Spin-singlet and spin-triplet pairing correlations in antiferromagnetically coupled Kondo systems

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Recent experiments in quantum critical heavy fermion metals have pushed to the fore the question about whether antiferromagnetic fluctuations can promote both spin-singlet and spin-triplet superconductivity. Here we address the issue through non-perturbative calculations in antiferromagnetically correlated Kondo systems. We identify Kondo-destruction quantum critical points in both the SU(2) symmetric and Ising-anisotropic cluster Bose-Fermi Anderson models. The spin-singlet pairing correlations are significantly enhanced near the quantum critical point in the SU(2) case; however, with adequate but still realistic degree of Ising anisotropy, the spin-triplet pairing correlations are competitive. Our results demonstrate that spin-flip processes strengthen the spin-singlet pairing at the Kondo-destruction quantum critical points, and point towards a way for antiferromagnetic criticality to drive spin-triplet pairing. Further implications of our findings in the broader context of strongly correlated superconductivity are discussed.

Quantum criticality has the potential to be a unifying theme in strongly correlated metals [1, 2]. A quantum critical point (QCP) arises at the point of continuous transition between two different types of ground states. Various types of novel order, including unconventional superconductivity, may emerge in its vicinity [3]. The materials in which this physics may be relevant include the cuprates [4], organic superconductors [5], heavy fermion metals [6, 7], and iron-based superconductors [8].

Heavy fermion metals represent a particularly important case study for the connection between quantum criticality and unconventional superconductivity. There are a large number — about 50 — of them which superconduct. In many cases, superconductivity develops out of a strange metal normal state, which is often associated with a QCP at the border of an antiferromagnetic (AF) order. Prototype examples are CeCu2Si2 [9], and CeRhIn5 [10–12]. Recently, superconductivity has been discovered at ultra-low temperatures in the canonical quantum critical heavy fermion metal, YbRh2Si2, which exhibits AF order and a field-induced QCP [9]. In addition to the superconducting phase at zero field, which has been interpreted as arising from the intrinsic electronic quantum criticality unmasked by the hyperfine coupling to nuclear spins [13], a new superconducting phase occurs near the critical magnetic field [14]. The latter appears to have spin-triplet pairing, raising a profound question of how antiferromagnetic correlations can drive spin-triplet pairing in quantum critical Kondo systems.

To make progress, it is necessary to start from a proper description of the quantum criticality in the normal state. It has been recognized that heavy fermion quantum criticality can go beyond the Landau description based on the slow fluctuations of a spin-density-wave (SDW) order [15–17]. Instead, a Kondo-destruction type of QCP [18–20], which involves a partial-Mott (delocalization-localization) transition and a small-to-large Fermi surface jump, plays an important role [10, 11, 21–25]. Essentially, the Kondo effect is destroyed at the QCP by the dynamical magnetic fluctuations. As such, the 4f electrons that manifest as the Kondo-driven delocalized composite fermions in the paramagnetic phase become localized in the AF-ordered phase, leading to a sudden jump of the Fermi surface from large to small.

The questions are, then, two-fold. First, does the Kondo destruction QCP necessarily drive superconductivity? Second, under what conditions does the quantum criticality promote spin-singlet or spin-triplet Cooper pairing? Theoretically, this problem is challenging because in the quantum critical regime there is no well-defined quasi-particle anywhere on the Fermi surface. It is thus necessary to search for microscopic models which possess this kind of QCP so that pairing correlations can be studied in a concrete setting.

Both of these questions can be addressed within cluster Bose-Fermi Anderson/Kondo models (BFAM/BFKM). These models involve multiple local moments coupled to each other through a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and simultaneously to both fermionic and bosonic baths. The bosonic bath captures the dynamical magnetic fluctuations of a Kondo lattice model, and formally develops from the later through a cluster extended dynamical mean field approach (C-EDMFT) [26]. In the Ising limit (with infinite Ising anisotropy), the cluster BFAM has been studied by the continuous-time quantum Monte Carlo (CT-QMC) method for its quantum critical behavior and associated pairing correlations [27]. Going beyond the pure Ising case, one can expect that the spin-flip processes associated with the transverse component of the RKKY interaction will significantly influence the nature of the pairing that develops. However, this is a challenging problem, because the introduction of transverse exchange couplings requires a triple expansion in the CT-QMC approach. Recently, we have laid the groundwork by introducing an SU(2) CT-QMC method for a single-impurity
BFAM that involves a double expansion in the hybridization and transverse Bose-Kondo coupling [28] such that it accesses an extended dynamical range in the quantum critical regime (see also, Ref. [29]).

In this Letter, we carry out the first study of an SU(2) symmetric cluster BFAM as well as its spin-anisotropic counterpart with finite Ising anisotropy. To do so, we develop the aforementioned triple-expansion scheme within the CT-QMC approach. We identify a Kondo-destruction QCP in the SU(2) symmetric model. Near the QCP, we find that spin-singlet pairing correlations are significantly enhanced, more strongly than its Ising-anisotropic counterpart. At the same time, the spin-triplet pairing correlations are suppressed, which is to be contrasted with what happens in the realistically Ising-anisotropic case. We understand both features from the physics that spin-flip processes strengthen the spin-singlet pairing at the Kondo-destruction QCPs.

Model and solution methods: The two-impurity SU(2) BFAM Hamiltonian is

\[ H = \sum_{i,\sigma} \epsilon_d d_{i\sigma}^\dagger d_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + I \sum_\alpha S_{\alpha}^b S_{\alpha}^g \]

\[ + \sum_{\mathbf{k}, \sigma} c_k c_{\mathbf{k}\sigma} + \sum_{i,k,\sigma} \left( V_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger \phi_{i\sigma}^\dagger + h.c. \right) \]

\[ + \sum_{p,\alpha} \omega_p \phi_p^\dagger \phi_p + g \sum_{p,\alpha} \left( S_1^\alpha - S_2^\alpha \right) (\phi_p^\dagger + \phi_p). \] (1)

The first line describes the interactions among the local degrees of freedom: \( d_{i\sigma}^\dagger \) creates an electron on site \( i = 1, 2 \) with spin \( \sigma = \uparrow, \downarrow \). \( \epsilon_d \) is the onsite energy, \( U \) is the coulomb repulsion and \( I \) is the RKKY interaction between the two impurities. \( S_{\alpha}^b = \frac{1}{2} \sum_{\mu,\nu} d_{\mu\sigma}^\dagger \sigma_{\mu\nu}^b d_{\nu\sigma} \) is the spin operator and \( \sigma_{\mu\nu}^b \) are the Pauli matrices. The second line describes the fermionic bath and its coupling with the impurities: \( c_{\mathbf{k}\sigma} \) creates a conduction electron with wave vector \( \mathbf{k} \), spin \( \sigma \) and energy \( \epsilon_{\mathbf{k}} \), which hybridizes with the local \( d \) electron through the matrix element \( V \). The third line describes the 3-component vector bosonic bath and its coupling to the anti-ferro component of the two local moments through coupling constant \( g \). \( \alpha \) is the spin index and it is summed over \( x, y \) and \( z \) such that the Hamiltonian is SU(2) invariant. We will also consider the Ising-anisotropic version of the model (see below).

For the fermionic bath, we consider a flat density of states \( \rho_F(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k) = \rho_0 \Theta(|D - \epsilon|) \), with a hybridization function \( \Gamma(\epsilon) = \Gamma_0 \Theta(|D - \epsilon|) \) and \( \Gamma_0 = \pi \rho_0 V^2 \). In addition, the impurity location \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) are set to be infinitely separated to avoid double counting of the RKKY interactions. The bosonic bath takes a sub-ohmic density of states specified by \( \rho_B(\omega) = \sum_p \delta(\omega - \omega_p) = K_0 \omega^e e^{-\omega/\Lambda} \Theta(\omega) \). The prefactor \( \rho_0 \) and \( K_0 \) are determined by the normalization conditions: \( \int_{-\infty}^{D} \rho_F(\epsilon) d\epsilon = 1 \) and \( \int_{0}^{\infty} \rho_B(\omega) d\omega = 1 \). The BFAM can be solved by a recently developed sign-problem-free CT-QMC method. The triple expansion method builds on prior work that has dealt with various double expansions [28–30]. Further details of the method are described in the Supplementary Material. In the calculation, we set \( D = 1, \Lambda = 1 \), and preserve particle-hole symmetry by choosing \( U = -2 \epsilon_d = 0.1 \). In addition, we take a sub-ohmic bosonic bath with exponent \( s = 0.6 \) and fix the hybridization parameter \( \Gamma_0 = 0.5 \). The RKKY interactions \( I \) and bosonic coupling \( g \) are tuning parameters to explore phase diagram and search for QCPs.

Quantum critical properties: Fig. 1 shows the \( T = 0 \) phase diagram of SU(2) symmetric BFAM in the \( g^2 - I \) parameter space obtained from CT-QMC. In the absence of the bosonic bath, the model reduces to the two impurity Anderson model [31], which has a single QCP from Kondo screened phase at small RKKY interaction to an impurity singlet (IS) phase at large RKKY interaction. Turning on the bosonic coupling \( g \), we find that the transition persists with the same critical behavior but at a reduced critical value of \( I \). At large bosonic coupling, there will be a second transition from the IS phase to an antiferromagnetic local moment (LM) phase. For \( I \) smaller than 0.3, the IS phase disappears and we have a direct transition between a Kondo screened phase and the LM phase. This turns out to be a Kondo destruction QCP that has not been studied before.

Given its “beyond-Landau” nature, we characterize the Kondo-destruction QCP with fidelity susceptibility that directly evaluates the changes of wavefunctions and detects quantum phase transition without introducing any order parameters [32]. The fidelity susceptibility \( \chi_F \) is defined as the second derivative of fi-
delity’s logarithm, where the fidelity measures the distance between the ground-state wavefunctions at two different values of parameters $V, V + 6V$. This definition can be extended to finite temperature: 
\[ \chi_F = \int_0^{3/2} \left( \langle T_\tau H_V(\tau)H_V \rangle - \langle H_V \rangle^2 \right) \tau d\tau, \]
where $H_V$ includes all the terms in the Hamiltonian that are proportional to the hybridization strength $V$ [33, 34]. Due to the sharp changes of ground-state wavefunctions near the QCP, we observe a singular behaviors of $\chi_F$:
\[ \chi_F(\beta, g)/\beta = \beta^{2/\nu} \chi \left( \beta^{1/\nu}(g - g_c)/g_c + A/\beta^{\delta/\nu} \right), \]
with $g_c = 0.66(2)$ and $\nu^{-1} = 0.31(6)$. The critical value and critical exponent are obtained by fitting the numerical data as shown in Fig. 2 (a), (b). The scaling behavior is consistent with a continuous transition and, moreover, suggests that $V$ is a relevant perturbation at QCP. Thus, the transition is indeed a Kondo destruction QCP.

Besides, we study the Binder cumulants and correlation length of the spin correlation function (Supplementary Material). The results are consistent with the conclusions drawn above from the fidelity susceptibility.

To further characterize the QCP, we analyze the static spin susceptibility, defined as $\chi_s(\tau) = \int_0^\tau \chi_s(\tau^\prime) d\tau^\prime$. As seen in Fig. 2 (c), $\chi_s(\tau)$ diverges as $\chi_s(\tau) \sim T^{-z}$ with $x = 0.60(1)$ at the QCP. The result is consistent with the relation $x = s$, suggesting that the critical behavior in the spin channel is completely determined by the properties of the bosonic bath. Note that this is one of the necessary conditions for the Kondo-destruction QCP to be realized in the lattice case [18].

Pairing susceptibilities: Within our 2-site construction we can study four different types of inter-site pairing, specified by the following pairing operators: 
\[ \Delta^{\uparrow\uparrow}(\tau, \pm 1) = \Delta^{\uparrow\downarrow}(\tau, 0) = \frac{\Delta^{\uparrow\downarrow}(\tau, 1) + \Delta^{\downarrow\uparrow}(\tau, 1)}{\sqrt{2}}, \]
and
\[ \Delta^{\uparrow\downarrow}(\tau, s, 0) = \frac{\Delta^{\uparrow\downarrow}(\tau, s, 1)}{\sqrt{2}}, \]
with $\Delta^{\uparrow\downarrow}(\tau, s, 1)$ for $\sigma, \sigma' \in \{\uparrow, \downarrow\}$. They are, respectively, the pairing operators in the triplet channel with $m_{tot}^z = \pm 1$, $m_{tot}^z = 0$ and the singlet channel with $m_{tot}^z = 0$, where $m_{tot}^z$ is the $z$ component of the total spin of the cooper pair. Accordingly we can define the dynamic and static pairing correlation functions respectively:
\[ \chi^{(a, m)}(\tau) = \langle T_\tau \Delta^{(a, m)}(\tau) \Delta^{(a, m)}(0) \rangle, \]
\[ \chi^{(a, m)}(T) = \int_0^\tau \chi^{(a, m)}(\tau) d\tau. \]

We study the behavior of the pairing susceptibility following a particular cut $(g^2, I) = (2.22\lambda, \lambda)$ illustrated in Fig. 2. This cut mimics the trajectories of the C-EDMFT self-consistent calculation, and will meet the line of Kondo destruction QCPs at $\lambda = \lambda_c = 0.2$. As shown in Fig. 3(a), the pairing susceptibility in the singlet channel $\chi^{(s, 0)}(0)$ increases as we move from the Kondo screened phase to the QCP, and is peaked slightly before the transition. There is also a large enhancement near the QCP as we lower the temperature: $\chi^{(s, 0)}(\tau)$ acquires a large anomalous dimension at the critical fixed point. In Fig. 3(b) we plot $\chi^{(s, 0)}(\tau)$ against the conformal form $\chi^{(s, 0)}(\tau) \sim (\pi T / \sin(\pi T))^{2-\eta}$. We observe a collapse across different temperatures, which suggests that $\chi^{(s, 0)}(\tau) \sim 1/\tau^{2-\eta}$, with an anomalous exponent $\eta \approx 0.6$.

At the same time, we find that the pairing susceptibility in the triplet channel is strongly suppressed and does not acquire any anomalous dimension.

SU(2) vs. Ising-anisotropic model For the SU(2) model, Fig. 4(a) displays the evolution of the pairing susceptibilities across the QCP. It clearly shows the enhancement of the spin-singlet pairing correlation near the QCP, and the concomitant suppression of the spin-triplet pairing correlation in all the three (degenerate) channels.

We now consider an Ising-anisotropic model. The extreme Ising-anisotropic model of Ref. [27] corresponds to having only the Ising component for both the bosonic-Kondo coupling and RKKY interaction. More realistically, we consider the model whose effective RKKY interaction is written in an anisotropic form:
\[ J_s S_1^z S_2^z + J_p (S_1^x S_2^x + S_1^y S_2^y). \]
Here $J_z$ and $J_p$ are respectively the longitudinal and spin-flip RKKY exchange interactions. The details of the model are described in the Supplementary Material.

We consider the parameters such that the Ising anisotropy near the QCP has a realistic $J_p/J_z \approx 0.2$. Fig. 4(b) shows that the pairing correlation in the $S_z = 0$ triplet channel is enhanced near the QCP, along with the spin-singlet pairing correlation. (By contrast, the pairing correlations in the $S_z = \pm 1$ triplet channels are suppressed.) In the case of extreme Ising anisotropy, with $J_p = 0$, the two dominant pairing susceptibilities are exactly equal to each other. Here, the pairing susceptibility in the $S_z = 0$ triplet channel is almost equal to its counterpart in the spin-singlet channel. An analysis of the Landau free-energy functional shows that, a Zeeman coupling will further enhance the $S_z = 0$ spin-triplet channel over the spin-singlet channel, thereby making the spin-triplet pairing dominate.

**Discussion and Summary:** Our findings shed light on the recent experiment in YbRh$_2$Si$_2$ near its field-driven QCP [13]. YbRh$_2$Si$_2$ has antiferromagnetic order at the ambient conditions. It has a strong $xy$-anisotropy in the spin space, which is turned to Ising-anisotropic by the applied magnetic field. Our results for the Ising-anisotropic cluster BFAM with an AF RKKY interaction suggest that the $S_z = 0$ spin-triplet pairing channel will be competitive against the spin-singlet pairing near the Kondo-destruction QCP, and can be further turned into the dominant pairing channel by the Zeeman coupling of the critical magnetic field. This provides a natural understanding of the surprising experimental results.

By contrast, when the spin anisotropy is relatively weak, our results derived from the SU(2) symmetric cluster BFAM suggests that the spin-singlet pairing dominates. This result lays the groundwork for the understanding of the superconductivity that has been experimentally observed in a host of antiferromagnetically correlated heavy fermion metals, such as CeRhIn$_5$ and CeCu$_2$Si$_2$.

Our results also shed light on other classes of strongly correlated metals. For example, UTe$_2$ has a strong Ising anisotropy in its spin response [38]. Recent inelastic neutron scattering experiments [37] show that both the normal and superconducting states are antiferromagnetically correlated; this raises the exciting possibility that, here too, antiferromagnetic correlations are primarily responsible for the potential spin-triplet pairing.

Going beyond the heavy-fermion context, the electronic delocalization-localization effect has been implicated by experiments in both the hole-doped cuprates [38] and organic charge-transfer salts [39]. Recently, based on analyses of related dynamical equations, it has been suggested that beyond-Landau quantum criticality that bears similarities to the Kondo-destruction QCP operates in doped Mott insulators [40]. These calculations have stayed at the spin-rotational invariant level. Our results suggest that in these models too, it would be instructive to analyze the role of spin anisotropy that may arise in doping Mott insulators such as Sr$_2$IrO$_4$.

To summarize, we have studied a cluster Bose-Fermi Anderson model as an effective Kondo system for beyond-Landau quantum criticality. In both the SU(2) symmetric and Ising anisotropic models, we identify Kondo-
destruction quantum critical points. The spin-singlet pairing correlations are more strongly enhanced near the QCP in the SU(2) symmetric case than its Ising-anisotropic counterpart. This reveals that spin-flip processes strengthen the spin-singlet pairing. In accordance with this insight, we find the $S_z = 0$ spin-triplet pairing channel to be competitive in the realistically Ising-anisotropic version of the model. The results provide a natural understanding of the recent experiments on the anisotropic version of the model. The results provide a natural understanding of the recent experiments on the anisotropic version of the model.

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CONTINUOUS-TIME QUANTUM MONTE CARLO METHOD

In the continuous-time quantum Monte Carlo method, we perform a unitary transformation [41, 42] to remove the $z$ component spin-boson coupling, using the generator $\mathcal{S} = g(S^z_1 - S^z_2) \sum_p \frac{1}{2} \phi^\dagger_p \phi_p$. The new Hamiltonian $\hat{H} = e^\mathcal{S} He^{-\mathcal{S}}$ can be separated into two parts $\hat{H}_0 + \hat{H}_1$, where $\hat{H}_0 = \epsilon_d \hat{d}^\dagger \hat{d}_\sigma + \sum_i \hat{U} n_{i\uparrow} n_{i\downarrow} + \hat{I} S^z_1 S^z_2 + \sum_{k,\sigma} c_k c^\dagger_k c_k \sigma + \sum_{p,\alpha} \omega_p \phi^\dagger p \phi_p$, $\hat{H}_1 = \sum_i (H_{e,i} + (-1)^i + H_{b,i}) + H + h.c.$, with $H_{e,i} = \sum_{k,\sigma} V(\sigma) d^\dagger_i c^\dagger_k c_{k\sigma}$, $H_{b,i} = g S^z_i \Phi_i$, and $H_1 = (I/2) \hat{S}^z_1 \hat{S}^z_2$. Here $\hat{d}_\sigma = e^{\epsilon_d \hat{d}_\sigma e^{-\frac{i}{2} \hat{S}^z_1}}$, $\sum_p \frac{1}{2} (\phi^\dagger_p - \phi_p)$ is the dressed fermionic operator, with $s_{\sigma} = \pm 1$ for $\sigma = \uparrow / \downarrow$ and $p_i = \pm 1$ for $i = 1, 2$. $\hat{S}^+_i = \hat{d}^\dagger_i \hat{d}_i$, $\Phi_i = 1/\sqrt{2} \sum_p ((\phi^\dagger_p + \phi_p) - i (\phi^\dagger_p - \phi_p))$. $\hat{U}$, $\hat{d}_\sigma$ and $\hat{I}$ are the renormalized coupling constant, given by $\hat{U} = U + (g^2/2) \sum_p 1/\omega_p$, $\hat{c}_\sigma = \epsilon_d - (g^2/4) \sum_p 1/\omega_p$ and $\hat{I} = I + 2g^2 \sum_p 1/\omega_p$.

Now, we are able to express the partition function $Z$ in terms of an expansion of $\hat{H}_1$ under the interaction representation of $\hat{H}_0$,

$$Z = \sum_{n_1, n_1', n_2, n_2'} (-1)^p \times \text{Tr} [e^{-\beta \hat{H}_0 \mathcal{T}}]$$

$$\times \frac{1}{n!} \left( \int_0^\beta H^I_i(\tau)d\tau \right)^{n_1} \left( \frac{1}{\hat{N}!} \left( \int_0^\beta H^I_i(\tau)d\tau \right)^{\hat{N}} \right)^{n_1'} \times \prod_{i=1,2} \frac{1}{n_i!} \left( \int_0^\beta H_{c,i}(\tau)d\tau \right)^{n_i} \frac{1}{\hat{N}_i!} \left( \int_0^\beta H_{c,i}(\tau)d\tau \right)^{\hat{N}_i} \times \frac{1}{n_b!} \left( \int_0^\beta H_{b,i}(\tau)d\tau \right)^{n_b} \frac{1}{\hat{N}_b!} \left( \int_0^\beta H_{b,i}(\tau)d\tau \right)^{\hat{N}_b}$$

(4)

where $p = n_1 + n_1' + n_2 + n_2' + n_i + n_I + n^{\prime I}$. Then each term in the expansion is sampled by the Metropolis-Hastings algorithm [43, 44].

The $(-1)^p$ factor in the expression could potentially cause a sign problem. However, it is always positive in this model. Notice that the number of conduction electrons at each site is a conserved quantity, meaning that $n^\xi = n^\xi'$. Besides, $S^z_1$, $S^z_2$, and number of bosons are all conserved quantity, such that $n_1 + n^i = n_1' + n', n_2 + n^I = n_2' + n^I$, and $n_1 + n_2 = n_1' + n_2'$. Under these conditions, $p$ is always even and thus $(-1)^p = 1$.

QUANTUM PHASE TRANSITION

To further establish the presence of a QCP between the Kondo screened phase and the LM phase, we calculate the Binder cumulant for a 3 components order parameter, $U_2 = 5/2 - 3/2(m \cdot \mathbf{m})^2/2(m \cdot \mathbf{m})^2$, and correlation length exponent $\xi$ of staggered spin correlation function $\chi^\xi(\tau)$ [45, 46]. Here $\mathbf{m}$ is the staggered magnetization with $m^\alpha = \langle \frac{1}{2} \int_0^\beta (S^\alpha_1(\tau) - S^\alpha_2(\tau)) d\tau \rangle$ and $\chi^\xi(\tau) = \langle \mathcal{T}_\tau (S^z_1(\tau) - S^z_2(\tau)) (S^z_1 - S^z_2) \rangle$ [28].

At the transition from Kondo screened to LM phase, both $U_2$ and $\xi/\beta$ should display a crossing at the critical coupling $g = g_c$, or in other words, become independent of $\beta$, the system size. As shown in Fig.3(a)(b), this is indeed what we have observed, where we plot $U_2$ and $\xi/\beta$ versus tuning parameter $g$ for various choices of $\beta$. In fact, the finite-size scaling hypothesis at a second-order QCP predicts that they should be described by the following scaling form near the QCP,

$$U_2(g, \beta) = \hat{U}_2 \left( \beta^{1/\nu} (g - g_c)/g_c + A/\beta^{\phi/\nu} \right),$$

(5)

$$\xi(g, \beta) = \hat{\xi} \left( \beta^{1/\nu} (g - g_c)/g_c + A/\beta^{\phi/\nu} \right).$$

(6)

$\hat{U}_2$ and $\hat{\xi}$ are universal functions, $g_c$ the critical coupling, $\nu$ the correlation length exponent. The term $A/\beta^{\phi/\nu}$ captures the correction to scaling from the leading irrelevant operator. By performing scaling collapse analysis, we find the optimal choices for $g_c$ and $\nu$ are $g_c = 0.66(1)$, $\nu^{-1} = 0.34(4)$ (from $U_2$) and $g_c = 0.67(1)$, $\nu^{-1} = 0.36(4)$ (from $\xi$). From this we estimate the actual critical value to be $g_c = 0.665(5)$ and the correlation length exponent of the Kondo destruction QCP to be $\nu^{-1} = 0.35(5)$, which are consistent with the results derived from fidelity susceptibility $\chi_F$. The discrepancy is due to the larger scaling corrections of $\chi_F$. 
To measure the pairing susceptibility, we use the formula of the four-point correlation function shown in Ref. [47]. However, due to the infinite separation in the SU(2) case, \( \langle T_\tau \Delta_{\downarrow \uparrow}^\dagger (\tau) \Delta_{\uparrow \downarrow} (\tau) \rangle \) and \( \langle T_\tau \Delta_{\uparrow \downarrow}^\dagger (\tau) \Delta_{\downarrow \uparrow} (\tau) \rangle \) cannot be measured via this formula, since they do not conserve the occupation number of \( d_{\sigma \sigma'} \). We can then utilize the SU(2) symmetry and obtain these pairing susceptibilities via:

\[
\langle T_\tau \Delta_{\downarrow \uparrow}^\dagger (\tau) \Delta_{\uparrow \downarrow} (\tau) \rangle = \langle T_\tau \Delta_{\uparrow \uparrow}^\dagger (\tau) \Delta_{\uparrow \uparrow} (\tau) \rangle - \langle T_\tau \Delta_{\uparrow \downarrow}^\dagger (\tau) \Delta_{\downarrow \uparrow} (\tau) \rangle
\]

and

\[
\langle T_\tau \Delta_{\uparrow \downarrow}^\dagger (\tau) \Delta_{\downarrow \uparrow} (\tau) \rangle = \langle T_\tau \Delta_{\downarrow \downarrow}^\dagger (\tau) \Delta_{\downarrow \downarrow} (\tau) \rangle - \langle T_\tau \Delta_{\downarrow \uparrow}^\dagger (\tau) \Delta_{\uparrow \downarrow} (\tau) \rangle.
\]

[48]
The Hamiltonian of Ising anisotropic BFAM is

\[ H = \sum_{i,\sigma} \epsilon_{d_\sigma} d_i^\dagger d_i + \sum_i U n_i \bar{n}_i + IS_i^z S_2^z \]

\[ + \sum_{k,\sigma} \epsilon_{k\sigma} c_k^\dagger c_{k\sigma} + \sum_{i,k,\sigma} \left( V e^{ik \cdot r_i} d_i^\dagger c_{k\sigma} + h.c. \right) \]

\[ + \sum_p \omega_p \phi_p^\dagger \phi_p^z + g \sum_p (S_i^z - S_2^z)(\phi_p^z + \phi_p^\dagger) \].

(7)

where only \( z \)-component of RKKY interaction and spin-boson coupling are kept. The effect of conduction electrons is described by two hybridization functions

\[ \Gamma(\epsilon) = \pi V^2 \sum_k \delta(\epsilon - \epsilon_k) \approx \Gamma_0 \Theta(D - |\epsilon|) \]

\[ \Gamma_a(\epsilon) = \pi V^2 \sum_k \delta(\epsilon - \epsilon_k) \cos(k \cdot (r_1 - r_2)) \approx \gamma \epsilon \Gamma_0 \Theta(D - |\epsilon|) \],

(8)

where \( \Gamma(\epsilon)(\Gamma_a(\epsilon)) \) describes the effective hybridization from fermionic bath between two \( d \) electrons of the same (different) sites [49]. By tuning parameter \( \gamma \), we are able to change the separation between two \( d \) electrons: \( \gamma = 0 \) denotes infinite separation \( |r_1 - r_2| = \infty \) and \( \gamma = 1 \) represents \( |r_1 - r_2| = a \) with \( a \) the lattice spacing. The finite separation generates an effective SU(2)-symmetric Heisenberg interactions of strength \( 2 \gamma^2 \Gamma^2/(\pi^2 U) \) between two \( d \) electrons. Thus, we can estimate the effective spin-spin interactions \( \tilde{J}_z S_i^z S_2^z + \tilde{J}_p (S_i^x S_2^x + S_i^y S_2^y) \) from fermionic bath, bosonic bath and RKKY interactions: \( \tilde{J}_z = I_z + 2 \gamma^2 + 2 \gamma^2 \Gamma^2/(\pi^2 U) \) and \( \tilde{J}_p = 2 \gamma^2 \Gamma^2/(\pi^2 U) \). In the calculation, we take \( \gamma = 0.2 \) and quantify the Ising anisotropy near QCP \( \tilde{J}_p/J_z \approx 0.2 \). Other parameters are taken to be \( U = -2 \epsilon_d = 0.001, \Gamma = 0.25, s = 0.8, D = 1, \Lambda = 1 \)