B}^{E} = \alpha_I \eta_x^2 + \beta_I (\eta_y^2)^2 + \gamma I \eta_x^2 (\eta_y^2)^2 + \gamma_1 \eta_x^2 (\eta_x^2 - 3\eta_y^2)^2 + \gamma_2 \eta_x^2 (3\eta_y^2 - \eta_x^2)^2 + \gamma_3 \eta_x^2 \eta_y^2 (\eta_x^2 - 3\eta_y^2)(3\eta_x^2 - \eta_y^2) \quad (4)$$

Once $\alpha_I$ changes sign the ground state will be $\eta = \eta_I(\cos \theta, \sin \theta)$, where the value of $\theta$ will depend on the value of the coefficients ($\gamma_I$) of the 6th order terms, and hence provides a viable mechanism for a transitions to a TRSB B phase.

For the 2D $E_{g/u}$ reps there are two possible TRS A states. We model the A–B transition as done before, with the A state being (1,0) possessing $D_4 \times T$ symmetry and (0,1) with $D_4^{(1)}(D_2) \times T$ symmetry [1]. The B state grows as $(1 + \tilde{\eta}_1, 0 + \tilde{\eta}_2)$, where $\tilde{\eta}_1$ belongs to the $A_1$ and $\tilde{\eta}_2$ belongs to $B_1$ reps of $D_4$, while for the (0,1) state, the situation is reversed. In that case the B state grows as $(0 + \tilde{\eta}_1, 1 + \tilde{\eta}_2)$, with $\tilde{\eta}_1$ having $B_1$ symmetry and $\tilde{\eta}_2$ belonging to the $A_1$ rep of $D_4$. The free energy will be the same as for the 1D order parameters

$$f_{A \rightarrow B} = \alpha_I \eta_1^2 + \beta_I \eta_1^4. \quad (5)$$

Interestingly due the absence of a Kerr measurement experiment, the $A_1$ rep is viable, and the same physics applies here as discussed for the $s + is$ states in the iron based superconductors [2,5]. These states are Kerr inactive, and can be ruled out depending on the result of a polar Kerr measurement in $U_{1-x}$Th$_x$Be$_{13}$.

For the 3D reps $T_{1g/u}$ and $T_{2u/9}$ there are four possible TRS A states, two for each $T$ reps, i.e. (1,0,0) and (1,1,1). However, as explained in the main text (1,0,0) is the only viable TRS A state which allows for a transition to a TRSB B state, due to the form of the coupling between superconductivity and AFM fluctuations. This state has
$D_4(C_4) \times \mathcal{T}$ and $D_4^{(2)}(D_2) \times \mathcal{T}$ symmetry for the $T_1$ and $T_2$ reps respectively. The A–B transition is modeled similar to PrOs$_4$Sb$_{12}$ i.e. $(1 + \tilde{\eta}_{11}, 0 + \tilde{\eta}_{21}, 0 + \tilde{\eta}_{31})$, except here $\tilde{\eta}_{11}$ belongs to the $A_1$ rep of $D_4$ and would again have the $s + is$ physics with the standard free energy for 1D reps

$$f_{A \rightarrow B} = \alpha I \tilde{\eta}_{11}^2 + \beta I \tilde{\eta}_{21}^4,$$  \hfill (6)

while $(\tilde{\eta}_{21}, \tilde{\eta}_{31})$ belong to the 2D Kerr active $E$ reps of $D_4$. The free energy for the $E$ rep is

$$f_{A \rightarrow B}^E = \alpha I \tilde{\eta}_i \tilde{\eta}_i + \beta_1 (\tilde{\eta}_i \tilde{\eta}_i)^2 + \beta_2 \tilde{\eta}_{21}^2 \tilde{\eta}_{31}^2.$$ \hfill (7)

For $\beta_2 > 0$ will pick the $\eta_{I}(1,0)$ and for $\beta_2 < 0$ the $\eta_{I}(1,1)$ state, both of which break time-reversal symmetry.

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