Bose-Fermi Anderson model with SU(2) symmetry: Continuous-time quantum Monte Carlo study
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I. INTRODUCTION

Heavy fermion systems serve as a prototype setting to study quantum criticality\(^1\). Experimental discoveries in various heavy fermion compounds open up the opportunity to explore beyond-Landau type quantum critical points (QCP) in the context of antiferromagnetic Kondo lattice systems. One prominent example is the Kondo destruction QCP\(^1\), where the phase transition at zero temperature not only involves the magnetic order parameter, but also the localization to delocalization transition of the 4 electrons constituting the local moments. Some of the hallmarks of the Kondo destruction type QCP are \(\omega/T\) scaling of the dynamical spin susceptibility as seen from inelastic neutron scattering, and jump of the fermi surface volume from magnetotransport and quantum oscillation measurements\(^6\). Such properties are inconsistent with predictions from the traditional description within the Landau framework, the spin-density-wave type QCP\(^7\)–\(^9\).

One of the simplest models that contain a Kondo destruction type QCP is the Bose-Fermi Kondo model (BFKM)\(^10\). It arises in the context of understanding the competition between Kondo effect and magnetic fluctuations in Kondo lattice model using extended dynamical mean field theory (EDMFT)\(^3\)\(^,\)\(^11\). It describes a local moment coupled to both itinerant electrons as well as free bosons, which are usually referred to as fermionic bath and bosonic bath. Typically the fermionic bath will assume a constant density of states, and the bosonic bath has a sub-ohmic spectrum: its density of states at low frequencies \(\rho_b(\omega)\) has a power-law form, \(\rho_b(\omega) \propto \omega^s\) with \(s < 1\). It characterizes the softened spectrum of the magnons near the magnetic QCP, which compete with the conduction electrons in their couplings to the local moment and causes the suppression of the Kondo effect.

This model is first treated with \(\epsilon\)-expansion renormalization group (RG) method, using \(\epsilon = 1 - s\) as a small parameter\(^3\)\(^,\)\(^11\)–\(^16\). It turns out the fixed points structure will depend on the symmetry of the spin boson coupling: for the SU(2) and XY symmetric cases, it has a Kondo screened stable fixed point (K) at strong coupling, a bosonic bath dominated stable fixed point (L) at intermediate coupling (so called critical phase), and an unstable critical point (C) describing the quantum phase transition. Both L and C can be accessed by the \(\epsilon\)-expansion; for the Ising anisotropic case, on the other hand, the critical phase controlled by L is unstable and is replaced by the local moment fixed point (L') at strong coupling. In all three cases, it is predicted that at the critical point (C) where the Kondo effect is critically destroyed, the local spin correlation function will behave as \(\chi_{\text{spin}}(\tau) \sim (1/\tau)^\eta\), with an exact relation \(\eta = \epsilon\)\(^15\)\(^,\)\(^16\). This has important implications for the EDMFT calculation of the Kondo lattice problem. For two dimensional magnetic fluctuations, it predicts a Kondo destruction QCP solution, provided that the relation \(\eta = \epsilon\) will remain valid at \(\epsilon \to 1\)\(^-\)\(^3\)\(^,\)\(^11\).

The numerical calculations of the Bose-Fermi Kondo model and the closely related Bose-Fermi Anderson model (BFAM) include treating it either as a standalone model using numerical renormalization group (NRG)\(^17\)\(^,\)\(^18\) and continuous-time quantum Monte Carlo (CT-QMC)\(^19\)\(^–\)\(^21\), or as an effective model under EDMFT\(^22\)\(^–\)\(^25\). Our focus in this work is on the CT-QMC method, from which a seeming controversy existed for...
the SU(2) symmetric BFAM: for \( s = 0.2 \), it was shown\(^\text{11} \) that the Kondo-destruction phase has the local-moment character instead of being critical; in the temperature dependence of the local spin susceptibility in this Kondo-destruction phase, it was found \( \chi^{\text{spin}} \sim 1/T \) instead of the \( \chi^{\text{spin}} \sim 1/T^\nu \) behavior predicted by \( \epsilon \)-expansion RG\(^\text{15,16} \) for the fixed point L.

To resolve this seeming inconsistency, we start with the observation that, if \( s \) is close to 1, the CT-QMC result must be consistent with that of the \( \epsilon \)-expansion RG in the range of coupling constants accessed by this expansion (again \( \epsilon = 1 - s \)). To make progress, in this article we develop the CT-QMC procedure for the BFAM such that it can reach sufficiently low temperatures while preserving the SU(2) symmetry. Using this procedure, we carry out a comprehensive study of the SU(2) BFAM for \( s \) ranging from close to 0 to close to 1. We study a variety of observables in order to identify all the QCPs between different phases, combined with detailed finite size scaling analysis to extract critical exponents.

Our analysis shows that the \( \epsilon \)-expansion\(^\text{15,16} \) and CT-QMC results are fully compatible with each other. Our results are summarized by the RG-flow diagrams of figure 1. We find that the fixed point structure will depend on the value of the bosonic bath exponent \( s \). For the \( s > s^* \) regime, we identify i) the critical point C separating the Kondo screened phase controlled by strong coupling fixed point K and critical phase governed by the intermediate coupling stable fixed point L, as predicted from \( \epsilon \)-expansion RG for the coupling constants accessible by the latter method; and ii) a separate critical point C’ and local moment fixed point L’, which occurs for larger values of the bosonic-Kondo coupling \( g \) inaccessible by \( \epsilon \)-expansion RG. For \( s < s^* \), the intermediate coupling fixed point L and the associated Kondo destruction fixed point C disappears, and there exists only a type ii) quantum phase transition C’ We also determine the correlation length exponent \( \nu \) at both C and C’ and show that they are indeed distinct. On the other hand, the anomalous dimension \( \eta \) in the critical spin correlation function at C and C’ are the same: they both satisfy the relation \( \eta = 1 - s \) within numerical uncertainty. Additionally, we find another unstable fixed point LC that controls the transition between the fixed points L and L’. Finally, we quantitatively estimate \( s^* \) (c.f. figure 15).

The remainder of the paper is organized as follows. In Sec. II we introduce the SU(2) Bose-Fermi Anderson model, and give an overview of the CT-QMC method as well as the physical quantities we will investigate in this work. We will present the numerical results in Sec. III. We will start with a detailed study for the \( s = 0.6 \) case in Sec. IIIA, followed by the \( s = 0.2 \) case in Sec. IIIB, before carrying through the analysis that leads to an estimate for the value of \( s^* \) in Sec. IIIC. We will discuss the implication of our results in Sec. IV and conclude the article in Sec. V.

II. MODEL AND METHOD

The Hamiltonian for the SU(2) symmetric BFAM reads,

\[
H = H_e + H_b + H_d + H_g + H_V, \tag{1}
\]
where $H_c$ and $H_b$ describes the bosonic and fermionic bath part, respectively,

$$H_c = \sum_{k, \sigma} \epsilon_k c_{k, \sigma}^{\dagger} c_{k, \sigma}, \quad H_b = \sum_{\alpha} H_{b\alpha} = \sum_{p, \alpha} \omega_p \phi_p^{\alpha\dagger} \phi_p^\alpha. \quad (2)$$

$H_d$ contains the local electron part,

$$H_d = \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\downarrow} d_{\downarrow}^{\dagger} d_{\uparrow}.$$

$H_V$ and $H_g$ couples the local orbital to the bosonic and fermionic bath,

$$H_V = \sum_{k, \sigma} V d_{\sigma}^{\dagger} c_{k, \sigma} + h.c., \quad H_g = \sum_{p, \alpha} g S_\alpha (\phi_p^{\alpha\dagger} + \phi_{-p}^\alpha) \quad (3)$$

where the summation over $\alpha$ runs through $x, y, z$, $S_\alpha = \sum_{\sigma, \tau} d_{\sigma}^{\dagger} \tau_{\sigma\tau}^{\alpha} d_{\sigma}$, and $\tau_{\sigma\tau}^{\alpha}$ being the three components of the Pauli matrices.

The properties of the fermionic and bosonic bath are specified by their density of states. For the fermionic bath, we choose a constant density of states,

$$\rho_F(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k) = \rho_0 \Theta(|D - \epsilon|), \quad (4)$$

which leads to a hybridization function $\Gamma(\epsilon) = \Gamma_0 \Theta(|D - \epsilon|)$, with $\Gamma_0 = \pi \rho_0 V^2$.

Unless specified otherwise, the density of states for the sub-Ohmic bosonic bath has an exponential cutoff, given by the following,

$$\rho_b(\omega) = \sum_q \delta(\omega - \omega_q) = K_0 (\omega / \Lambda)^q e^{-\omega / \Lambda} \Theta(\omega). \quad (5)$$

Throughout the text we fix $D = 1$, $\Lambda = 1$, and stays at the particle-hole symmetric point $U = -2\epsilon_d = 0.1$. The prefactor $\rho_0$ and $K_0$ in the density of states of the fermionic bath and bosonic bath are determined from the normalization condition $\int_{-D}^{D} \rho_F(\epsilon) d\epsilon = 1$ and $\int_0^\infty \rho_b(\omega) d\omega = 1$. We will use either the amplitude of the hybridization function $\Gamma_0$ or the spin-boson coupling $g$ as our tuning parameter.

**A. Monte-Carlo procedure**

We will employ the CT-QMC algorithm, first introduced in reference 26,27 and then generalized to treat the BFAM in references 19–21. We start with removing the $z$ component of the spin-boson coupling by employing a Firsov-Lang transformation $\tilde{H} = e^S H e^{-S}$ with $S = g S_\Sigma \sum_p \frac{1}{\omega_p} (\phi_p^{\uparrow\dagger} + \phi_{-p}^{\downarrow})$ (similar to Ref. 28) and work with the transformed Hamiltonian $\tilde{H}$,

$$\tilde{H} = H_c + H_b + H_d + H_V + H_g$$

$$\tilde{H}_d = \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^\dagger d_{\downarrow} d_{\downarrow}^{\dagger} d_{\uparrow}$$

$$\tilde{H}_V = V \sum_{k, \sigma} (d_{\sigma}^{\dagger} c_{k, \sigma} + \sum_{\epsilon} \frac{2}{\omega_p} (\phi_{\sigma}^{\dagger} - \phi_{\sigma}^\dagger) + h.c.)$$

$$\tilde{H}_g = \sum_{p} (g \sqrt{2}) (S_\uparrow \phi_p^{\uparrow\dagger} e^{-\sum_{\epsilon} \frac{2}{\omega_p} (\phi_{\uparrow}^{\dagger} - \phi_{\uparrow}^\dagger)} + S_\downarrow \phi_p^{\downarrow\dagger} e^{-\sum_{\epsilon} \frac{2}{\omega_p} (\phi_{\downarrow}^{\dagger} - \phi_{\downarrow}^\dagger)}), \quad (6)$$

where we have defined the renormalized parameters $\tilde{\epsilon}_d = \epsilon_d - (g^2 / 4) \sum_q (1 / \omega_q)^2$, $\tilde{U} = U + (g^2 / 2) \sum_q (1 / \omega_q)^2$, $s_{\sigma} = \pm 1 / 2$ for $\sigma = \uparrow / \downarrow$, and recombined the $x$ and $y$ components of $S_\alpha$ and $\phi_\alpha$ into $S_\alpha = d_\alpha^\dagger d_\alpha$, $S_{\alpha} = d_\alpha^\dagger d_\alpha$, $\phi_\alpha = (1 / \sqrt{2}) (\phi_{\alpha}^{\uparrow} + \phi_{\alpha}^{\downarrow}) \pm i (\phi_{\alpha}^{\uparrow} - \phi_{\alpha}^{\downarrow})$. The partition function is constructed by expanding in the non-diagonal terms 19–21, 26,27, $H_V$ and $H_g$ under the interaction representation of $H_0 = \tilde{H}_b + H_c + \tilde{H}_d$. It has the following form 19–21.

$$Z = Z_0 \sum_m \int \prod_{i=1}^{m} d\tau_{\uparrow}^{i} d\tau_{\downarrow}^{i} \prod_{\sigma = \uparrow, \downarrow} \prod_{i=1}^{n_\sigma} \left( \int \prod_{i=1}^{n_\sigma} d\tau_{\sigma}^{i} d\tau_{\bar{\sigma}}^{i} \right)$$

$$w_d(\{\tau^{tot}\}_{n_{tot}}) \prod_{\sigma = \uparrow, \downarrow} \prod_{i=1}^{n_\sigma} \left( \int \prod_{i=1}^{n_\sigma} d\tau_{\sigma}^{i} d\tau_{\bar{\sigma}}^{i} \right)$$

where $Z_0 = Tr[e^{-\beta H_\Sigma}] | Tr[e^{-\beta H_b}] | Tr[e^{-\beta (H_c + H_d)}]$ is the partition function of the bath, $\beta$ being the inverse temperature: $\beta = \frac{1}{T}$. $\int \prod_{i=1}^{n_\alpha} d\tau_{\sigma}^{i} d\tau_{\bar{\sigma}}^{i} = \int_{0}^{\beta} d\tau_{\sigma}^{1} \cdots \int_{0}^{\beta} d\tau_{\sigma}^{n_\alpha} \int_{0}^{\beta} d\tau_{\bar{\sigma}}^{1} \cdots \int_{0}^{\beta} d\tau_{\bar{\sigma}}^{n_\alpha}$. $\{\tau^{\alpha}\}_n$ denotes the set of imaginary time of all the operators of a given type $\alpha$ in the expansion: $\{\tau^{\alpha}\}_n = \{\tau^{\sigma}_1, \tau^{\bar{\sigma}}_1, \ldots, \tau^{\sigma}_n\}$. $\alpha \in \{s, s', d\sigma, d\bar{\sigma}\}$ represents $S_\uparrow, S_\downarrow, d_\uparrow^\dagger, d_\downarrow^\dagger$, or $d_\sigma, d_{\bar{\sigma}}, n = m$ or $n_\sigma$ denotes the number of pairs of $S_+, S_-$ or $d_\uparrow^\dagger, d_\downarrow^\dagger$, also labeling the expansion order. $\{\tau^{tot}\}_{n_{tot}}$ refers to all the $\{\tau^{\alpha}\}_n$ combined, with $n_{tot} = 2(\sum_n n_\sigma + m)$. The integrand, or so-called weight, factorizes into multiple components. In the following we will present the form of each part explicitly.

$$w_d(\{\tau^{tot}\}_{n_{tot}})$$

is the contribution from the local d electron part. It describes valence spin fluctuations of the local orbitals,

$$w_{d}(\{\tau^{d\sigma}\}_{n_\sigma}, \{\tau^{d\bar{\sigma}}\}_{n_\sigma})$$

is the contribution from the
conduction electron with spin index $\sigma$,

$$w_c^\sigma = V^{2n_a} \left( \prod_{s=1}^{n_a} \sum_{k,k'} Tr [T_T e^{-\beta H_i} c_{k,\sigma} (\tau^{d\sigma}_{n_a}) \times c_{k',\sigma} (\tau^{d\sigma}_{n_a})] / Tr [e^{-\beta H_i}] \right) = \det (F^\sigma).$$

It can be expressed as a determinant of matrix $F^\sigma$, whose matrix element is given by

$$F^\sigma_{ij} = \sum_k V^2 Tr [e^{-\beta H_i} T_T c_{k,\sigma} (\tau^{d\sigma}_{j}) c_{k',\sigma} (\tau^{d\sigma}_{i})] / Tr [e^{-\beta H_i}],$$

(9)

$$w_z (\{\tau^{tot}_i\}_{i=1}^{n_{tot}})$$

comes from the $z$ component bosonic bath part$^{19,20}$,

$$w_z = Tr [e^{-\beta H_i} \prod_{i=1}^{n_{tot}} \sum_{\{s\}} \sum_{\{\tau^{tot}_i\}} (s^g/\omega_T) (\phi^p (\tau^{tot}_i) - \phi^\dagger (\tau^{tot}_i))] / Tr [e^{-\beta H_i}]$$

$$= \exp \left( -g^2 \sum_{1<i<j<n_{tot}} s_i s_j (B(\tau_i - \tau_j) - B(0)) \right),$$

where $s_i = \pm s_a$ or $\pm 1$ when the operator $O (\tau^{tot}_i)$ at $\tau^{tot}_i$ corresponds to $d^\dagger / d_{\sigma}$ or $S^\dagger$, and

$$B(\tau_j - \tau_i) = \sum_p Tr [T_T e^{-\beta H_i} \phi^p_T (\tau_i) \phi^\dagger (\tau_j)] / \omega^2 \text{Tr} [e^{-\beta H_i}] + (\tau_i \leftrightarrow \tau_j).$$

(11)

Finally, $w_p (\{\tau^p\}_m, \{\tau^s\}_m)$ involves the bosonic bath in the transverse direction$^{21}$, forming a permanent,

$$w_p = (g/\sqrt{2})^m \left( \prod_{i=1}^m \sum_{p_i,p'_i} Tr [e^{-\beta (H_i + H_H)} T_T \phi^p_T (\tau^p_m) \times \phi^\dagger (\tau^s_m)] / \omega^2 \text{Tr} [e^{-\beta (H_i + H_H)}] \right)$$

$$= \sum_{p \in S_m} \prod_{i=1}^m P_{i,p}(i).$$

(12)

The summation extends over $S_m$, representing all permutations of $1, 2, \cdots, m$. The matrix element of $P$ is the following,

$$P_{ij} = (g^2/2) \sum_p Tr [e^{-\beta (H_i + H_H)} T_T \phi^p_T (\tau^p_j) \phi^\dagger (\tau^s_j)] / \text{Tr} [e^{-\beta (H_i + H_H)}]$$

$$\equiv (g^2/2) J(\tau^p_j - \tau^s_j).$$

(13)

Now the partition function can be interpreted as integrating a probability distribution function over some configuration space. Here, each configuration is specified by all sets of different $\{\tau^\sigma\}_n$ and a particular permutation $p \in S_m$, which is then sampled through a Metropolis algorithm with a probability proportional to $w_d \times w_z \times w^+_c \times w^+_e \times \prod_{i=1}^m P_{i,p}(i)$.

We now describe the Monte Carlo updates. We inherit the updates from the Ising BFM$^{19,20}$, namely the insertion, removal and shift of $d^\dagger c_{k,\sigma} c_{k',\sigma} d_{\sigma}$ pair, and also adopt the insertion/removal of $S^\dagger \phi^- / S^- \phi^+$ and the sampling of the permutation $S_m$ introduced in reference$^{21}$ (named updates (a)-(c) there). In addition we introduce a swap update that swaps $S_+ (\tau^\dagger)$ with a pair of $d^\dagger$ and $d_\downarrow$ ( $d^\dagger_1$ and $d_\downarrow_1$). For example consider the $S_a$ case. We first randomly pick a pair of $S_+ (\tau_i^\dagger)$, $S_- (\tau_j^\dagger)$ from the $m$ pairs of $S_+$ and $S_-$ that is connected by one of $J(\tau)$. Then we choose a $d^\dagger (\tau^\dagger_k)$ with a probability

$$P_k = J(\tau^\dagger_k - \tau^\dagger_j) / \left( \sum_{n=1}^{n_{\tau}} J(\tau^\dagger_n - \tau^\dagger_j) \right)$$

from the $n_{\tau}$ operators. We then swap the position of $S_+ (\tau_i^\dagger)$ and $d^\dagger (\tau^\dagger_k)$. Finally, we find the $d^\dagger (\tau^\dagger_j)$ that is closest to $d^\dagger (\tau^\dagger_k)$ before the swap, and move it to $d^\dagger (\tau^\dagger_j')$. The direction $\tau^\dagger_j$ is randomly selected within an interval of length $l_{max}$, which is the distance between two creation operators in the $\sigma = \downarrow$ orbital next to $S_+$ before the swap. The corresponding proposal probability is given by

$$P_{prop} = \frac{1}{l_{max}m} \times \frac{J(\tau^\dagger_j - \tau^\dagger_j')}{\sum_{n=1}^{n_{\tau}} J(\tau^\dagger_n - \tau^\dagger_j')}.$$ 

Likewise we can find the proposal probability for the inverse update,

$$P_{prop}^{inv} = \frac{1}{l_{max}m} \times \frac{J(\tau^\dagger_j - \tau^\dagger_j')}{\sum_{n \neq k}^{n_{\tau}} J(\tau^\dagger_n - \tau^\dagger_j) + J(\tau^\dagger_j - \tau^\dagger_j')}.$$ 

(14)
The weight ratio between the proposed configuration and the current configuration is given by

\[
\frac{w_{\text{new}}}{w_{\text{old}}} = \frac{w_c^d(\{\tau_{\text{d}}\}^\text{new}_{n^2}, \{\tau_{\text{d}}\}^\text{new}_{n^1}, \{\tau_{\text{d}}\}^\text{new}_{n^0})}{w_c^d(\{\tau_{\text{d}}\}^\text{old}_{n^2}, \{\tau_{\text{d}}\}^\text{old}_{n^1}, \{\tau_{\text{d}}\}^\text{old}_{n^0})}
\]

\[
\times \frac{w_d(\{\tau_{\text{tot}}\}^\text{new}_{n^0})w_z(\{\tau_{\text{tot}}\}^\text{old}_{n^0})w_{\tau_{\text{tot}}}(\tau_{\text{d}} - \tau_{\text{d}}')}^{\text{new}}}{w_d(\{\tau_{\text{tot}}\}^\text{old}_{n^0})w_z(\{\tau_{\text{tot}}\}^\text{old}_{n^0})w_{\tau_{\text{tot}}}(\tau_{\text{d}} - \tau_{\text{d}}')}^{\text{old}},
\]

where \(\{\tau_{\text{d}}\}^\text{new}_{n^i}\) is \(\tau_{\text{d}}\) replaced by \(\tau_{\text{d}}^i\) with \(\tau_{\text{d}}^i\) replaced by \(\tau_{\text{d}}^i\) and \(\tau_{\text{d}}^i\) is replaced by \(\tau_{\text{d}}^i\). The detailed balance condition is satisfied by adopting the acceptance ratio \(\max[R, 1]\), with \(R\) given by

\[
R = \frac{w_{\text{new}}}{w_{\text{old}}} \times \frac{P_{\text{prop}}^{\text{new}}}{P_{\text{prop}}^{\text{old}}},
\]

where \(\nu_n = 2\pi n/\beta\), \(n \in \mathbb{Z}\) is the Matsubara frequencies. There are two ways to calculate \(J(\tau)\). We can either perform the integration over the density of states first,

\[
J(\nu_n) = \int_0^\infty \frac{2\omega}{\omega^2 - \nu_n^2} \rho_b(\omega) d\omega,
\]

followed by the Matsubara summation,

\[
J(\tau) = \frac{1}{\beta} J(\nu_n = 0) + \frac{2}{\beta} \sum_{\nu_n > 0} J(\nu_n) \cos(\nu_n \tau).
\]

Or we can first do the Matsubara summation, then integrate over the density of states,

\[
J(\tau) = \int_0^\infty \frac{e^{(\beta - \tau)\omega} + e^{\tau\omega}}{e^{\beta\omega} - 1} \rho_b(\omega) d\omega.
\]

In practice we find the summation in equation (20) converges too slow when \(\beta\) is large. So using equation (21) is recommended.

On the other hand, \(J(\tau)\) is related to \(B(\tau)\) by being its second derivative: \(J(\tau) = d^2 B(\tau)/d\tau^2\). \(B(\tau)\) is most easily evaluated using the following formula,

\[
B(\tau) - B(0) = J(\nu_n = 0) \frac{\tau (\tau - \beta)}{2\beta} + \sum_{\nu_n > 0} J(\nu_n) \frac{1 - \cos(\nu_n \tau)}{\nu_n^2}.
\]

Because of the extra \(1/\nu_n^2\) factor here, the summation actually converges very quickly.

**B. Observables**

In this subsection we introduce all the quantities we will calculate using CT-QMC.

We start with the local magnetization,

\[
\langle m_\alpha \rangle = \langle \frac{1}{\beta} \int_0^\beta S_\alpha(\tau) d\tau \rangle, \quad \alpha = x, y, z,
\]

which is related to most of the quantities we discussed below.

Because the sampling will preserve spin rotation symmetry, the actual measured \(\langle m_\alpha \rangle\) is always 0. Instead we measure its root mean square,

\[
\sigma_\alpha = \sqrt{\langle m_\alpha^2 \rangle},
\]

which is also related to the static spin susceptibility

\[
\chi_\alpha^{\text{spin}}(0) = \int_0^\beta \chi_\alpha^x(\tau) d\tau = \int_0^\beta \langle T_\tau S_\alpha(\tau) S_\alpha \rangle d\tau
\]

by,

\[
\chi_\alpha^{\text{spin}} = \beta \sigma_\alpha^2.
\]

where we have also defined the dynamical spin correlation function \(\chi_\alpha^x(\tau)\). From \(\chi_\alpha^x(\tau)\) we can also extract the spin correlation length \(\xi_\alpha\) along the imaginary-time axis,

\[
\xi_\alpha = \frac{1}{\nu_1} \sqrt{\frac{\chi_\alpha^{\text{spin}}(\nu_1)}{\chi_\alpha^{\text{spin}}(0)}} - 1.
\]
Here $\chi_\alpha^\lambda(\nu_0)$ is the Fourier transform of $\chi_\alpha^\lambda(\tau)$, $\nu_0$ is the zero Matsubara frequency, and $\nu_1$ the first nonzero Matsubara frequency. This is in close analogy with extracting the spatial correlation length from the momentum dependence of the structure factor, where $q^2$ is accompanied by $\xi^2$ in the small-\( q \) limit. As $L$ goes to infinity, in a disordered state $\xi_d$ approaches constant, so $\xi_d/L$ goes to zero, while in an ordered state $\xi_d/L$ diverges because the condensate makes $S(q = 0)$ diverge. Finally, at the critical point, the system is scale invariant, thus $\xi_d/L$ will assume a universal value, independent of $L$. The ratio $\xi_d/L$ has been used extensively in numerical calculation of lattice spin systems to detect magnetic ordering. For quantum impurity model, we can define $\xi_d$ in terms of the temporal Fourier transform of the imaginary time correlation function $\chi_\alpha^\lambda(\tau)$ defined over $\tau \in (0, \beta)$ in exactly the same fashion, and treat the inverse temperature $\beta$ as the system size. Thus $\xi_\alpha$ will represent the correlation length of the spin correlation along the imaginary time axis. By analogy with the spacial-dependent case described above, we expect $\xi_d/\beta$ to be independent of $\beta$ at a critical point. Note, however, whether this leads to a crossing point in a plot of $\xi_d/\beta$ vs. the control parameter depends on the nature of the involved phases; see the next section for further discussion.

As we will always preserve spin SU(2) symmetry, in the following we will drop the subscript a labeling different spin components in any vector quantity.

We will also look at the Binder cumulant, generalized to an $n$-component order parameter, to an $n$-component order parameter:

$$U_2 = \frac{n + 2}{2} \left( 1 - \frac{n}{n + 2} \frac{(m \cdot m)^2}{(m \cdot m)^2} \right),$$

(27)

In essence, $U_2$ probes the probability distribution function $P(m)$ of the order parameter $m$, by forming the ratio between the forth moment and square of the second moment of $P(m)$. The precise form of $U_2$ is constructed such that $U_2$ approaches 1 in the ordered state and 0 in the disordered state. This can be understood as follows. In the disordered state, $P(m)$ follows a n-dimensional Gaussian distribution. It can be shown that $\langle (m \cdot m)^2 \rangle / (m \cdot m)^2 = (n + 2)/n$ so that $U_2 = 0$. Deep in the ordered state, $P(m) \propto \delta(m^2 - \langle m^2 \rangle)$, so $\langle (m \cdot m)^2 \rangle / (m \cdot m)^2 = 1$ and $U_2 = 1$. At the critical point, $\langle (m \cdot m)^2 \rangle$ and $\langle m \cdot m \rangle$ has the same scaling dimension by construction thus $U_2$ take a universal value irrespective of system size $\beta$. So one can look for crossing in $U_2$ to detect a phase transition.

Quantities like $\langle (m \cdot m)^2 \rangle$ will involve 4-point correlation functions of different components of $S_\alpha$, which would require implementing worm type algorithm. In the presence of spin SU(2) symmetry, we can utilize the relation $\langle (m \cdot m)^2 \rangle = 5/3 \langle m^2 \rangle$ and $\langle m \cdot m \rangle = 3/2 \langle m^2 \rangle$ to simplify the expression (here $n = 3$ since $m$ has 3 components),

$$U_2 = \frac{5}{2} \left( 1 - \frac{1}{3} \frac{\langle m^2 \rangle}{\langle m^2 \rangle} \right).$$

(28)

Another interesting quantity that can be used to study quantum phase transition is the fidelity susceptibility $\chi_f^\lambda$. Suppose the Hamiltonian is composed of two parts $H = H_{\lambda=0} + \lambda H_\lambda$, with $\lambda$ being some tuning parameter. The fidelity is defined as the modulus of the overlap between the ground state $|\psi_0\rangle$ at $\lambda$ and $\lambda + \delta\lambda$: $F(\lambda, \delta\lambda) = |\langle \psi_0(\lambda) | \psi_0(\lambda + \delta\lambda) \rangle|^{37}$. Since the two phases separated by a QCP are described by two types of ground states, the fidelity will be minimized as $\lambda$ passes through the QCP with $\delta\lambda \to 0^+$. The fidelity susceptibility, which is defined as the second derivative of $F$ with respect to $\delta\lambda^{38}$, $\chi_f^\lambda = -\partial^2 F/\partial \delta\lambda^2$, picks up this singularity. To calculate the fidelity susceptibility using CT-QMC, we need to generalize the zero temperature definition to finite temperature. One can express $\chi_f^\lambda$ under perturbation theory and relate it to the imaginary time correlation function of $H_\lambda$. Then it can be straightforwardly generalized to finite temperature with the following expression (for details, see Ref. 39),

$$\chi_f^\lambda(T) = \int_0^{\beta/2} \langle \langle H_\lambda(\tau) H_\lambda \rangle - \langle H_\lambda \rangle^2 \rangle \, d\tau.$$

(29)

In general, $\chi_f^\lambda$ is a smooth function of $\lambda$. But it is singular and even diverges at a QCP. At a second order quantum phase transition, $\langle H_\lambda(\tau) \rangle := H_\lambda \sim (1/\tau)^2 \text{Dim}[\lambda]$. Here : $H_\lambda :$ denotes normal ordering: $H_\lambda := H_\lambda - \langle H_\lambda \rangle$ and $\text{Dim}[\lambda]$ denotes scaling dimension of $H_\lambda$. As we require $\int_0^{\beta/2} \tau \, d\tau H_\lambda$ to be scale invariant, we have $\text{Dim}[H_\lambda] = 1 \sim \text{Dim}[\lambda]$.

Therefore $\chi_f^\lambda$ can be used to detect the location of a QCP, without knowing the actual order parameter. It turns out that for hybridization expansion CT-QMC, if we choose $\lambda$ to be the hybridization strength $V$, then the corresponding fidelity susceptibility, which we denoted by $\chi_f^V$, can be calculated by a very simple formula:

$$\chi_f^V = \langle k_L k_R \rangle_{M.C.} - \frac{\langle k_L \rangle_{M.C.} \langle k_R \rangle_{M.C.}}{2V^2}.$$

(31)

Here, $k_L$ and $k_R$ refer to the number of hybridization vertices $H_V$ (the filled and empty circles in Fig.2) residing in the range $[0, \beta/2]$ and $[\beta/2, \beta)$ of the imaginary time axis, in a particular configuration during the Monte Carlo sampling. $(\ldots)_{M.C.}$ denotes the expectation value under Monte Carlo sampling. Intuitively this formula measure the covariance of $k_L$ and $k_R$. At the QCP, fluctuation is the most violent, which means the covariance is the greatest, and $\chi_f^V$ is maximized.
III. QUANTUM PHASE TRANSITIONS AND PHASE DIAGRAM

We now present the CT-QMC results. We describe the details of our analysis in the representative cases of $s = 0.6$ in section III A and $s = 0.2$ in section III B. We then consider the dependence on $s$ in the range $0 < s < 1$ appropriate for sub-ohmic bosonic bath in section III C.

A. $s = 0.6$

We start by presenting our analysis at $s = 0.6$, which belongs to the case of RG flow specified in figure 1 (a). The RG fixed point $C'$ controls the transition from the local moment phase to the Kondo phase; a stable fixed point $L$ represents the critical phase; and, correspondingly, we have two additional unstable fixed points $C$ and $LC$, respectively describing the transition to the Kondo phase and the local moment phase from the critical phase. In the following, we will present numerical evidence for each of the three QCPs.

1. Critical phase-Kondo transition

First we stay at $g = 0.5$, and gradually increase $\Gamma_0$. In figure 3(a) we plot $\xi/\beta$ versus $\Gamma_0$ from $\beta = 200$ all the way to $\beta = 6400$. For $\Gamma_0 \lesssim 0.08$, we find $\xi/\beta$ is almost independent of $\beta$ (system size), suggesting the system being scale invariant for a range of $\Gamma_0$. This is the signature of the critical phase. At larger $\Gamma_0$, $\xi$ grows slower than the system size $\beta$, signifying short time correlation between the impurity spin as the impurity is Kondo screened. At some critical value of $\Gamma_0$ we expect a quantum phase transition separating the two phases. But the exact location is hard to pin-point, as we do not see any crossing in $\xi/\beta$ (The fact that $\xi/\beta$ is universal at the QCP does not necessarily guarantee a crossing. In order to have a crossing, $\xi/\beta$ need to be increasing/decreasing with $\beta$ to the left/right of the critical point, or vice versa. But here $\xi/\beta$ stays at a constant value for $\Gamma_0 \lesssim 0.08$ due to the nature of the critical phase). In section III A 3 we will show that $\xi/\beta$ does have a crossing at the local moment to Kondo QCP.

One observable we can utilize is the root mean square magnetization $\sigma$ defined in equation (24). We expect that a scaling form as follows should hold,

$$\sigma(\Gamma_0, \beta) = \beta^{-\nu(1-x)/2} \bar{\sigma} \left( \beta^{1/\nu} (\Gamma_0 - \Gamma_c) / \Gamma_c + A / \beta^{2/\nu} \right).$$

(32)

where $\bar{\sigma}$ is the universal function, $\Gamma_c$ the critical coupling, $\nu$ the correlation length exponent, and $A / \beta^{2/\nu}$ is the subleading terms.

In the universal function $\bar{\sigma}$, the dependence of the tuning parameter only comes in through the combination of $\beta^{1/\nu} (\Gamma_0 - \Gamma_c)$ (ignoring sub-leading corrections). This can be justified from RG or understood phenomenologically based on the consideration that at a QCP the system only depends on the ratio $\beta/\xi$ and $\xi$ diverges, $\xi \propto |\Gamma_0 - \Gamma_c|^{-\nu}$. One subtlety here is that the correlation length diverges in the entire critical phase. So one could question whether such a scaling form still applies in the region of $\Gamma_0 < \Gamma_c$. The prefactor $\beta^{-(1-x)/2}$ comes from equation (25) and that at the QCP we expect $\chi^{spin} \propto \beta^x$ with the exact relation $x = s$ based on $\epsilon$-expansion RG result. Here instead of imposing this relation we allow $x$ to adjust freely. As shown in figure 3(b), the quality of the scaling collapse suggests that equation (32) is the correct scaling hypothesis. In addition the correspondingly determined $\Gamma_c = 0.08(1)$ and $\nu^{-1} = 0.26(3)$ are consistent with what we obtained from $\chi_f^V$. We also find $x = 0.63(4)$, consistent with the prediction $x = s$.

Based on the $\epsilon$-expansion to the second order, we obtain $\nu^{-1} = \epsilon/2 + \epsilon^2/6 \approx 0.23$, in reasonably good agreement with the numerical value.

Unlike the $\chi^{spin}(T) \sim 1/T$ local moment behavior in the $s = 0.2$ case previously found in reference 21, here the temperature dependence of the spin susceptibility obeys a nontrivial power-law, as shown in figure 4. We find $x = 0.66, 0.67, 0.66, 0.65$ for $\Gamma_0 = 0.04, 0.05, 0.06, 0.07$, respectively. We interpret this as implying that, for
$\Gamma_0 < \Gamma_c$, the system will flow under RG towards the critical phase fixed point $L$ with $\chi^{\text{spin}}(T) \sim A_1/T^s$. Notice that according to $\epsilon$-expansion the leading irrelevant operator has a very small scaling dimension $y_i = -\epsilon/2 + O(\epsilon^2)$, so the deviation from the exact relation $x = s$ is most likely due to corrections to scaling. At $\Gamma_0 = \Gamma_c$, we have $x = 0.61$. This is also consistent with the predicted critical behavior $\chi^{\text{spin}}(T) \sim A_2/T^s$ at fixed point $C$ from $\epsilon$-expansion RG\textsuperscript{15,16}.

![Graph showing temperature dependence of spin susceptibility](image)

**FIG. 4:** Temperature dependence of the spin susceptibility across the critical phase to Kondo QCP at $g = 0.5$, $s = 0.6$. Dashed line shows the $T^{-s}$ behavior expected in the critical phase ($\Gamma_0 \lesssim 0.08$) as well as at the QCP ($\Gamma_0 \simeq 0.08$). The errorbar is less than 1% of the value of $\chi^{\text{spin}}(T)$.

2. Critical phase-local moment transition

So far we have considered the regime accessible by the $\epsilon$-expansion of the SU(2) model, namely when both the fermionic and bosonic couplings are small. Unlike the Coulomb-gas expansion of the Ising case\textsuperscript{12,13,15,16}, the $\epsilon$-expansion here does not reach the regime of large $g$. In order to simplify the calculation we set $\Gamma_0 = 0$ in this section. We have also performed calculations at small but nonzero $\Gamma_0$ and the conclusion remains the same.

First let us look at the behavior of the correlation length as a function of $g$, plotted in figure 5. The low temperature behavior of $\xi/\beta$ for $g \lesssim 0.5$ resembles the critical phase behavior in figure 3(a), both converging to a value around 0.3. For $g \gtrsim 0.8$, on the other hand, $\xi/\beta$ rises as temperature decreases, which suggests local moment phase behavior.

A more quantitative way of studying the transition between these two phases is by looking at the temperature dependence of the mean square magnetization $\sigma^2$. Following reference\textsuperscript{21}, the low temperature behavior of $\chi^{\text{spin}}(T)$ can be described by the following ansatz,

$$\chi^{\text{spin}}(T) = M_0/T + 1/T^2 T_B^{-z}. \quad (33)$$

Here $M_0$ is the Curie constant, $T_B$ the crossover temperature scale above which the critical fluctuation part $T^{-x}$ will dominate. This together with equation (25) leads to

$$\sigma^2(T) = M_0 + (T/T_B)^{1-x}. \quad (34)$$

Our result for $\sigma^2(T)$ is plotted in figure 6. For $g \leq 0.5$, the data can be described by equation (34) with $M_0 = 0$ and $x = 0.68, 0.67, 0.66$ for $g = 0.3, 0.4, 0.5$. This is the critical phase and the exponent is very close to what we obtained at Sec.III A 1. For $g \geq 0.8$, fitting $\sigma^2(T)$ using the same equation gives a finite $M_0$. This indicates we are entering the local moment phase. While we have obtained $x = 0.60$ for $g > 1$, we have $x = 0.67, 0.65, 0.64$ for $g = 0.8, 0.9, 1.0$, reflecting corrections to scaling not captured by equation (34).

![Graph showing temperature dependence of mean square magnetization](image)

**FIG. 5:** (a) Reduced correlation length as a function of $g$. The distinct behavior at small and large $g$ each corresponds to critical phase and local moment phase. (b) Effective Curie constant extracted using equation (33) as a function of $g$. Dashed lines are power law fits according to $M_0 \propto (g - g_0)^{\gamma_1}$ up to $g \geq g_{\text{min}}$ with three different choice of $g_{\text{min}}$.

**FIG. 6:** Temperature dependence of mean square magnetization across the critical phase-local moment transition. Red (Blue) lines are fits according to equation (34) with zero (finite) Curie constant $M_0$, which is expected in the critical (local moment) phase.
The extracted $M_0$ is plotted in figure 5(b). Close to the transition point at $g = g_c$, we expect $M_0$ to vanish as $M_0 \propto (g - g_c)^{\beta_1}$. We attempt to use this relation to find the value of $g_c$ by fitting over the $M_0$ versus $g$ data. Bearing in mind that for $0.8 \leq g \leq 1$ the value of $x$ obtained from equation (34) is larger than $s$, it is likely that we will be overestimating $M_0$ in this region, so we only use $M_0$ down to $g \geq g_{\text{min}}$, and vary $g_{\text{min}}$ from 0.8 to 1. Depending on the cutoff $g_{\text{min}}$, the obtained $g_c$ lands within the range $g_c \in [0.74, 0.88]$. Notice that the fitting with different $g_{\text{min}}$ all describe the $g \geq 1$ part of the data quite well. We thus take our final estimate of $g_c$ to be $g_c = 0.8 \pm 0.1$.

3. Local moment-Kondo transition

Now that we have established that the system resides in the local moment phase for $g > g_c \approx 0.8$ at $\Gamma_0 = 0$, we consider a path to the Kondo screened phase by turning on the hybridization while fixing $g = 1$. As expected, we observe a crossing in $\xi/\beta$, and a divergence in $\chi^V_f$, both around $\Gamma_0 = 0.4$ (cf. figure 7).

![Diagram](https://example.com/diagram.png)

**FIG. 7:** Reduced correlation length $\xi/\beta$ (a) and fidelity susceptibility $\chi^V_f$ (b) vs. $\Gamma_0$ across the local moment-Kondo transition from $\beta = 200$ to $\beta = 6400$ at $g = 1$, $s = 0.6$. Near the QCP $\xi/\beta$ exhibits crossing and $\chi^V_f$ shows up a peak. The errorbar of $\xi/\beta$ is much smaller than symbol size.

Similar to what we have done for $\sigma(\Gamma_0, \beta)$ in equation (32), we consider the following finite size scaling hypothesis for $\xi$ and $\chi^V_f$:

$$\xi(\Gamma_0, \beta) = \beta^\xi \left( \beta^{1/\nu}(\Gamma_0 - \Gamma_c) / \Gamma_c + A/\beta^{\phi/\nu} \right), \quad (35)$$

$$\chi^V_f(\Gamma_0, \beta) = \beta^{2/\nu} \chi \left( \beta^{1/\nu}(\Gamma_0 - \Gamma_c) / \Gamma_c + A/\beta^{\phi/\nu} \right). \quad (36)$$

As seen in figure 8, close to the critical point the data fall nicely under a single universal curve. We obtain $\Gamma_c = 0.35(2), \nu^{-1} = 0.39(6)$ from $\xi$ and $\Gamma_c = 0.34(2), \nu^{-1} = 0.37(5)$ from $\chi^V_f$. Our final estimated value are $\Gamma_c = 0.35(2)$ and $\nu^{-1} = 0.38(5)$. The value of $\nu^{-1}$ obtained here for the critical point $C'$ is in sharp contrast with that for the critical point $C$ with $\nu = 0.25(4)$. This further establishes that $C$ and $C'$ are two distinct critical points.

![Diagram](https://example.com/diagram.png)

**FIG. 8:** Finite size scaling of correlation length (a) and fidelity susceptibility (b) for the local moment to Kondo transition. Inset shows blow up view of the data obtained near $\Gamma_0 = \Gamma_c$. Note that due to incorporating the sub-leading term in the scaling ansatz, it is no longer centered around 0. The errorbar of $\xi/\beta$ is much smaller than symbol size.

We now turn to the critical behavior of spin susceptibility. In figure 9, we plot $\chi^{\text{spin}}$ vs. $T$ at different $\Gamma_0$. At the critical coupling $\Gamma_0 = \Gamma_c \simeq 0.35$, $\chi^{\text{spin}}(T)$ can be fitted with a power law $\chi^{\text{spin}}(T) \propto T^{-\alpha}$ with $\alpha = 0.65$. Inside the local moment phase at $\Gamma_0 = 0.1$, it can be described by equation (33) with a finite $M_0 = 0.10$ for the $M_0/T$ term and a sub-leading $1/T^{1-x}T_B^{1-x}$ term with $x = 0.62$. These are consistent with the critical spin fluctuations being dominated by a $T^{-\alpha}$ behavior. Thus we infer that the local spin susceptibility at $C'$ should also diverge as $\chi^{\text{spin}} \sim 1/T^\alpha$. 

![Diagram](https://example.com/diagram.png)
B. $s=0.2$

We now turn to the model at $s = 0.2$. This is also the case investigated in reference\textsuperscript{21} at the $U = \infty$ limit. We will fix $g = 0.5$ and gradually increase $\Gamma_0$ to find the QCP from the local moment phase to the Kondo screened phase.

We first plot the dependence on $\Gamma_0$ of the Binder cumulant $U_2$ and the reduced correlation length $\xi/\beta$ in figure 10(a) and figure 10(b), where we have identified crossing points for both quantities. This suggests a transition from a local moment phase at small $\Gamma_0$ to a Kondo screened phase at large $\Gamma_0$. The crossing points have a sizable drift as we lower the temperature, which can be seen more clearly by plotting the crossing points between curves at $\beta$ and $2\beta$ in figure 11. We see that the crossing points obtained from $U_2$ and $\xi/\beta$ are approaching to the same critical value $\Gamma_c$ in the $T = 0$ limit from the opposite directions. By extrapolating the crossing points $\Gamma_{\text{cross}}$ to $T = 0$ using a simple power-law relation $\Gamma_{\text{cross}} = \Gamma_c + aT^b$, we find $\Gamma_c = 0.48(1)$.

We can then repeat the analysis done in Sec.III.A.1 for the same type of transition at $s = 0.2$ by considering scaling collapse of the form in equation (35) for the correlation length $\xi$ and similarly for the Binder cumulant $U_2$,

$$U_2(\Gamma_0, \beta) = \tilde{U}_2 \left( \beta^{1/\nu}(\Gamma_0 - \Gamma_c)/\Gamma_c + A/\beta^{\phi/\nu} \right)$$ (37)

where the presence of the sub-leading term $A/\beta^{\phi/\nu}$ can take into account the finite temperature shift of the crossing point.

It turns out these ansatzes describe the data very well. The collapsed data using equation (37) and equation (35) are plotted in figure 12(a), and they give consistent estimates for the value of the critical coupling $\Gamma_c$ and correlation length exponent $\nu$. We obtain $\Gamma_c = 0.49(1)$, $\nu^{-1} = 0.42(3)$ from $U_2$ and $\Gamma_c = 0.48(1)$, $\nu^{-1} = 0.43(3)$ from $\xi$.

We further test the applicability of the fidelity susceptibility in this case, which serves as another independent tool to detect the QCP. As shown in figure 10(c) the measured $\chi_f^\nu$ appears to converge near our estimated $\Gamma_c$. A finite size scaling analysis can be performed as well. For consistency we consider the same type of scaling form of $\chi_f^\nu$ as appeared in equation (36).

The result, plotted in figure 12(b), gives $\Gamma_c = 0.46(2)$ and $\nu^{-1} = 0.48(3)$, in fairly good agreement with what we have obtained from $U_2$ and $\xi$. Our final estimates are $\Gamma_c = 0.48(1)$ and $\nu^{-1} = 0.44(5)$.

Having identified the location of the QCP, we now look at the temperature dependence of the spin susceptibility $\chi_{\text{spin}}^s$ across the QCP, shown in figure 13(a). It turns out the critical behavior of $\chi_{\text{spin}}^s$ is much harder to study for the $s = 0.2$ case compared to the $s = 0.6$ case. For $\Gamma_0 < \Gamma_c$, the dominant behavior of $\chi_{\text{spin}}^s(T)$ is Curie-Weiss like, reflecting the localized nature of the impurity spin. For
suggest that this is due to the fact that $\chi$ at $\Gamma$ temperature is lowered. Data are extracted from fig. 10(a)(b). Upper panel: scaling collapse of fidelity susceptibility with $\Gamma$. $c$ is still in the initial cross-over regime. To see this, we determine the critical coupling $\Gamma_c$ via a variety of independent methods and obtained unambiguous results for the presence and the location of the QCP. Then we attempt to verify the critical behavior of $\chi^{spin}(T)$ directly. Unfortunately from figure 13(b) it seems that, in contrast to the case of $s = 0.6$, accessing the asymptotic critical regime requires even lower temperatures for $s = 0.2$. We have seen earlier that in the $s = 0.6$ case it is much easier to access the asymptotic critical behavior of $\chi^{spin}(T)$.

$T^s \chi^{spin}(T)$ at different $T$. But there the crossing point has significant drift versus temperature, which is consistent with an evolving $\alpha(T)$ in our calculation. Here we determine the critical coupling $\Gamma_c$ via a variety of independent methods and obtained unambiguous results for the presence and the location of the QCP. Then we attempt to verify the critical behavior of $\chi^{spin}(T)$ directly. Unfortunately from figure 13(b) it seems that, in contrast to the case of $s = 0.6$, accessing the asymptotic critical regime requires even lower temperatures for $s = 0.2$. We have seen earlier that in the $s = 0.6$ case it is much easier to access the asymptotic critical behavior of $\chi^{spin}(T)$.

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$J(\tau)$, we directly adopt a $J(\tau)$ that has the correct $1/\tau^{1+s}$ dependence as our input without specifying the actual form of $\rho_0(\omega)$. To be specific, we choose $J(\tau)$ to be the following,

$$J(\tau) = \left[ \frac{\pi/\beta}{\sin(\pi \tau/\beta)} \left( 1 + e^{-\beta} - e^{-\tau} - e^{-(\beta - \tau)} \right) \right]^{1+s}.$$  \hspace{1cm} (38)

The exponential factor will make $J(\tau)$ finite at the end points: $\lim_{\tau \to 0} J(\tau) = \lim_{\tau \to \infty} J(\tau) = 1$. Also $J(\tau)$ is even under reflection about $\tau = \beta/2$.

We can then integrate $J(\tau)$ twice to get $B(\tau)$,

$$B(\tau) - B(0) = \int_0^\tau \int_0^{\tau'} J(\tau'') d\tau' d\tau'' + a \tau.$$ \hspace{1cm} (39)

with $a = -\int_0^{\beta/2} J(\tau'') d\tau''$ determined from the condition $dB(\tau)/d\tau|_{\tau^{\beta/2}} = 0$.

Using equation (38) and equation (39) as input we have obtained the dynamical spin correlation function $\chi^s(\tau)$ for different value of $g$ and $s$. In figure 14(a) we present the result of $\chi^s(\tau)$ vs. $\tau$ at several different value of $\beta$ for the specific case of $g = 0.4, s = 0.2$. At each $\beta$, $\chi^s(\tau)$ drops from $1/4$ at $\tau = 0$ and reaches its minimum at $\tau = \beta/2$.

As $\beta$ is increased, $\chi^s(\tau = \beta/2)$ converge to a finite value.

![FIG. 14: (a) Dynamical spin correlation function $\chi^s(\tau)$ from $\tau = 0$ up to $\tau = \beta/2$ at different $\beta$. For large $\beta$, $\chi^s(\beta/2)$ converges to a finite value around 0.05. Arrow marks the value of $\chi^s(\beta/2)$ at $\beta = 4500$ (b) Effective susceptibility $\chi^s(\beta/2)$ vs $s$ at different value of $g$. Increasing $s$ reduces the size of $\chi^s(\beta/2)$. Dashed lines are linear extrapolation of $\chi^s(\beta/2)$ to $\chi^s(\beta/2) = 0$, the intersections with the horizontal axis give the critical values $s_c(g)$ for each $g$. Arrow marks the value of $s_c$ obtained at $g = 0.5$.](image)

![FIG. 15: Phase diagram of the pure bosonic problem. For $s > s^* \simeq 0.47$, increasing $g$ will induce a transition from the critical phase to the local moment phase. For $s < s^*$, the critical phase disappears.](image)

We then plot the evolution of $\chi^s(\tau = \beta/2)$ obtained at low temperature, as a function of $s$ for four different choices of $g$ in figure 14(b), up to the smallest value of $\chi^s(\tau = \beta/2)$ that we can reach convergence. We can identify $\chi^s(\tau = \beta/2)$ obtained here as an effective Curie constant, and use it as the order parameter for the local moment phase. We see that for fixed $g$, $\chi^s(\tau = \beta/2)$ decreases smoothly as a function of $s$. Furthermore, we can extrapolate each curve to larger value of $s$ until $\chi^s(\tau = \beta/2)$ vanishes at some critical value $s = s_c(g)$. This gives the value of $s$ where the corresponding $g$ is the critical value between the local moment phase and the critical phase.

The dependence of $s_c(g)$ on $g$ maps out the phase boundary between the local moment phase and the critical phase, which is shown in figure 15. Note that the shape of the phase boundary will depend on the specific form of $J(\tau)$ that is employed. As we can see the dependence of $s_c(g)$ on the value of $s$ is fairly weak and it reaches the $g^2 = 0$ axis at around $s = s^* \simeq 0.47$. We note that the simple extrapolation scheme performed in figure 15(a) could introduce some error in this estimate.

IV. DISCUSSION

Our result is best summarized in figure 1. We have shown that the $\epsilon$-expansion RG result remains valid when $s > s^* (\epsilon < 1 - s^*)$ and provide numerical evidence for the existence of the intermediate coupling local moment fixed point $L$ and the associated Kondo destruction critical point $C$ in this model for the first time. In addition, we find a second local moment fixed point $L'$ at strong coupling, associated with a second Kondo destruction critical point $C'$, neither of which is accessible by the $\epsilon$-expansion approach. For $s < s^*$, only $L'$ and $C'$ sur-
vive and our result is fully compatible with the result of Ref. 21 for $s = 0.2$. In terms of the quantum critical properties of $C$ and $C'$, we find that while they have different correlation length exponents, the anomalous dimension of the local spin correlation function follows the same relation $\eta = 1 - s$.

Our findings have important implications for the quantum criticality in Kondo lattice model within the EDMFT framework. In the EDMFT solution of the Kondo lattice model, the Kondo destruction QCP of the lattice problem is embedded in the impurity QCP of an effective BFKM. For two dimensional magnetic the lattice problem is embedded in the impurity QCP EDMFT framework. In the EDMFT solution of the regardless of whether $\eta$ dimension of the local spin correlation function follows the different correlation length exponents, the anomalous destruction QCP is still expected, even though $C$ and $C'$ have different correlation length exponents and belong to different universality classes. This is quite surprising until we realize that the argument that leads to $\eta = \epsilon$ only relies on the condition $\eta = \epsilon + 2\beta(g)/g|_{g=\epsilon,J=J^*}$, which is shown to be valid to all orders in $\epsilon$ in reference. The relation $\eta = \epsilon$ then follows at any intermediate coupling fixed point $g = g^*, J = J^*$, where $\beta(g)/g|_{g=\epsilon,J=J^*} = 0$, regardless of whether $g^*$ and $J = J^*$ is of the order $\epsilon$. Thereby this argument can be extended to $C'$ as well.

V. CONCLUSIONS

We have studied the SU(2) Bose-Fermi Anderson model using CT-QMC, focusing on the Kondo destruction type QCP. We find two type of such QCPs: one from Kondo screened phase to a local moment phase, the other to a critical phase. The second type QCP only exists when $s > s^*$, in which case the critical properties we have calculated agree with those from an $\epsilon$-expansion RG. At both types of QCP, our results suggest the spin correlation function obeys the power law $\chi^{\text{spin}}(\tau) \sim (1/\tau)^{\eta}$ with $\eta = 1 - s$.

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1. Q. Si and F. Steglich, Science 329, 1161 (2010).
2. P. Coleman and A. J. Schofield, Nature 433, 226 (2005).
3. Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature 413, 804 (2001).
4. P. Coleman, C. Pépin, Q. Si, and R. Ramazashvili, J. Phys. Cond. Matt. 13, R723 (2001).
5. T. Senthil, M. Vojta, and S. Sachdev, Phys. Rev. B 69, 035111 (2004).
6. Q. Si and S. Paschen, physica status solidi (b) 250, 425 (2013).
7. J. A. Hertz, Physical Review B 14, 1165 (1976).
8. A. Millis, Physical Review B 48, 7183 (1993).
9. T. Moriya, Spin fluctuations in itinerant electron magnetism, vol. 56 (Springer Science & Business Media, 2012).
10. Q. Si, J. H. Pixley, E. Nica, S. J. Yamamoto, P. Gogwmi, R. Yu, and S. Kirchner, Journal of the Physical Society of Japan 83, 061005 (2014).
11. Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Physical Review B 68, 115103 (2003).
12. Q. Si and J. L. Smith, Physical review letters 77, 3391 (1996).
13. J. Smith and Q. Si, EPL (Europhysics Letters) 45, 228 (1999).
14. A. M. Sengupta, Physical Review B 61, 4041 (2000).
15. L. Zhu and Q. Si, Physical Review B 66, 024426 (2002).
16. G. Zarà and E. Demler, Physical Review B 66, 024427 (2002).
17. M. T. Glosso and K. Ingersent, Physical review letters 95, 067202 (2005).
18. M. T. Glosso and K. Ingersent, Physical Review B 75, 104410 (2007).
19. J. Pixley, S. Kirchner, M. Glosso, and Q. Si, in Journal of Physics: Conference Series (IOP Publishing, 2011), vol. 273, p. 012050.
20. J. Pixley, S. Kirchner, K. Ingersent, and Q. Si, Physical Review B 88, 245111 (2013).
21. J. Otuki, Physical Review B 87, 125102 (2013).
22. D. Grempel and Q. Si, Physical review letters 91, 026401 (2003).
23. J.-X. Zhu, D. Grempel, and Q. Si, Physical review letters
24 M. T. Glossop and K. Ingersent, Physical review letters 99, 227203 (2007).
25 J.-X. Zhu, S. Kirchner, R. Bulla, and Q. Si, Physical review letters 99, 227204 (2007).
26 P. Werner, A. Comanac, L. DeMedici, M. Troyer, and A. J. Millis, Physical Review Letters 97, 076405 (2006).
27 P. Werner and A. J. Millis, Physical Review B 74, 155107 (2006).
28 P. Werner and A. J. Millis, Physical review letters 99, 146404 (2007).
29 K. Steiner, Y. Nomura, and P. Werner, Physical Review B 92, 115123 (2015).
30 A. W. Sandvik, A. Avella, and F. Mancini, in AIP Conference Proceedings (AIP, 2010), vol. 1297, pp. 135–338.
31 R. K. Kaul, Physical review letters 115, 157202 (2015).
32 T. Sato, M. Hohenadler, and F. F. Assaad, Physical review letters 119, 197203 (2017).
33 S. Pujari, T. C. Lang, G. Murthy, and R. K. Kaul, Physical review letters 117, 086404 (2016).
34 K. Binder, Zeitschrift für Physik B Condensed Matter 43, 119 (1981).
35 P. Gunacker, M. Wallerberger, E. Gull, A. Hausoel, G. Sangiovanni, and K. Held, Physical Review B 92, 155102 (2015).
36 P. Gunacker, M. Wallerberger, T. Ribic, A. Hausoel, G. Sangiovanni, and K. Held, Physical Review B 94, 125153 (2016).
37 P. Zanardi and N. Paunković, Physical Review E 74, 031123 (2006).
38 W.-L. You, Y.-W. Li, and S.-J. Gu, Physical Review E 76, 022101 (2007).
39 A. F. Albuquerque, F. Alet, C. Sire, and S. Capponi, Physical Review B 81, 064418 (2010).
40 L. C. Venuti and P. Zanardi, Physical review letters 99, 095701 (2007).
41 L. Wang, Y.-H. Liu, J. Imriška, P. N. Ma, and M. Troyer, Physical Review X 5, 031007 (2015).
42 L. Wang, H. Shinaoka, and M. Troyer, Physical review letters 115, 236601 (2015).