Universal scaling in the Knight-shift anomaly of the doped periodic Anderson model

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We report a dynamical cluster approximation investigation of the doped periodic Anderson model to explain the universal scaling in the Knight-shift anomaly predicted by the phenomenological two-fluid model and confirmed in many heavy-fermion compounds. We calculate the quantitative evolution of the orbital-dependent magnetic susceptibility and reproduce correctly the two-fluid prediction in a large range of doping and hybridization. Our results confirm the presence of a temperature/energy scale $T^*$ for the universal scaling and show distinctive behaviors of the Knight-shift anomaly in response to other “orders” at low temperatures. However, comparison with the temperature evolution of the calculated resistivity and quasiparticle spectral peak indicates a different characteristic temperature from $T^*$, in contradiction with the experimental observation in CeCoIn$_5$ and other compounds. This reveals a missing piece in the current model calculations in explaining the two-fluid phenomenology.

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I. INTRODUCTION

The NMR Knight-shift anomaly has been detected in a few families of materials, including the cuprates [1–3], heavy-fermion compounds CeCu$_2$Si$_2$, UPt$_3$, and URu$_2$Si$_2$ [4,5], and most recently iron-based superconductors AFe$_2$As$_2$ ($A = K$, Rb, Cs) [6]. As a ubiquitous non-Fermi liquid behavior in correlated systems, it manifests itself as the breakdown of the proportionality between the Knight shift and magnetic susceptibility as seen in normal Fermi liquids. For example, in the CeMIn$_5$ ($M =$ Rh, Ir, or Co) class of heavy-fermion materials [7–9], the Knight shift $K$ is proportional to the susceptibility at high temperatures. However, this simple relation fails below a material-dependent crossover temperature $T^* \sim 10–100$ K, which reflects the onset of lattice coherence or hybridization between conduction electrons and localized $f$ electrons. More interestingly, the Knight-shift anomaly has been observed to obey a universal scaling in a particular temperature regime across a dozen heavy-fermion materials, which has attracted considerable attention [10] among various exotic behaviors of heavy-electron materials.

Theoretically, the Knight-shift anomaly has been argued to be due to a temperature-dependent hyperfine interaction [11] or the crystal field occupations of the $4f$ ($5f$) electrons in the rare-earth or actinide ions [12]. However, these developments have been criticized because of the much higher energy scale of the hyperfine coupling compared with the Kondo and crystal field interactions [13]. To understand diverse non-Fermi liquid behaviors observed in heavy-electron materials including the universality of the Knight-shift anomaly, a phenomenological two-fluid theory has been developed as a promising framework [14–19]. Specifically, this two-fluid model argues that below a material-dependent coherence temperature, $T^*$, an itinerant heavy-electron Kondo liquid, which displays non-Fermi liquid scaling behavior, emerges as the localized $f$ electrons collectively hybridize with the conduction electrons. This emergent Kondo liquid coexists with a spin liquid formed by the lattice moments of $f$ electrons whose magnitude is reduced by the hybridization. Below $T^*$ both the residual unhybridized local moments and the emergent Kondo liquid contribute to the Knight shift but with different weights so that the Knight shift is no longer proportional to the total susceptibility. Moreover, the relative weight of the local moments is continuously reduced with decreasing temperature whereas the weight of the Kondo liquid increases. These two components compete over a broad range of temperatures below $T^*$ until the onset of either long-range order antiferromagnetism or superconductivity as ground states [14–20]. Although the intertwined two-fluid picture has gained much interest in accounting for several anomalous heavy-fermion properties, a minimal microscopic model that can clarify the nature of the two fluids and provide a comprehensive and quantitative understanding is still lacking [18].

To this end, one of us (M.J.) has performed a determinant quantum Monte Carlo (DQMC) simulation to gain some insight into the universal scaling behavior of the Knight-shift anomaly reported in experiments and the two-fluid theory [21]. That previous work confirmed the expectation that the different temperature evolution of orbital-dependent magnetic susceptibilities plays a key role [22]. They were able to derive the universal behavior of the Knight-shift anomaly below a crossover temperature $T^*$, in qualitative agreement with experiments and the two-fluid prediction. However, while this provides the first theoretical support of the Kondo liquid scaling, the calculations are limited to the half-filled periodic Anderson model (PAM) due to the notorious sign problem in DQMC simulations. This is in contrast with the metallic nature of the usual heavy-fermion systems. For example, in a recent study, the particular fillings $\langle n_f \rangle \sim 1$, $\langle n_c \rangle \sim 0.9$ were used for the Ce-115 family of heavy-fermion materials to investigate the $d$-wave superconductivity in the frustrated PAM [23]. It is therefore necessary to study the PAM away from the half filling.
The paper is organized as follows: Section II discusses the PAM Hamiltonian and dynamical cluster approximation (DCA) methods including the calculation of magnetic susceptibilities. Section III first provides a brief overview of the NMR Knight-shift anomaly and then illustrates its occurrence in the doped PAM from DCA simulations. Section IV focuses on our key results, namely the universal scaling of the Knight-shift anomaly in terms of both hybridization and doping level. Section V examines the spectral properties and quasiparticle scattering rate and compares their behavior with the Knight-shift anomaly. Section VI summarizes our results.

II. MODEL AND METHODOLOGY

Here we extend our previous investigation to the doped system by means of the dynamical cluster approximation (DCA) [24,25]. Absent the severe sign problem, the DCA allows us to explore how the universal scaling behavior observed in the half-filled PAM [21] evolves in hole-doped systems. In the past decades, the PAM has been extensively studied via dynamical mean field theory (DMFT) and its various extensions, e.g., the DCA and cellular DMFT, aiming to explore its phase diagram [26,27], d-wave superconductivity [23], Mott metal-insulator transition [28–30], strange metallicity [31], existence of ferromagnetism [32], charge order [33], or generalized versions of the PAM, for example, in the presence of disorder [34], attractive interaction [35], or triangular lattices [36].

The PAM on a square lattice is conventionally believed to capture the essential physics of heavy-fermion materials via triangular lattices [36], or generalized versions of the PAM, for example, in the presence of disorder [34], attractive interaction [35], or triangular lattices [36].

We note that the Hamiltonian reads as

\[ \mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + c_{j \sigma}^\dagger c_{i \sigma}) - V \sum_{i \sigma} (c_{i \sigma}^\dagger f_{i \sigma} + f_{i \sigma}^\dagger c_{i \sigma}) + U \sum_i \left( n_{f \uparrow}^i - \frac{1}{2} \right) \left( n_{f \downarrow}^i - \frac{1}{2} \right) - \sum_{i \sigma} (\mu_c n_{c \sigma}^i + \mu_f n_{f \sigma}^i), \]

which is same as the model employed in our previous work [21]. For more details on the relevant basic physics of the PAM and extensive review of another closely related Kondo lattice model, we refer the reader to Refs. [21,37]. \( c_{i \sigma}, c_{j \sigma}^\dagger \) and \( f_{i \sigma}, f_{j \sigma}^\dagger \) are creation (annihilation) operators for the conduction and local \( f \) electrons on site \( i \) with spin \( \sigma \), respectively. \( n_{c \sigma}^i, n_{f \sigma}^i \) are the associated number operators. \( t \) is the hopping parameter of the conduction electrons on nearest-neighbor sites \( \langle ij \rangle \) of a square lattice, \( U \) the local repulsive interaction in the \( f \) orbital, and \( V \) the hybridization between the conduction and \( f \) electrons. \( \mu_c, \mu_f \) denotes the orbital-dependent chemical potential. \( t = 1 \) sets the energy scale throughout the paper.

We remark that differently from the model settings in [23], here we adopt the fixed \( \langle n_{c \uparrow} \rangle \approx 1 \) by taking the chemical potential for the conduction electron to be \( \mu_c = 0 \), while the \( f \)-electron orbital is doped with varying occupancy spanning from the Kondo regime \( \langle n_f \rangle \approx 1 \) to the mixed-valence regime (\( \langle n_f \rangle < 1 \)). This is done via tuning an “artificially” orbital-dependent chemical potential \( \mu_{c,f} \) in order to explicitly examine the impact of \( f \)-orbital occupancy, which is difficult to be realized if we simply fix the total occupancy via a “global” chemical potential \( \mu = \mu_c = \mu_f \). In this way, we focus on the doping effects in the \( f \)-orbital on the Knight-shift anomaly and its universality in terms of temperature and doping level. We note that \( \langle n_c \rangle \approx 1 \) resides in a special situation where the Van Hove singularity in the density of states of the conduction electrons in a tight-binding model such as the PAM with nearest-neighbor hopping in a square lattice may play a role. This allows us to compare directly with previous results obtained using DQMC where we had both \( n_c = 1 \) and \( n_f = 1 \). On the other hand, we found that the essential physics is not altered for more generic cases, e.g., with a fixed total occupancy in spite of the charge redistribution between conduction and \( f \) electrons.

As an extension of the dynamical mean field theory (DMFT) [38], the DCA represents the bulk lattice problem by a finite number of cluster degrees of freedom embedded in a self-consistent mean-field host via a coarse-graining procedure of the Green’s function, in which the Brillouin zone is divided into \( N_c \) patches and the self-energy is assumed to be constant on these patches. In this way, the DCA deals with all correlations within the cluster, while the longer range correlations outside the cluster are described in the mean-field level. This gives an approximation of the thermodynamic limit and the exact solution of the lattice model can be reproduced in the limit of infinite cluster size. In practice, the most time-consuming part of the DCA self-consistent loop is the cluster solver, which includes either perturbative techniques such as the fluctuation-exchange approximation or nonperturbative techniques such as quantum Monte Carlo (QMC) or exact diagonalization. One widely used approach is the continuous-time QMC (CT-QMC), which is based on a diagrammatic expansion of the partition function to all orders [39]. We will adopt a particular version of CT-QMC, namely the continuous-time auxiliary-field (CT-AUX) algorithm, which is based on an interaction expansion combined with an auxiliary-field decomposition of the interaction vertices owing to its accuracy and efficiency [40].

For later usage, we mention that the local magnetic susceptibility is calculated in the CT-AUX cluster solver after achieving the DCA self-consistency as

\[ \chi_{\alpha \beta} = \frac{1}{N_c} \sum_i \int_0^\beta d\tau \left[ n_{f \uparrow}^i(\tau) - n_{f \downarrow}^i(\tau) \right] \left[ n_{f \uparrow}^i(0) - n_{f \downarrow}^i(0) \right] \]

with \( \alpha, \beta \) denoting the conduction- and \( f \)-electron orbitals in the PAM, respectively. In principle, because the self-consistency in the DCA is achieved only at the single-particle level, e.g., for self-energy, the two-particle coarse-grained quantities such as \( q \)-dependent charge/spin susceptibility are not identical to those of the cluster [24]. In fact, it is much more involved and time-consuming to calculate the two-particle quantities within the DCA [24,25] and recently developed DCA+ algorithm [41,42]. However, the local cluster quantities such as \( \chi_{\alpha \beta} \) presented here are identical to the local lattice ones. We emphasize that in our simulations the Knight-shift...
anomaly usually occurs at relatively high temperatures, where
the local susceptibilities do not differ much from their uniform
(q = 0) counterpart, which implies that the DCA cluster size
plays a minor role. For the same reason, it is reasonable that the
correlation strength \( U \) does not play a significant role either.
Therefore, we focus on the particular parameters: \( U/t = 4, N_c = 16 \).
We have confirmed that other \( U, N_c \), and even different band structures,
e.g., finite next-nearest-neighbor hoppings ' \( \nu \) for conduction electrons and/or hybridization
between orbitals, do not modify the results throughout the
paper qualitatively.

III. NMR KNIGHT-SHIFT ANOMALY

The hyperfine interactions coupling the nuclear spins \( \vec{i} \) to
the electron spins \( \vec{S} \) significantly perturb the nuclear spins,
which enables the nuclei to probe the susceptibility of the
electron quasiparticles [22]. Specifically, this is reflected in the
Knight shift that measures the percentage shift of the nuclear
magnetic resonance (NMR) frequency from that of an isolated
nucleus. In real materials, the hyperfine coupling is generally
not isotropic but rather a tensor quantity \( \mathcal{H}_{\text{hyp}} = \vec{I} \cdot \sum \vec{A}_i \cdot \vec{S} \),
so that the Knight shift also has a tensor form \( \mathcal{K} = \vec{A} \cdot \chi \),
where \( \vec{A}_i \) is the hyperfine interaction matrix and \( \chi \) is the
magnetic susceptibility of the electrons. Note that in those
systems with local moments such as rare-earth materials, the
hyperfine coupling can be both on-site coupling to itinerant
electron spins \( \vec{S} \) and transferred coupling to localized electron
spins \( \vec{S} \), the latter of which plays an important role in materials
with localized electrons. For the nucleus located at the site
of the local moment such as lanthanide and actinide atoms,
the on-site hyperfine coupling can be so large that the fast
relaxation rate results in difficulty in detecting spin echo [22].
Therefore, the transferred hyperfine coupling of ligand nuclei
to their neighboring local moments is often more useful. From
now on, we only consider the nuclear spins on the ligand sites
and rewrite the hyperfine coupling as
\[
\mathcal{H}_{\text{hyp}} = \vec{I} \cdot (A \vec{S}_c^c + B \vec{S}_f^f),
\]
where \( A \) denotes the on-site hyperfine interaction with the
conduction-electron spin and \( B \) is a transferred hyperfine
interaction with the \( f \)-electron spin. Note that the tensor
notation is dropped for simplicity. If the electron spins are
polarized via an external magnetic field \( \vec{H} \), then \( \vec{S}_c^c = (\chi_{cc} + \chi_{cf}) \vec{H} \) and
\( \vec{S}_f^f = (\chi_{cf} + \chi_{ff}) \vec{H} \), where \( \chi_{cc}, \chi_{cf}, \chi_{ff} \) denote
three components of the susceptibilities, so that the total
susceptibility and Knight shift are
\[
\chi(T) = \chi_{cc}(T) + 2 \chi_{cf}(T) + \chi_{ff}(T),
\]
\[
K(T) = A \chi_{cc}(T) + (A + B) \chi_{cf}(T) + B \chi_{ff}(T).
\]

FIG. 1. Distinct temperature evolution of three types of local
magnetic susceptibility for \( (\vec{n}_i) = 0.9 \) implies the emergence of the
Knight-shift anomaly.

Theoretically, as argued in the two-fluid theory [14–18],
\( T^* \) corresponds to the coherence temperature of the Kondo
lattice below which the local moment and itinerant degrees
of freedom become entangled and the heavy-electron Kondo
fluid begins to emerge. Our previous work in the half-filled
PAM [21] also numerically illustrated the existence of this
coherence temperature scale. The purpose of the present paper
is to show that all essential properties on the Knight-shift
anomaly reported in [21] persist in the more general doped
systems.
Figure 1 provides evidence of the distinct temperature evolutions of three types of susceptibilities $\chi_{cc}$, $\chi_{cf}$, and $\chi_{ff}$ for varying hybridization $V$, which signifies the possibility of the Knight-shift anomaly. Although the present study focuses on the relatively high temperature regime, namely $T/t \gtrsim 0.1$, due to the scale of the crossover temperature $T^{*}$ discussed later, it is informative to discuss the whole temperature evolution of the susceptibilities. For weak hybridization (small $V$), the conduction electrons only weakly interact with the $f$-electron moments so that $\chi_{cc}$ is expected to exhibit a $T$-independent Pauli behavior at low temperatures. However, Fig. 1(a) displays a gradual increase with lowering temperature. In fact, even the flatness of $\chi_{cc}(T)$ anticipated for strong hybridization at low temperature disappears. This issue was attributed to the Van Hove singularity in the density of states associated with the half-filled conduction band [21]. Here the lack of $T$-independent $\chi_{cc}$ in the doped PAM stems from both the Van Hove singularity and overcomplete screening of $f$-electron local moments $(n_{c} = 1.0, n_{f} = 0.9)$. Appendix A includes more discussions and comparison between DQMC and DCA results. Figure 1(b) shows the behavior of the interorbital susceptibility $\chi_{cf}$, which is negative due to the antialignment between the conduction- and $f$-electron spins. As expected, a stronger hybridization leads to a larger $\chi_{cf}$ at the high-temperature regime. However, lowering $T$ induces a nonmonotonic evolution of $\chi_{cf}(V)$ with the critical $V$ around the quantum critical hybridization separating $f$-electron antiferromagnetism and $c$-$f$ singlet phases, which also occurs for $(n_{c} = 1.0, n_{f} = 0.9)$ [21]. Naturally, the small $|\chi_{cf}|$ originates from the weak hybridization at small $V$ and the constraint due to the singlet formation at large $V$. Figure 1(c) displays the Curie-like divergence of $\chi_{ff}$ for weak hybridization, while stronger hybridization induces antialignment between $c$-$f$ electron spins to form spin singlets, as manifested in the gradual flatness of the temperature evolution of $\chi_{ff}$.

With the temperature evolution of $\chi_{cc}$, $\chi_{cf}$, and $\chi_{ff}$, we can plot $K$ versus $\chi$ with $T$ as an implicit parameter, namely the Clogston-Jaccarrino plot [43]. Note that experimentally the Knight shift and magnetic susceptibility can be measured independently. If there is only a single spin component that gives rise to the magnetic susceptibility, then the data will form a straight line, which is not generic in the PAM with two orbitals. We remark that, without loss of generality, the hyperfine couplings are chosen as $A = 0.2$ and $B = 1.0$ throughout the paper [44]. For large enough hybridization $V$ in the half-filled PAM [21], the curves of $K(\chi)$ show counterclockwise turnaround with decreasing temperature, which originates from the peak structure of the total susceptibility $\chi(T)$. Figure 2 illustrates that this feature persists in the doped PAM for $V/t \gtrsim 1.2$ but with a second clockwise turnaround, which is due to the continual increase of the total susceptibility in Fig. 3 at lower temperature. The peak value of total susceptibility decreases with increasing $V$, which leads to the compression of the $K(\chi)$ curve towards the origin. Note that experimentally both clockwise and counterclockwise of traversal have been observed, depending on the particular values and signs of the hyperfine coupling tensors $A$ and $B$, whose determination are nontrivial in practice [22].

As done in the half-filled PAM [21] and experimentally [5], the high-temperature regime of $K(\chi)$ can be fitted with a straight line [45], $K = B_{\text{eff}} \chi + K_{0\text{eff}}$. Figure 3 illustrates the Knight-shift anomaly by comparing $\chi$ and $K = (K - K_{0\text{eff}})/B_{\text{eff}}$, which clearly shows the deviation between $\chi$ and $K$ below a $V$-dependent temperature scale for a wide range of hybridizations. For large hybridization, the total susceptibility has a peak characterizing the formation of the hybridized local moment. At lower temperatures, as discussed in Fig. 1, the continual increase of the total susceptibility is attributed to both the Van Hove singularity and the mismatch of the $c$-$f$ orbital occupations. Note that the peak value decreases with increasing $V$, which is consistent with the trend in Fig. 2 that the turnaround point for large $V$ precedes that for small $V$. 
The Knight-shift anomaly below the V-dependent temperature $T^*$ for a wide range of hybridization for $(n_f) = 0.9$, $K_{HF}$ and $T^*$ are free parameters for fitting $K_{HF}(T)$ with Eq. (5). The black curve shows the scaling function $(1 - T/T^*)^{3/2}[1 + \ln(T^*/T)]$ for comparison. $T^*$ increases with the hybridization $V$, reflecting the enhancement of coherence between $c$-$f$ electrons, while the prefactor $K_{HF}^0$ decreases with the hybridization. See text for more discussion.

**IV. UNIVERSAL SCALING WITH VARYING HYBRIDIZATION AND DOPING**

The Knight-shift anomaly below the V-dependent temperature scale $T^*$ in Fig. 3 implies that the physical quantity $K_{HF} = \bar{K} - \chi$ reflects the increasingly important role of hybridization between the $f$-electron spins and the conduction-electron spins. The two-fluid model [14–19] argues that below $T^*$ the hybridization-induced heavy electrons and residual unhybridized $f$-local moments coexist and both contribute to the Knight shift but with different weights so that $K$ is no longer proportional to the total susceptibility. $K_{HF}$ strongly depends on the hybridization $V$ (not shown here), which is reminiscent of its material dependence in experiments. One remarkable feature associated with the Knight-shift anomaly is its scaling behavior observed in a wide range of heavy-fermion materials [4], which provides strong support for the two-fluid model [17]. Empirically, $K_{HF}$ has been found to exhibit a universal logarithmic divergence with decreasing temperature below $T^*$ [16]:

$$K_{HF}(T) = K_{HF}^0(1 - T/T^*)^{3/2}[1 + \ln(T^*/T)],$$

where $K_{HF}^0$ and $T^*$ are material-dependent constants. Figure 4 displays the scaling behavior of $K_{HF}(T)$ by fitting it near $T^*$ with Eq. (5) using parameters $K_{HF}^0$ and $T^*$ for a wide range of hybridization. The intriguing universal logarithmic scaling below a $V$-dependent temperature $T^*$ provides a microscopic demonstration of the Knight-shift anomaly, suggesting that heavy-electron materials can be described in a unified way only with distinct crossover temperature $T^*$. In Appendix B, we discuss the results for generic $n_c$ away from the Van Hove singularity. We fix the total occupancy $n_c + n_f$ and find that there is a charge redistribution between conduction and $f$ electrons with temperature. However, the same universal scaling seems robust in spite of this complication.

Figure 4 reveals several noticeable features of the Knight-shift anomaly in the doped PAM. Evidently, the scaling of $K_{HF}$ only applies between $T^*$ and a lower temperature scale $T_0$, which is consistent with experimental observations and reflects the intervention of other effects at temperatures below $T_0$ [17]. The low-temperature behaviors of $K_{HF}$ differ distinctively between weak and strong hybridizations. In particular, at small $V$ and absent antiferromagnetism, $K_{HF}$ keeps increasing and the deviation from the scaling formula originates in part from the interplay between the residual $f$ moments and the conduction electrons. In the presence of long-range antiferromagnetic order, the Knight-shift anomaly is typically suppressed, owing to the competition between the heavy-electron formation and the localization caused by the magnetic ordering. This is termed relocalization of heavy electrons, as has been observed in CeRhIn$_5$, CePt$_3$In$_7$, and other heavy-fermion antiferromagnets [5,46]. In either case, the $f$-electron moments remain partially screened and partially localized and one expects a continuing competition between the itinerant and localized behavior, causing possible coexistence of long-range antiferromagnetism (or a spin liquid in the absence of long-range order) and unconventional superconductivity [17]. While at large $V$, $K_{HF}$ is seen to saturate below $T_0$, the constant behavior at low temperatures reflects complete hybridization of the $f$-electron moments and the ground state is a heavy Fermi liquid. Between these two regimes, one finds a minimal deviation of $K_{HF}$ from the two-fluid scaling at an intermediate $V/t \sim 1.2$. This corresponds roughly to the quantum critical point between antiferromagnetism and the Fermi liquid, suggesting that the two-fluid scaling has less intervention by low-temperature "orders". We note that the onset temperature $T^*$ increases with the hybridization $V$, reflecting the enhancement of coherence between $c$-$f$ electrons. On the other hand, the prefactor $K_{HF}^0$, which is relevant to the concept of hybridization effectiveness in the two-fluid model, decreases with the hybridization. In the two-fluid model, $K_{HF}^0$ is inversely proportional to $T^*$ [17], which may partially explain the change in $K_{HF}^0$.

Figure 5 provides a systematic study of the Knight-shift anomaly for varying $(n_f)$ in all three regimes of hybridizations. Similarly to the case in Fig. 4, $K_{HF}$ displays universal scaling behavior below $T^*$ down to a breakdown temperature $T_0$. For weak hybridization, $K_{HF}$ approaches gradually the scaling formula at low temperatures with decreasing $(n_f)$, indicating the weakening of the local-moment effect away from half filling. For intermediate and strong hybridizations, $K_{HF}$ below $T_0$ first approaches the universal scaling but then deviates again. This nonmonotonic variation with $(n_f)$ reflects the crossover from the heavy-fermion regime $(n_f) = 1$ to the mixed-valence regime. In particular, it suggests two different Fermi liquid states for $(n_f) \sim 1$ and $(n_f) \ll 1$ at strong hybridization, probably separated by an intermediate non-Fermi liquid phase around $(n_f) \sim 0.75$. Interestingly, for all doping levels illustrated including half filling, the onset temperature of the Knight-shift anomaly, $T^*$, grows rapidly with the hybridization parameter $V$ as expected, but only weakly on $(n_f)$ as shown in Fig. 6. This suggests that the variation of $(n_f)$ plays a less important role in determining the magnitude of the hybridization compared to $V$. Figure 6 also shows the decrease of the prefactor $K_{HF}^0$ with $(n_f)$ and
FIG. 5. Universal logarithmic scaling of $K_{HF}$ with varying $f$-electron occupancy $\langle n_f \rangle$ for three hybridization regimes. The black curve shows the scaling function $(1 - T/T^*)^{3/2}[1 + \ln(T^*/T)]$ for comparison. Doping strongly modifies the behavior of $K_{HF}$ after the scaling breakdown at low temperatures in comparison with the scaling curve. A crossover is seen around $V = 1.2$, possibly corresponding to the transition between heavy-fermion and strong mixed-valence regimes.

hybridization $V$, which provides a strong hint on two extreme cases, namely strong enough hybridization and/or very low $\langle n_f \rangle$, where $K_{HF}^0$ vanishes leading to the suppression of the Knight-shift anomaly in those systems. In fact, as argued in the two-fluid model, the crucial ingredient for the occurrence of an obvious Knight-shift anomaly is the existence of two competing fluids, which is missing in both extreme cases where only one fluid dominates: the heavy electrons for strong hybridization $V$ and the conduction electrons for low enough $\langle n_f \rangle$. Our DCA simulations confirmed the suppression of the Knight-shift anomaly in both cases.

V. COMPARISON WITH THE DENSITY OF STATES AND THE QUASIPARTICLE SCATTERING RATE

One essential piece of the two-fluid model is that the density of states (DOS) of the heavy-electron Kondo liquid has the same universal scaling form as the Knight-shift anomaly. Undoubtedly, it is important to numerically examine how these two universalities are correlated in PAM. To this end, we calculate the local density of states (DOS) for $f$ electrons $N_f(\omega)$ via analytical continuation of the local imaginary-time Green’s function $G_f(\tau) = \sum_J \langle c_J^\dagger(\tau)c_J(0) \rangle$ by inverting

$$G_f(\tau) = \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau}e^{-\beta\omega} + 1 N_f(\omega)$$

FIG. 6. Evolution of $T^*$ and $K_{HF}^0$ with doping and hybridization based on the results in Fig. 4 and Fig. 5. For all doping levels including half filling, $T^*$ grows rapidly with $V$ but only weakly with doping. $K_{HF}^0$ decreases with both $\langle n_f \rangle$ and hybridization $V$, which implies the suppression of the Knight-shift anomaly in systems with either strong enough hybridization or very low $\langle n_f \rangle$. Our DCA simulations confirmed the suppression of the Knight-shift anomaly in both cases.
FIG. 7. Temperature evolution of $f$-electron local density of states for two typical hybridizations for $\langle n_c \rangle = 1.0$, $\langle n_f \rangle = 0.9$. The spectral peak shifts towards the Fermi energy with lowering $T$, which is accompanied by the increase of the peak height.

FIG. 8. The peak temperature of the temperature derivative of the quasiparticle scattering rate $Q(T)$ (solid lines) and the temperature scale below which the peak height of the local DOS of $f$ electrons (dashed lines with markers) shows a rapid increase roughly agree, especially for small dopings and strong hybridizations. This temperature scale grows with $V$ but is much lower than the onset temperature $T^*$ of the Knight-shift anomaly.
different from that of CeCoIn$_5$. In either case, it would be important to clarify the conditions for which the three quantities exhibit similar/different $T^*$. Possible extensions would be to perform calculations taking into account additional bosonic excitations such as spin fluctuations or phonons, which might lead to dynamical renormalization of the hybridization $V$ and a large reduction of the coherence temperature [54]. This might give an additional control parameter to tune $T^*$ for fitting with the experimental findings.

VI. CONCLUSION

We extend previous theoretical study of the NMR Knight shift in the half-filled periodic Anderson model to the doped case using the DCA method. Our simulations show that the universal scaling of the Knight-shift anomaly persists in the moderate doping levels and hybridization regime and represents a robust property of the Anderson lattice. Our work provides a plausible basis for developing a microscopic understanding of the phenomenological two-fluid model. However, it also indicates that some essential physics is missing in the current model calculations, as it cannot reproduce the common $T^*$ for the magnetic, transport, and spectral properties observed in CeCoIn$_5$ and many other heavy-fermion compounds. This reveals a missing piece in explaining the two-fluid phenomenology in the current model calculations, which may be the key for a thorough solution of the heavy-fermion problem.

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APPENDIX A: COMPARISON OF LOCAL SUSCEPTIBILITIES BETWEEN DQMC AND THE DCA IN THE HALF-FILLED PAM

The main text aims to extend the previous DQMC study on the half-filled PAM [21] to the generally doped PAM using the DCA method. Therefore, it is valuable to compare the three orbital-dependent local susceptibilities in the half-filled case from two numerical methods.

Adopting a characteristic common DQMC lattice size and DCA cluster size $4 \times 4$, Fig. 9 illustrates the excellent agreement between DQMC and the DCA of all three local susceptibilities at high temperatures for half filling. Nevertheless, at lower temperatures, they deviate for weak hybridization $V = 0.8$ because the presence of the nonlocal antiferromagnetic correlation is treated in essentially different ways. The DCA incorporates the host outside of the cluster in a self-consistent mean-field manner, while DQMC normally considers the bulk system by employing the periodic boundary conditions. It is well known that DQMC simulations exhibit strong finite-size effects for weak correlations or when the itinerancy of conduction electrons is strong [55]. Figure 9 shows the approach of DQMC’s local susceptibilities to DCA curves via two larger lattice sizes, $N = 6 \times 6, 8 \times 8$. Apparently, the deviation between DQMC and DCA curves is expected to completely vanish in the limit of the infinite DQMC lattice or DCA cluster size. As expected, this difference is hidden for strong hybridization $V = 1.6$ due to the locality.
especially for weak hybridization.

of the singlet formation via hybridization so that both DQMC’s finite-size effects and the DCA’s dependence on cluster size can be neglected.

FIG. 10. Top: Universal scaling of the Knight-shift anomaly for fixed total orbital occupancy \(\langle n_c + n_f \rangle = 1.9\) at \(T^*\) and \(K_{HF}^0\) are close to the values in Fig. 4, indicating the robustness of the universality against the orbital occupancy distribution. Bottom: Orbital occupancy as a function of temperature indicates that the hole doping mainly affects the conduction-electron occupancy at low temperatures, especially for weak hybridization.

APPENDIX B: FIXED TOTAL ORBITAL OCCUPANCY

As mentioned in the main text, we adopt the fixed \(\langle n_c \rangle \sim 1\) but varying \(\langle n_f \rangle\) via tuning an “artificially” orbital-dependent chemical potential \(\mu_{c,f}\) in order to explicitly examine the impact of \(f\)-orbital occupancy. As discussed in Fig. 1 and Appendix A, \(\langle n_c \rangle \sim 1\) leads to the Van Hove singularity in the density of states causing the lack of Pauli-like behavior in \(\chi_{cc}(T)\) for small \(V\). Hence, it is interesting to check our major result, namely the universal scaling of the Knight-shift anomaly in Fig. 4, in more generic settings.

The upper panel of Fig. 10 shows that the universal scaling of the Knight-shift anomaly persists for fixed total orbital occupancy \(\langle n_c + n_f \rangle = 1.9\) via tuning a “global” chemical potential \(\mu = \mu_c = \mu_f\). Remarkably, even \(T^*\) and \(K_{HF}^0\) are quite close to the values in Fig. 4. The bottom panel shows the orbital occupancy as a function of temperature, which indicates that the hole doping mainly affects the conduction-electron occupancy at low temperatures, especially for weak hybridization, while the singlet formation for strong hybridization results in more even distribution between orbitals. Figure 10 provides evidence of the robustness of the universal Knight-shift anomaly against the orbital occupancy distribution, supporting the major results in the main text.
