Effects of an additional conduction band on the singlet-antiferromagnet competition in the periodic Anderson model

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The competition between antiferromagnetic (AF) order and singlet formation is a central phenomenon of the Kondo and periodic Anderson Hamiltonians and of the heavy fermion materials they describe. In this paper, we explore the effects of an additional conduction band on magnetism in these models, and, specifically, on changes in the AF-singlet quantum critical point (QCP) and the one particle and spin spectral functions. To understand the magnetic phase transition qualitatively, we first carry out a self-consistent mean field theory (MFT). The basic conclusion is that, at half filling, the coupling to the additional band stabilizes the AF phase to larger $f$ $d$ hybridization $V$ in the PAM. We also explore the possibility of competing ferromagnetic phases when this conduction band is doped away from half filling. We next employ quantum Monte Carlo (QMC) which, in combination with finite size scaling, allows us to evaluate the position of the QCP using an exact treatment of the interactions. This approach confirms the stabilization of AF order, which occurs through an enhancement of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. QMC results for the spectral function $A(q,\omega)$ and dynamic spin structure factor $\chi(q,\omega)$ yield additional insight into the AF-singlet competition and the low temperature phases.

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I. INTRODUCTION

The periodic Anderson model (PAM) describes the hybridization between mobile ($d$ band) free electrons in a metal with strongly correlated $f$ electrons. The PAM has been extensively studied since its first introduction [1] and can successfully account for a variety of remarkable $f$-electron (rare-earth and actinide) phenomena including heavy-fermion physics [2–6], valence fluctuations [7,8], volume collapse transitions [9–16], and unconventional superconductivity [17].

At low temperatures, as the hybridization strength is varied in the PAM, there is a competition between the RKKY interaction [18–20], which favors magnetically ordered $f$ band local moments, and the Kondo effect [21,22], which screens the local moments and induces singlet states. Kondo screening can also occur at the interface between metallic and strongly correlated materials [23,24], a situation which has given rise to additional theoretical and numerical investigation of the PAM and its geometrical variants [25–27]. Here the metallic band is viewed as arising from material on one side of an interface, and the correlated band describes the other side of the interface, as opposed to originating from strongly and weakly correlated orbitals of atoms in a single, homogeneous material.

A natural generalization of models which couple a single conduction band to localized, magnetic, orbitals is to consider similar physics when several conduction bands are present. The new qualitative physics to be explored is how the third band, and the resulting imbalance between the numbers of conduction and localized electrons, alters the strong correlation phenomena of the two band PAM: RKKY-induced AF order at weak $V$, the nature of the Kondo gap at strong $V$, and, finally, the position of the AF-singlet transition between these limits.

Besides these interesting fundamental questions, such a model is also worthy of investigation as a first step towards experiments [28] on $f$-electron superlattices like CeIn$_3$(n)/LaIn$_3$(m). In these systems, by varying the thicknesses n,m of the different materials, the effective dimensionality can be tuned and hence the 2D-3D crossover of Kondo physics and AF order.

Recent theoretical investigations of the effect of immersing a Kondo insulator, or a superlattice thereof, in a 3D metal has been undertaken by Peters et al. [29]. The focus there was on the evolution of the density of states $\rho(\omega)$ and, especially, features like the Fermi level hybridization gap of the Kondo sheet. A key conclusion is that the Kondo gap is modified to a pseudogap, with quadratically vanishing $\rho(\omega)$ from coupling to the metallic layer, and that the 3D $\rho(\omega)$ of the metallic layer adjacent to the Kondo layer develops 2D features. Changes to $\rho(\omega = 0)$ in the singlet phase will be a key feature of our results here.

A bilayer heavy fermion system comprising a Kondo insulator (KI), represented by a symmetric PAM, coupled to a simple metal (M) has been proposed and studied employing the framework of DMFT [6] at half filling. The main goal of the work was to determine the ground state phase diagram from a Kondo screened Fermi liquid to a Mott insulating phase as a function of interaction strength and interlayer coupling. More generally, the possibility of the coexistence of spectral functions with distinct behaviors near the Fermi surface, despite the presence of interband hybridization, is the topic of studies of orbitally selective transitions [30,31].

While we focus here on the influence of an additional metallic band on the properties of the PAM, similar extensions to include electron-phonon coupling [32], dilution [33], and
$f$-electron hybridization [34] have similarly explored the ways in which AF-singlet competition can be influenced by the inclusion of further energy scales and degrees of freedom in the Hamiltonian.

In this paper, we employ the determinant quantum Monte Carlo (DQMC) method [35,36], which provides an approximation-free solution to strong correlations, to study the magnetic structure of the bilayer KI-M system. By finite size scaling, we reliably extract the AF order parameter the quantum critical point (QCP) of the AF-singlet phase transition of the half-filled PAM, the $t' = 0$ limit, with higher accuracy than in previous literature [37]. The DQMC work is mainly focused on the particle-hole symmetric (half-filled) limit where there is no sign problem in the simulation. We also implemented a mean-field theory (MFT) calculation both at and away from half filling as a supplement to DQMC. Our work is distinguished from previous work [6,29] by its consideration of a PAM rather than a coupling to local (Kondo) spins and its treatment of intersite magnetic correlations which are suppressed in the paramagnetic DMFT used in earlier work.

II. MODEL AND METHODS

We consider the bilayer KI-M Hamiltonian on a square lattice,

$$
H = -t \sum_{\langle \mathbf{k}, \mathbf{k}' \rangle} (c_{\mathbf{k} \downarrow} c_{\mathbf{k}' \uparrow} + c_{\mathbf{k} \uparrow} c_{\mathbf{k}' \downarrow}) + \epsilon^c \sum_{\mathbf{k}_o} n^c_{\mathbf{k}_o} - t' \sum_{\langle \mathbf{k}, \mathbf{k}' \rangle} (d_{\mathbf{k} \downarrow} d_{\mathbf{k}' \uparrow} + d_{\mathbf{k} \uparrow} d_{\mathbf{k}' \downarrow}) + \epsilon^d \sum_{\mathbf{k}_o} n^d_{\mathbf{k}_o} + U_f \sum_{\mathbf{k}} \left( n^f_{\mathbf{k} \downarrow} - \frac{1}{2} \right) \left( n^f_{\mathbf{k} \uparrow} - \frac{1}{2} \right) + \epsilon^f \sum_{\mathbf{k}_o} n^f_{\mathbf{k}_o} - t' \sum_{\langle \mathbf{k}, \mathbf{k}' \rangle} (c_{\mathbf{k} \downarrow} d_{\mathbf{k}' \downarrow} + c_{\mathbf{k} \uparrow} d_{\mathbf{k}' \uparrow}) - V \sum_{\mathbf{k}} (d_{\mathbf{k} \downarrow} f_{\mathbf{k} \downarrow} + d_{\mathbf{k} \uparrow} f_{\mathbf{k} \uparrow}).
$$

$t$ is the intralayer hopping parameter, which, for simplicity, we chose to be the same in the uncorrelated $c$ and $d$ bands. $t'$ is the interlayer hopping parameter between the $c$, $d$ bands. $V$ is the hybridization strength between the $d$, $f$ bands. $U_f$ is the Coulomb repulsion in the $f$ band. Finally, $\epsilon^a$ are the orbital energies of the $a = c,d,f$ bands, and $n^a_{\mathbf{k}_o} \equiv \langle a_{\mathbf{k} \sigma}^\dagger a_{\mathbf{k} \sigma} \rangle$ are the density operators. The model is shown pictorially in Fig. 1, where $f$ and $d$ bands belong to the KI layer, and $c$ band belongs to the metal layer. Within the KI formed by the $d$ and $f$ bands, $V$ controls the competition between antiferromagnetic (AF) and singlet phases.

In this work, we set $t = 1$ as our energy scale and mainly consider the particle-hole symmetric limit where $\epsilon^c = 0$, so each of the three bands is individually half filled. We also implement the MFT calculation away from half filling.

At half filling, the Hamiltonian can be solved exactly in the noninteracting limit ($U_f = 0$). Unlike the PAM in which $V$ opens a gap at half filling and which hence is a band insulator there, the KI-M system is metallic at half filling. This follows from the fact that the Hamiltonian has an odd number of bands (three): The Fermi level lies in the middle of the central band. This metallic character at half filling can be made more precise by going to momentum space $\alpha = c,d,f$.

$$
H = \sum_{\mathbf{k},\sigma} (\epsilon^c_{\mathbf{k} \sigma} d^c_{\mathbf{k} \sigma} + d^c_{\mathbf{k} \sigma} \epsilon^c_{\mathbf{k} \sigma}) \left[ \begin{array}{ccc} \epsilon^c_{\mathbf{k} \sigma} & t'_{\mathbf{k} \sigma} & 0 \\ -t'_{\mathbf{k} \sigma} & \epsilon^c_{\mathbf{k} \sigma} & -V \\ 0 & V & \epsilon^c_{\mathbf{k} \sigma} \end{array} \right] d^c_{\mathbf{k} \sigma}.
$$

Here $\epsilon^c_{\mathbf{k}} = -2t'(\cos(k_x) + \cos(k_y))$. Diagonalizing the Hamiltonian Eq. (2) yields the three energy bands. In general, these bands cross and, at $\epsilon^c = 0$, are all partially filled. However, in certain limits, e.g., $V = 0$ and $t' > 4t$, band gaps are present. Even so, in these situations the central band is half filled and the system remains metallic.

The focus of our work will be the implications of the additional metallic ($c$) band on the competition between the RKKY interaction-induced AF and the Kondo regime of screened singlets, both central to the behavior of heavy-fermion materials [2–4] and captured in the solution of the PAM ($t' = 0$). A natural expectation is that, with the increase of $t'$, the RKKY interaction between the local $f$ moments is enhanced, due to the additional conduction band channels, while the Kondo energy scale, set by $V$ and $U_f$, remains roughly fixed. This should lead to an overall movement of the quantum critical point to larger values of $V$.

To understand the precise effect of $t'$ on the AF-singlet transition, we first carried out a self-consistent mean field theory (MFT). We then turned to a more exact, DQMC solution.

III. RESULTS: MEAN FIELD THEORY

Together with Kondo phases, ferromagnetic, antiferromagnetic, and mixed order are all possible in the PAM and related Hamiltonians [38,39]. In the MFT treatment presented here, we thus consider three possible phases, the AF phase, the
ferromagnetic (F) phase, and the singlet phase. The AF MFT ansatz is

$$\langle n_{\nu^f} \rangle = \frac{n_f}{2} + \sigma m_f (\beta - 1)/2,$$

where $\sigma$ is spin up (↑) or spin down (↓) and $m_f$ is the $f$ band AF order parameter. While the F MFT ansatz is

$$\langle n_{\nu^f} \rangle = \frac{n_f}{2} + \sigma m_f (\beta - 1)/2,$$

where $\sigma$ follows the same definition and $m_f$ is the $f$ band ferromagnetic order parameter. In order to fix the particle densities $n_c$, $n_d$, and $n_f$, the terms $N_n, \epsilon_c, N_n, \epsilon_d$, and $N_n, \epsilon_f$ must be subtracted from the original Hamiltonian, Eq. (1) reported in Ref. [40].

The AF MF decoupling of the interaction then gives a quadratic Hamiltonian in which momenta $Q$ where

$$E = \text{EFFECTS OF AN ADDITIONAL CONDUCTION BAND ON . . . PHYSICAL REVIEW B}$$

$$\text{total ground state energy}$$

$$\text{boundary, are computed self-consistently by minimizing the}$$

$$\text{where}$$

$$\text{denotes \sigma \text{MF \ decoupling of the interaction then gives a}$$

$$\text{AF MF decoupling leads to}$$

$$\text{The evolution of}$$

$$\text{whose location agrees with previous work [37]. The evolution of}$$

$$\text{is smoother for}$$

$$\text{as a function of}$$

$$\text{On the other hand, the F MF decoupling leads to}$$

$$\text{and}$$

$$\text{where}$$

$$\text{stands for}$$

$$\text{and the matrix is}$$

$$\text{Hence,}$$

$$\text{and the corresponding MFT phase boundary, are computed self-consistently by minimizing the}$$

$$\text{We first explore the AF MFT ansatz at half filling. Results}$$

$$\text{for}$$

$$\text{as a function of}$$

$$\text{with}$$

$$\text{A sharp QCP is evident at}$$

$$\text{whose location agrees with previous work [37]. The evolution of}$$

$$\text{in which momenta}$$

$$\text{where}$$

$$\text{and}$$

$$\text{which characterizes the behavior of the ground state order parameter. While}$$

$$\text{is varied greatly from 0.2 to 1.8, the magnitude of the order parameter stays in a small range from 0.85 to 0.89,}$$

FIG. 2. MFT results for the AF order parameter $m_f$ as a function of $V$ for several KI-M hybridizations, $t' = 0.1, 2, 3.4$. Each band is fixed at half filling. The on-site interaction in the KL, $U_f = 4$, is fixed. At $t' = 0$, where the system is insulating in the noninteracting limit, the order parameter rises from zero steeply, i.e., with the expected exponent $t' = 1/2$ for $V < V_c$. For $t' \neq 0$, $m_f$ exhibits a more gradual behavior. This smoother crossover is a consequence of the diverging density of states at the Fermi surface and reflects the persistence of AF order at large $V$. A ‘crossover value’ $V_c$ is identified as described in the text. Calculations shown are for lattice sizes of linear extent $L = 60$ and verified to have converged. (See inset.)

Nevertheless, a crossover $V_c$ is still evident in Fig. 2, especially for modest $t'$. We assign a quantitative value by choosing the point of $m_f(V)$ of largest slope and extrapolating linearly to $m_f = 0$ as shown. These crossover values for $V_c$ will be compared with the critical hybridization obtained by DQMC in the following section.

To determine the ground state phase away from half filling, we compare results from both the AF MFT ansatz and the F MFT ansatz, as shown in Fig. 3. We denote the corresponding ground state energies $E_{AF} (E_F)$ and, for the singlet (paramagnetic) phase, $E_{S}$. In Fig. 3(a), $E_{AF} - E_{S}$ and $E_{F} - E_{S}$ are shown as a function of the density $n_c$ with fixed $n_d = 1$, $n_f = 1$, that is, by doping the additional conduction band. We have chosen $t' = 1$, $V_f = 1$, $U_f = 4$, and $L = 200$. For these parameters, $E_{AF}$ is always lowest for all densities $n_c$. In Fig. 3(b), the optimal $m_f$ from the AF MFT ansatz (denoted as $m_f^{\text{AF}}$) and the optimal $m_f$ from the F MFT ansatz (denoted as $m_f^{\text{F}}$) are shown as a function of density $n_c$. Since the ground state phase is AF, red triangular data characterizes the behavior of the ground state order parameter. While $n_c$ is varied greatly from 0.2 to 1.8, the magnitude of the order parameter stays in a small range from 0.85 to 0.89,
showing that the $c$ band has limited effects on the $f$ band magnetic structure.

In Fig. 3(c), $E_{AF} - E_{S}$ and $E_{F} - E_{S}$ are shown as a function of the hybridization strength $V$ with fixed $n_{t} = 0.8, n_{d} = 1, n_{f} = 1, \tau' = 1$, $U_{f} = 4$, and $L = 200$. Below the critical point $V_{c} \approx 1.75$, $E_{AF}$ is lower than $E_{F}$ and $E_{S}$. Above the critical point, the AF order gives way to the singlet phase in a second order phase transition. In Fig. 3(d), the explicit behaviors of $m_{F}^{c}$ and $m_{F}^{s}$ with respect to $V$ are presented, in agreement with results of Fig. 3(c). Red triangular data points characterize the behavior of the ground state order parameter. Notably, by moving away from half filling, the smooth transition observed at the half-filling limit returns to the conventional MFT transition behavior with order parameter exponent $\beta = 1/2$.

IV. RESULTS: DETERMINANT QUANTUM MONTE CARLO

In contrast to MFT, DQMC provides an exact treatment of the interactions in the KI-M Hamiltonian. This is accomplished through the construction of a path integral expression for the partition function and the introduction of an auxiliary field to decouple the exponential of the quartic interaction term into a quadratic form [35]. The fermion trace can be done exactly, and the auxiliary field is then sampled to produce measurements of one and two particle correlation functions.

The DQMC method works on lattices of finite spatial extent, necessitating an extrapolation to the thermodynamic limit as described below. A “Trotter error” is also introduced in the separation of the kinetic and potential energy pieces of the Hamiltonian. We work with an imaginary time discretization small enough such that the Trotter error is negligible, i.e. it is less than our statistical sampling errors. All the following DQMC results are presented at the particle-hole symmetric limit.

To explore the magnetic behavior, we first study the $f$ band real space equal time spin-spin correlation function,

$$C^{f}(\mathbf{r}) = \langle S_{i+r\downarrow}^{f} S_{i\downarrow}^{f} \rangle = \langle (n_{i+r\uparrow}^{f} - n_{i\uparrow}^{f}) (n_{i\downarrow}^{f} - n_{i \downarrow}^{f}) \rangle. \quad (8)$$

$C^{f}(\mathbf{r})$ measures the correlation between the $z$ component of a spin on site $i$ with that on a site $\mathbf{r}$ away. Although the definition in Eq. (8) only involves the $z$ component, we average all three components (which are equal by rotational symmetry).

In addition to the spatial decay of the $f$ band spin correlation function of Eq. (8), we also study the Kondo singlet correlation function [41], defined as:

$$C^{f,d} = \langle \tilde{S}_{i}^{f} \cdot \tilde{S}_{i}^{d} \rangle, \quad (9)$$

where $\tilde{S}_{i}^{f} = \{ f_{i}^{\uparrow}, f_{i}^{\downarrow} \} \bar{\sigma} [ t_{f_{i}}^{\uparrow} ]$ and $\tilde{S}_{i}^{d} = \{ d_{i}^{\uparrow}, d_{i}^{\downarrow} \} \bar{\sigma} [ t_{d_{i}}^{\uparrow} ]$ and $\bar{\sigma}$ are the Pauli matrices.

At a KI-M coupling $t' = 1$, the DQMC result for the $f$ band spin-spin correlation function $C^{f}(\mathbf{r})$ shown in Fig. 4 reveals nonzero (long range) AF correlations at hybridization strength $V = 1.06$. This value is well above the pure KI ($t' = 0$) critical point, indicating that AF order is stabilized by $t'$. The right panel of Fig. 4 shows the variation of the singlet correlation function $C^{f,d}$ with hybridization strength. As $V$ increases, the system switches from a small $C^{f,d}$ regime where singlet correlations are absent (the AF phase dominates) to a large $C^{f,d}$ regime where Kondo singlets are well formed (and AF correlations are absent). As has been previously noted [37], the position of the most rapid increase in magnitude of $C^{f,d}$ gives an approximate location to the AF-singlet QCP.
In addition to the manner in which the spin correlation function decays with spatial separation, the imaginary time evolution also offers a window into the AF-singlet transition. Specifically, the f band dynamic local moment,

\[
(m^2)_{\text{dyn}} = \frac{1}{\beta} \int_0^\beta d\tau \frac{C^f(r = 0, \tau)}{C^f(r = 0, \tau)} = \frac{1}{\beta} \int_0^\beta d\tau \left( S^f_{\xi}(\tau) S^f_{\xi}(0) \right)
\]

is the integral of the spatially local, unequal time spin correlation function \(C^f(r = 0, \tau)\). Here \(S^f_{\xi}(\tau) = e^{iH \tau} S^f_{\xi} e^{-iH \tau}\). As with our previous equal time \(C^f(r)\), we average this correlation function over all spin directions to improve statistics. In a situation where the spin operator commutes with the Hamiltonian, e.g., at \(V = 0\) where one has isolated moments, the instantaneous, \(C^f(r = 0, \tau = 0)\), and dynamic moments \((m^2)_{\text{dyn}}\) are equal. Quantum fluctuations from the hybridization \(V\) cause the spin correlation to decay in imaginary time, reducing the dynamic moment.

As seen in Fig. 5 there are two quite different behaviors of \(C^f(r = 0, \tau)\) when \(V\) is nonzero. \(C^f(r = 0, \tau)\) decays to zero rapidly at \(\tau/\beta = 0.5\) for \(t' = 1\), while it decays smoothly to a nonzero value at \(\tau/\beta = 0.5\) for \(t' = 3\). Integrating \(C^f(r = 0, \tau)\) yields the dynamic local moments shown in the inset to Fig. 5. Increasing \(t'\) from 1 to 3, induces a very large change in \((m^2)_{\text{dyn}}\), which implies the shifting of the system from a Kondo singlet to an AF phase.

The rapid decay of \(C^f(r = 0, \tau)\) with \(\tau\) is associated with the presence of a singlet gap. An alternate way of interpreting the data of Fig. 5 is that by enhancing the AF tendency, increasing \(t'\) causes the vanishing to the singlet gap and a large increase in \((m^2)_{\text{dyn}}\).

The f-band structure factor \(S^f(k)\) is the Fourier transform of the f-band equal time spin-spin correlation function \(C^f(r)\) and is defined as:

\[
S^f(k) = \sum_\tau e^{i k r} C^f(r). \tag{11}
\]

We present results for \(k = Q\), the AF structure factor, since this is the dominant ordering wave vector at half filling.

If there is long range AF order in the system, \(C^f(r)\) remains nonzero to large separations \(r\) and hence the spatial sum to form \(S^f(Q)\) yields a quantity which increases linearly with the system size \(N\). Spin wave theory [42] provides the analytic form for the finite size correction

\[
\frac{3S^f(Q)}{N} = \frac{a}{L} + \frac{m^2_{\text{AF}, f}}{N^2}. \tag{12}
\]

Here \(m_{\text{AF}, f}\) is the AF order parameter in the thermodynamic limit and \(L = \sqrt{N}\) is the linear lattice size. The correction factor \(a\) can be reduced by excluding short range terms \(C^f(r = 0)\) from the sum used to build the full structure factor, since spin correlations at short distances are enhanced over the square of the order parameter \(m_{\text{AF}, f}\). An improved estimator (lower finite size effects) is therefore [43]

\[
S^f_n(Q) = \frac{N}{N^2 - n} \sum_{r,|r|>l_c} e^{i k r} C^f(r), \tag{13}
\]

where \(n\) is the number of separations \(r\) shorter than \(l_c\), which are excluded from the sum. In our DQMC measurements, we chose \(l_c = 0\) and \(n = 1\), removing only the fully local spin-spin correlation \(C^f(0,0)\). (This is the off-vertical scale data point in Fig. 4.)

To locate the phase transition point accurately, we measure the structure factor \(S^f(Q)\) according to Eq. (12) and then extrapolate to get the order parameter \(m_{\text{AF}, f}\). The results are shown in Fig. 6. Fixing \(t' = 1, U_f = 4, \beta = 25\), then for \(t' = 1\), \(m_{\text{AF}, f}\) has a negative extrapolation at \(V = 1.13\) but is positive at \(V = 1.08\). These bracket the QCP which we estimate to be at \(V_c = 1.10 \pm 0.03\). Similarly, for \(t' = 2\), we conclude \(V_c = 1.70 \pm 0.04\); for \(t' = 3\), we have \(V_c = 2.58 \pm 0.04\); and finally for \(t' = 4\), we find \(V_c = 3.54 \pm 0.08\).

Although our focus here is on the KI-M model and ascertaining the effect of additional metallic bands on the AF-singlet transition, we also have determined \(V_c\) more accurately for the PAM (\(t' = 0\)). To our knowledge, the original DQMC results [37] have not been re-examined. The main panel of Fig. 7 shows the \(U_f - V\) phase diagram and the AF and singlet regions at \(t' = 0\). The critical points are deduced from the scaling of \(S^f(Q)\). A representative plot is shown in the inset for \(U_f = 3, V = 0.90\) (zero intercept) and \(V = 0.87\) (nonzero intercept), bracketing a critical value \(V_c = 0.89 \pm 0.02\) at \(U_f = 3\). Similarly, for \(U_f = 4\), we conclude \(V_c = 0.99 \pm 0.02\) and for \(U_f = 6\), we conclude \(V_c = 1.18 \pm 0.02\). The dotted line showing the MFT results has been discussed in the previous section.

We now consider the phase diagram for the full KI-M Hamiltonian with \(t' \neq 0\). Here we chose to fix \(U_f = 4\) and
focus on the effect of coupling the KI to the metal with $t'$. The phase diagram is shown in Fig. 8. With the increase of $t'$, the critical value $V_c$ increases in both DQMC and MFT calculations, quantifying the degree to which interlayer hybridization did not reveal as great a difference in $V_c$. This suggests the increase found here is associated with the van-Hove singularity in the DOS.

In an AF ordered phase, the presence of low energy spin wave excitations leads to a vanishing of the gap in $\text{Im}\chi_f(q,\omega)$ at the ordering wave vector $[\pi,\pi]$. In an AF ordered phase, the presence of low energy spin wave excitations leads to a vanishing of the gap in $\text{Im}\chi_{f}(q,\omega)$ at the ordering wave vector $[\pi,\pi]$.

In Fig. 9 and 10, we show the one particle spectral function $A_f(q,\omega)$ and the spin spectral function $\text{Im}\chi_f(q,\omega)$, which are calculated using the maximum entropy method [46,47], for the PAM model and the KI-M model, respectively. $\text{Im}\chi_f(q,\omega)$ complements the data for the equal time spin and singlet correlators of Fig. 4. In their AF phases (left panels) the PAM and KI-M models are both characterized by a single particle gap in $\text{Im}\chi_f(q,\omega)$ at the ordering wave vector $[\pi,\pi]$.

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Although the singlet phase dynamic spin response of the KI-M is considerably broader, a natural consequence of the larger value of $V$ required to destroy AF order and of the hybridization to an additional band.

The singlet phase of the KI-M is distinguished from the PAM by a nonzero $A_f(q,\omega)$ at $\omega = 0$ and also a very broadly distributed spectral weight $\text{Im}\chi_f(q,\omega)$ (Fig. 10, bottom right). The distinction between the singlet phases of the KI-M and the PAM is further confirmed by the dynamic spin structure factors, given by $\text{Im}\chi_f(\omega) = \sum_q \text{Im}\chi_f(q,\omega)$ for both models, as shown in Fig. 11.

VI. CONCLUSIONS

A considerable body of existing theoretical and numerical work [27,48–54] has examined coupling of a single band Hubbard model to additional conduction electrons as a model of metal-insulator interfaces, and the possibility of penetration of AF and Mott insulator features of strong interaction into the metal, and vice versa. Qualitative similarities exist between phenomena like singlet formation between electrons in distinct bands and between electrons in two conjoined materials. In this paper we have first shown that within a self-consistent MFT there is a tendency towards expansion of the region of AF stability in a three band extension of the PAM.

We next employed the DQMC method to confirm these findings with an exact, beyond MF, treatment of the correlations and thereby identify quantitatively the critical $f d$ hybridization in the plane of interaction strength $U_f$ and hopping $t'$ between the PAM and the metal. In the process, we improved on the previously known $V_c$ in the PAM ($t' = 0$) limit. Our primary observables in the characterization of the phases were the AF structure factor, the singlet correlator, and the dynamical moment, which all provide a consistent picture of the location of the phase boundary. Work within DMFT [29], which focuses on the paramagnetic phase, is complementary to what we have done here.

Although the AF phase of the KI-M is stabilized by contact with the metal, the behavior of $\text{Im}\chi_f(q,\omega)$ is not dramatically different from the PAM. $\text{Im}\chi_f(q,\omega)$ has a gap $\Delta$, at low frequencies in the singlet phase but has nonzero low frequency spectral weight in the AF phase associated with spin-wave excitations.

In contrast, the single particle spectral weight $A_f(q,\omega)$, and the momentum-integrated density of states, behave differently in the KI-M than the PAM. The PAM has a nonzero charge gap.
\( \Delta_r \) in both the AF and singlet phases [37], with \( \Delta_r / \Delta_c \to 1 \) as \( V \) increases to deep in the singlet phase. We find here that for the KI-M there are peaks in \( A(q, \omega) \) near \( q = (\pi, 0) \) and \( q = (\pi/2, \pi/2) \) and hence also in \( \gamma(q, \omega) = \sum_q A(q, \omega) \). We believe this distinction to originate in the fact that even though the AF order is lost, the additional \( c \) electrons still strongly interact with the \( d \) and \( f \) bands of the KI, so that there is no longer an insulating Kondo gap.

The Hamiltonian Eq. (1) includes \( cd \) and \( cf \) hybridizations. We have also done some studies of the effect of on-site \( cf \) hopping. In order to keep the lattice bipartite and avoid a sign problem we have altered the \( df \) hybridization to a near-neighbor form also used, for example, in Ref. [44]. This change does not shift the critical \( V \) from the on-site value to within our error bars. Having verified this, we then added \( cf \) hopping and find that it, also, leaves the critical point at the same value. We conclude that more complex (and realistic) forms of the electronic kinetic energy have little effect on the qualitative and quantitative results of our paper: an enhancement of the regime of AF order.

Our work on a two layer metal-PAM represents a first step in the application of DQMC to the more general investigation of \( f \)-electron-metal superlattices, where, on the experimental side, dimensionality can be controlled [28]. Theoretical and numerical studies within dynamical mean field theory [29,55–57] of these structures have already led to great insight. Including the full spatial structure of each layer, as done in DQMC, makes the full superlattice problem challenging.

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[1] P. W. Anderson, Localized magnetic states in metals, Phys. Rev. 124, 41 (1961).
[2] G. R. Stewart, Heavy-fermion systems, Rev. Mod. Phys. 56, 755 (1984).
[3] P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Theories of heavy-electron systems, Comments Condens. Matter Phys. 12, 99 (1986).
[4] A. Georges, A. Kotliar, W. Krauth, and M. J. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, Rev. Mod. Phys. 68, 13 (1996).
[5] N. S. Vidhyadhiraja and D. E. Logan, Dynamics and scaling in the periodic Anderson model, Eur. Phys. J. B 39, 313 (2004).
[6] S. Sen and N. S. Vidhyadhiraja, Quantum critical Mott transitions in a bilayer Kondo insulator-metal model system, Phys. Rev. B 93, 155136 (2016).
[7] A. C. Hewson, The Kondo Problem to Heavy Fermions (Cambridge University Press, Cambridge, 1993).
[8] R. Shinzaki, J. Nasu, and A. Koga, DMFT study for valence fluctuations in the extended periodic Anderson model, J. Phys. Conf. Ser. 683, 012041 (2016).
[9] J. W. Allen and R. M. Martin, Kondo Volume Collapse and the \( \gamma \to \alpha \) Transition in Cerium, Phys. Rev. Lett. 49, 1106 (1982).
[10] J. W. Allen and L. Z. Liu, \( \alpha \to \gamma \) transition in Ce. II. A detailed analysis of the Kondo volume-collapse model, Phys. Rev. B 46, 5047 (1992).
[11] M. Lavagna, C. Lacroix, and M. Cyrot, Volume collapse in the Kondo lattice, Phys. Lett. A 90, 210 (1982).
[12] O. Gunnarsson and K. Schönhammer, Electron spectroscopies for Ce compounds in the impurity model, Phys. Rev. B 28, 4315 (1983).
[13] A. K. McMahan, C. Huscroft, R. T. Scalettar, and E. L. Pollock, Volume Collapse transitions in the rare earth metals, J. Comput.-Aided Mater. Des. 5, 131 (1998).
[14] M. J. Lipp, D. Jackson, H. Cynn, C. Aracne, W. J. Evans, and A. K. McMahan, Thermal Signatures of the Kondo Volume Collapse in Cerium, Phys. Rev. Lett. 101, 165703 (2008).
[29] R. Peters, Y. Tada, and N. Kawakami, Kondo effect in \(f\)-electron superlattices, Phys. Rev. B 88, 155134 (2013).

[30] A. Liebsch, Single Mott transition in the multiorbital Hubbard model, Phys. Rev. B 70, 165103 (2004).

[31] R. Arita and K. Held, Orbital-selective Mott-Hubbard transition in the two-band Hubbard model, Phys. Rev. B 72, 201102(R) (2005).

[32] P. Zhang, P. Reis, K. Tam, M. Jarrell, J. Moreno, F. Assaad, and A. K. McMahan, Periodic Anderson model with electronphonon correlated conduction band, Phys. Rev. B 87, 121102(R) (2013).

[33] S. Sen, J. Moreno, M. Jarrell, and N. S. Vidhyadhiraja, Spectral changes in layered \(f\)-electron systems induced by Kondo hole substitution in the boundary layer, Phys. Rev. B 91, 155146 (2015).

[34] A. Euverte, S. Chiesa, R. T. Scalettar, and G. G. Batrouni, Finite \(f\)-electron bandwidth in a heavy fermion model, Phys. Rev. B 88, 235123 (2013).

[35] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Monte Carlo calculations of coupled boson-fermion systems. I, Phys. Rev. D 24, 2278 (1981).

[36] E. Loh and J. Gubernatis, in Modern Problems of Condensed Matter Physics, edited by W. Hanke and Y. V. Kopaev (North Holland, Amsterdam, 1992), Vol. 32, p. 177.

[37] M. Vekic, J. W. Cannon, D. J. Scalapino, R. T. Scalettar, and R. L. Sugar, Competition Between Antiferromagnetic Order and Spin Liquid Behavior in the Two–Dimensional Periodic Anderson Model at Half–Filling, Phys. Rev. Lett. 74, 2367 (1995).

[38] B. H. Bernhard and C. Lacroix, Coexistence of magnetic order and Kondo effect in the Kondo-Heisenberg model, Phys. Rev. B 92, 094401 (2015).

[39] R. Eder, K. Grube, and P. Wróbel, Antiferromagnetic phases of the Kondo lattice, Phys. Rev. B 93, 165111 (2016).

[40] N. C. Costa, J. P. Lima, and R. R. dos Santos, Spiral magnetic phases on the Kondo Lattice Model: A Hartree-Fock approach, J. Magn. Magn. Mater. 423, 74 (2017).

[41] C. Huscroft, A. K. McMahan, and R. T. Scalettar, Magnetic and Thermodynamic Properties of the Three-Dimensional periodic Anderson Hamiltonian, Phys. Rev. Lett. 82, 2342 (1999).

[42] D. A. Huse, Ground-state staggered magnetization of two-dimensional quantum Heisenberg antiferromagnets, Phys. Rev. B 37, 2380 (1988).

[43] C. N. Varney, C.-R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Quantum Monte Carlo study of the 2D fermion hubbard model at half-filling, Phys. Rev. B 80, 075116 (2009).

[44] K. Held, C. Huscroft, R. T. Scalettar, and A. K. McMahan, Similarities between the Hubbard and Periodic Anderson Models at Finite Temperatures, Phys. Rev. Lett. 85, 373 (2000).

[45] M. Jarrell and J. E. Gubernatis, Bayesian inference and the analytic continuation of imaginary-time quantum Monte Carlo data, Phys. Rep. 269, 133 (1996).

[46] J. E. Gubernatis, M. Jarrell, R. N. Silver, and D. S. Sivia, Quantum Monte Carlo simulations and maximum entropy: Dynamics from imaginary-time data, Phys. Rev. B 44, 6011 (1991).

[47] K. S. D. Beach, Identifying the maximum entropy method as a special limit of stochastic analytic continuation, arXiv:cond-mat/0403055.

[48] A. Ohmoto, D. Muller, J. Grazul, and H. Hwang, Artificial charge-modulation in atomic-scale perovskite titanate superlattices, Nature (London) 419, 378 (2002).

[49] M. Potthoff and W. Nolting, Metallic surface of a Mott insulator–Mott insulating surface of a metal, Phys. Rev. B 60, 7834 (1999).

[50] M. Potthoff and W. Nolting, Surface metal-insulator transition in the Hubbard model, Phys. Rev. B 59, 2549 (1999).

[51] S. Okamoto and A. J. Millis, Spatial inhomogeneity and strong correlation physics: A dynamical mean-field study of a model Mott-insulator-band–insulator heterostructure, Phys. Rev. B 70, 241104 (2004).

[52] H. Zenia, J. K. Freericks, H. R. Krishnamurthy, and T. Pruschke, Appearance of “Fragile” Fermi Liquids in Finite-Width Mott Insulators Sandwiched between Metallic Leads, Phys. Rev. Lett. 103, 116402 (2009).

[53] H. Ishida and A. Liebsch, First-order metal-to-metal phase transition and non-Fermi-liquid behavior in a two-dimensional Mott insulating layer adsorbed on a metal substrate, Phys. Rev. B 85, 045112 (2012).

[54] R. W. Helmes, T. A. Costi, and A. Rosch, Kondo Proximity Effect: How Does a Metal Penetrate into a Mott Insulator? Phys. Rev. Lett. 101, 066802 (2008).

[55] S. Okamoto and T. A. Maier, Enhanced Superconductivity in Superlattices of High-Tc Cuprates, Phys. Rev. Lett. 101, 156401 (2008).

[56] Y. Tada, R. Peters, and M. Oshikawa, Dimensional crossover in layered \(f\)-electron superlattices, Phys. Rev. B 88, 235121 (2013).

[57] R. Peters and N. Kawakami, Surface density of states of layered \(f\)-electron materials, Phys. Rev. B 89, 041106 (2014).